Euclidean Distance Geometry via Convex Optimization

Jon Dattorro

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for Jennie Columba

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◊ Antonio

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and Sze Wan

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Chapter 1

Prelude

People are so afraid of convex analysis.

−Claude Lemaréchal, 2003

Convex Analysis is the calculus of inequalities while Convex Optimization is its application. Analysis is inherently the domain of the mathematician while Optimization belongs to the engineer. It can be difficult for the engineer to apply theory without understanding Analysis. Boyd & Vandenberghe's book *Convex Optimization* [1] is a marvelous bridge between the two disciplines; rigorous though accessible to non-mathematicians. Their text was conventionally published in 2004 having been taught at Stanford University and made freely available on the world-wide web for ten prior years;[1.1] a dissemination motivated by the belief that a virtual flood of new applications would follow by epiphany that many problems hitherto presumed non-convex could be transformed or relaxed into convexity. [2] [3] [4] [5] [6] [7, §4.3, p.316-322] [8] [9] [10] Subsequently there were great advances, particularly in the electronic circuit design industry. [7, §4.7] [11] [12]-[21]

[1.1] Its influence has already great impact; the web holds countless copies in bits and pieces spanning the book's evolution.

These pages constitute the author's journal over a six year period filling some remaining gaps between mathematician and engineer. Consequently there is heavy cross-referencing and very much background material provided in the text, footnotes, and appendices so as to be more self-contained and to provide an understanding of fundamental concepts. Material contained in Boyd & Vandenberghe is, for the most part, not duplicated here although in some instances (*e.g.*, matrix-valued functions and calculus (§3), linear algebra, geometry, nonorthogonal and orthogonal projection, semidefinite programming (§6), *etcetera*) we expand or elaborate topics found particularly useful in the study of Euclidean distance geometry, the main focus of the present work. In that sense, this journal may be regarded as a companion to Boyd & Vandenberghe.

1.1 Overview

The study of Euclidean distance matrices (EDMs) fundamentally asks what can be known geometrically given only distance information between points in Euclidean space. Each point may represent simply location or, abstractly, any entity expressible as a vector in finite-dimensional Euclidean space: thus inclusive of nearly all contemporary discrete signals and systems; *e.g.*, the discrete Fourier transform (DFT).[1.2] The answer to the question posed is that very much can be known; the mathematics is rich and deep. Throughout we cite beacons of historical accomplishment in this area of geometry. The application of EDMs has already proven invaluable in discerning biological molecular conformation. [22] The emerging practice of localization in wireless sensor networks or the global positioning system (GPS) will certainly simplify and benefit from this theory as well.

We study the pervasive convex bodies and their various representations. In particular, we make convex polyhedra, cones, and dual cones more visceral through illustration in chapter **2**, and we study the geometric relation of polyhedral cones to nonorthogonal bases (biorthogonal expansion). The conic analogue to linear independence, called *conic independence*, is introduced as a new tool in the study of classical cone theory; the logical next step in the progression: linear, affine, conic.

[1.2] Yet to date there is no recorded appearance of EDMs in this particular field of engineering except §4.15.1 herein.

The concept of faces and extreme points and directions of convex bodies is explained here in chapter **2**; crucial to the understanding of convex optimization problems in later chapters, as all convex optimization problems have quite visual geometric analogues. Any convex optimization problem has a geometric interpretation. This is, in fact, the main attraction of convex optimization; the ability to visualize geometry of a problem. This chapter provides tools to make those visualizations easier.

Chapter **3** presents pertinent results for multidimensional convex functions ignored in the literature; tricks and tips for determining their convexity and discerning their geometry.

The Euclidean distance matrix (EDM) is studied in chapter **4**, its properties and relationship to positive semidefinite (PSD) and Gram matrices. Problem types solvable via EDMs, and EDM problems posed as convex optimization is discussed; *e.g.*, we generate an isotonic map of the United States using only comparative distance information (no distance information, only distance inequalities). The DFT is related to EDMs, a connection to *digital signal processing* of which we are previously unaware.

In chapter **5** we illustrate the geometric relationship between EDM and PSD cones. In particular we explain geometric requirements for projection of a candidate matrix on the PSD cone that establish its membership to the EDM cone. The faces of the EDM cone are described, but still open is the question whether all its faces are exposed as they are for the PSD cone. The classic Schoenberg criterion relating EDM and PSD cones is revealed to be a discretized membership relation (a generalized inequality, a new Farkas'-like lemma) between the EDM cone and its ordinary dual.

Semidefinite programming is reviewed in chapter **6** with particular attention to optimality conditions of the primal and dual programs, their interplay, and the perturbation method of rank reduction of optimal solutions (extant but not as well known as should be).

Chapter **7** explores methods of solution to a few fundamental and prevalent Euclidean distance matrix proximity problems emphasizing projection methods on polyhedral cones of eigenvalues (spectral projection) for rank minimization, and their relation to convex optimization and Procrustes techniques (§C.2). We also derive a novel expression for the EDM cone as an intersection and vector sum of two subspaces and the PSD cone.

Chapter **8** investigates Euclidean distance matrix completion problems and their relationship to convex optimization. What is the least amount of data contained in an incomplete EDM that makes the corresponding points in Euclidean space uniquely discernible to within an isometry? We demonstrate a novel procedure for partitioning a large problem into many small problems whose solutions are unique, easy to solve, and can be assembled into the solution of the original large problem.

Chapter 2

Convex geometry

Convexity has an immensely rich structure and numerous applications. On the other hand, almost every "convex" idea can be explained by a two-dimensional picture.

−Alexander Barvinok [23]

There is relatively less published pertaining to matrix-valued convex sets and functions. [24] [25, §6.6] As convex geometry and linear algebra are inextricably bonded, we provide much linear algebra background material (especially in the appendices) although it is assumed the reader is comfortable with [26], [27], [28], or any other intermediate-level text. The essential references to convex analysis are [29] [30]. The reader is referred to [31] [23] [32] [33] [1] [34] [35] for a more comprehensive treatment of convexity.

2.1 Convex set

A set $\mathcal{C}$ is convex iff for all $Y, Z \in \mathcal{C}$ and $0 \le \mu \le 1$,

$$\mu Y + (1 - \mu)Z \in \mathcal{C} \tag{1}$$

Under that defining constraint on μ, the linear sum in (1) is called a *convex combination* of Y and Z. If Y and Z are points in Euclidean vector space $\mathbb{R}^n$ or $\mathbb{R}^{m \times n}$, then (1) represents the closed line segment joining them. All line segments are thereby convex sets. Apparent from the definition, a convex set is a connected set. [36, §3.4, §3.5] [33, p.2]

The idealized chicken egg, an ellipsoid (Figure **2.1**(c)), is a good organic icon for a convex set in three dimensions $\mathbb{R}^{\mathbf{3}}$.

2.1.0.1 subspace

A subset of Euclidean vector space $\mathbb{R}^n$ is called a *subspace* (§2.4) if every vector of the form $\alpha x + \beta y$, for $\alpha, \beta \in \mathbb{R}$, is in the subset whenever x and y are. [37, §2.3] A subspace is a convex set containing the origin, by definition. [30, p.4] It is not difficult to show

$$\mathbb{R}^n = -\mathbb{R}^n \tag{2}$$

as is true for any subspace $\mathcal{R}$, because $x \in \mathbb{R}^n \Leftrightarrow -x \in \mathbb{R}^n$.

Any subspace not constituting the entire ambient vector space is a *proper subspace*; *e.g.*, any line through the origin in two-dimensional Euclidean space $\mathbb{R}^{\mathbf{2}}$. The vector space $\mathbb{R}^n$ is itself a conventional subspace, inclusively, [38, §2.1] although not proper.

2.1.0.2 affine set

An *affine set* (from the word *affinity*) is any subset of $\mathbb{R}^n$ that is a translation of some subspace, hence convex; *e.g.*, $\emptyset$, point, line, plane, hyperplane (§2.3.2), subspace, *etcetera*. The intersection of an arbitrary collection of affine sets remains affine. The *affine hull* of a set $\mathcal{C} \subseteq \mathbb{R}^n$ (§2.2.1) is the smallest affine set containing it.

2.1.0.3 dimension

Dimension of an arbitrary set $\mathcal{S}$ is the dimension of its affine hull; [32, p.14]

$$\dim \mathcal{S} \triangleq \dim \operatorname{aff} \mathcal{S} \tag{3}$$

the same as dimension of the subspace parallel to that affine set. Hence dimension is synonymous with *affine dimension.* [29, A.2.1]

2.1.0.4 relative interior

Whenever a point x lies *interior* to some set $\mathcal{C} \subseteq \mathbb{R}^n$, then we say its interior $\operatorname{int} \mathcal{C}$ is a *neighborhood* of x. [36, §2.1.1] We distinguish interior from *relative interior* throughout. [31] [32] [35] The relative interior of a convex set $\mathcal{C}$ is its interior relative to its affine hull.[2.1] Thus defined, it is common (though confusing) for the interior of $\mathcal{C}$ to be empty while its relative interior is not: this happens whenever dimension of its affine hull is less than dimension of the *ambient space* ($\dim \operatorname{aff} \mathcal{C} < n$, *e.g.*, were $\mathcal{C}$ a flat piece of paper in $\mathbb{R}^{\mathbf{3}}$) or in the exception when $\mathcal{C}$ is a single point; [36, §2.2.1]

$$\operatorname{rel int}\{x\} \triangleq \operatorname{aff}\{x\} = \{x\}\,, \qquad \operatorname{int}\{x\} = \emptyset\,, \qquad x \in \mathbb{R}^n \tag{4}$$

In any case, the *closure* of the relative interior of a convex set always yields the closure of the set itself; $\overline{\operatorname{rel int} \mathcal{C}} = \overline{\mathcal{C}}$.

2.1.0.5 emptiness

Emptiness of a set $\emptyset$ is handled differently than *interior* in the classical literature. It is common for a nonempty convex set to have empty interior; [29, §A.2.1] *e.g.*, paper in the real world. Thus the term *relative* is the conventional fix to this ambiguous terminology:[2.2]

> An ordinary flat piece of paper is a nonempty convex set having relatively nonempty interior.

[2.1] Likewise for *relative boundary*, although *relative closure* is superfluous. [29, §A.2.1]

[2.2] Superfluous mingling of terms as in *relatively nonempty set* would be an unfortunate consequence.

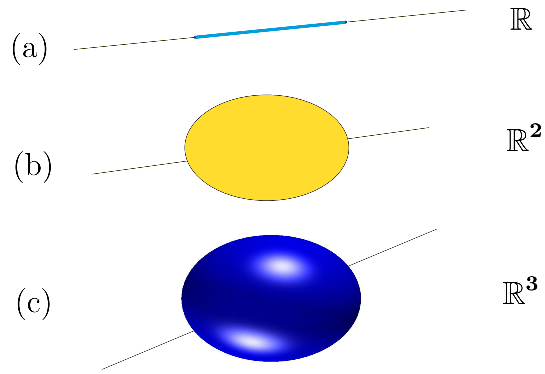


Figure 2.1: Showing intersection of line with boundary of convex Euclidean object can be a point: **(a)** Boundary consists of two points. Intersection of line with ellipsoid in $\mathbb{R}$, **(b)** in $\mathbb{R}^2$, **(c)** in $\mathbb{R}^3$.

2.1.0.6 classical boundary

The classical definition of *boundary* of a set $\mathcal{C}$ is the closure of $\mathcal{C}$ less its interior presumed nonempty; [39, §1.1]

$$\partial\mathcal{C} = \overline{\mathcal{C}} \setminus \operatorname{int}\mathcal{C} \tag{5}$$

which follows from the fact $\overline{\operatorname{int}\mathcal{C}} = \overline{\mathcal{C}}$ assuming nonempty interior. One implication is: an open set has a boundary defined although not contained in the set.

2.1.0.7.1 Example. *Orthant*: Name given to a closed convex set that is the higher-dimensional generalization of *quadrant* from the classical Cartesian partition of $\mathbb{R}^2$. The most common is the nonnegative orthant $\mathbb{R}^n_+$ or $\mathbb{R}^{n\times n}_+$ (analogue to quadrant I) to which membership denotes all nonnegative vector- or matrix-entries respectively;

$$\mathbb{R}^n_+ \triangleq \{x \in \mathbb{R}^n \mid x_i \geq 0 \ \forall i\} \tag{6}$$

The nonpositive orthant $\mathbb{R}^n_-$ or $\mathbb{R}^{n\times n}_-$ (III) denotes negative and 0 entries. The orthant $\mathbb{R}^n_{i-}$ for example, identifies the region in $\mathbb{R}^n$ whose members' sole negative coordinate is their i^{th} (II or IV). Orthant convexity[2.3] is easily verified by definition (1). $\square$

2.1.0.8 sum, product, difference

The *vector sum* of two convex sets $\mathcal{C}_1$ and $\mathcal{C}_2$

$$\mathcal{C}_1 + \mathcal{C}_2 = \{x + y \mid x \in \mathcal{C}_1\ ,\ y \in \mathcal{C}_2\} \tag{7}$$

and *Cartesian product*

$$\mathcal{C}_1 \times \mathcal{C}_2 = \left\{ \begin{bmatrix} x \\ y \end{bmatrix} \mid x \in \mathcal{C}_1\ ,\ y \in \mathcal{C}_2 \right\} \tag{8}$$

remain convex. By additive inverse, we can similarly define the *vector difference* of two convex sets

$$\mathcal{C}_1 - \mathcal{C}_2 = \{x - y \mid x \in \mathcal{C}_1\ ,\ y \in \mathcal{C}_2\} \tag{9}$$

which is convex. Applying this definition to nonempty convex $\mathcal{C}_1$, the self-difference $\mathcal{C}_1 - \mathcal{C}_1$ is generally nonempty, nontrivial, and convex.

Convex results are also obtained for scaling $\kappa\,\mathcal{C}$, rotation/reflection $Q\,\mathcal{C}$, or translation $\mathcal{C} + \alpha$ of a convex set $\mathcal{C}$; all similarly defined.

Given any operator T and convex set $\mathcal{C}$, we are prone to write $T(\mathcal{C})$ meaning

$$T(\mathcal{C}) \triangleq \{T(x) \mid x \in \mathcal{C}\} \tag{10}$$

Given linear operator T , it therefore follows from (7),

$$\begin{aligned} T(\mathcal{C}_1 + \mathcal{C}_2) &= \{T(x+y) \mid x \in \mathcal{C}_1\ ,\ y \in \mathcal{C}_2\} \\ &= \{T(x) + T(y) \mid x \in \mathcal{C}_1\ ,\ y \in \mathcal{C}_2\} \\ &= T(\mathcal{C}_1) + T(\mathcal{C}_2) \end{aligned} \tag{11}$$

2.1.0.9.1 Theorem. *Intersection.* [1, §2.3.1] [30, §2] The intersection of an arbitrary collection of convex sets is convex. $\diamond$

Note that the converse is implicitly false in so far as a convex set can be formed by the intersection of sets that are not.

[2.3] All orthants are self-dual simplicial cones. (§2.8.3.2, §2.7.3.0.1)

Together with the theorems of §E.8.0.0.1 it can be shown, for example, that a line can intersect the boundary of a convex set in any dimension at a point. This is intuitively plausible because a line intersects the boundary of the similar convex objects in Figure **2.1** at a point in $\mathbb{R}$, $\mathbb{R}^{\mathbf{2}}$, and $\mathbb{R}^{\mathbf{3}}$.

2.1.0.10.2 Theorem. *Image, Inverse image.* [30, §3] [1, §2.3.2]
Let f be a mapping from $\mathbb{R}^{p\times k}$ to $\mathbb{R}^{m\times n}$.

- The image of a convex set $\mathcal{C}$ under any affine function (§3.1.1.1)

$$f(\mathcal{C}) = \{f(X) \mid X\in\mathcal{C}\} \subseteq \mathbb{R}^{m\times n} \tag{12}$$

  is convex.

- The inverse image[2.4] of a convex set $\mathcal{F}$,

$$f^{-1}(\mathcal{F}) = \{X \mid f(X)\in\mathcal{F}\} \subseteq \mathbb{R}^{p\times k} \tag{13}$$

  a single or many-valued mapping, under any affine function f is convex.

$\diamond$

In particular, any affine transformation of an affine set remains affine. [30, p.8]

Each converse of this two-part theorem is generally false; *id est*,[2.5] given f affine, a convex image $f(\mathcal{C})$ does not imply that set $\mathcal{C}$ is convex, and neither does a convex inverse image $f^{-1}(\mathcal{F})$ imply set $\mathcal{F}$ is convex. A counterexample is easy to visualize when the affine function is an orthogonal projector [26] [37]:

2.1.0.11.3 Corollary. *Projection on subspace.* [30, §3][2.6]
Orthogonal projection of a convex set on a subspace is another convex set.

$\diamond$

Again, the converse is false. Shadows, for example, are umbral projections that can be convex when the object providing the shade is not.

[2.4] See §2.6.6.3.4 for an example.

[2.5] The expansion of common Latin terms reflects the author's disdain for acronyms; *e.g.*, `www`. Yet we will substitute the abbreviation *e.g.* in place of the Latin *exempli gratia*.

[2.6] The corollary holds more generally for projection on hyperplanes (§2.3.2); [32, §6.6] hence, for projection on affine subsets (§2.2.1, nonempty intersections of hyperplanes). Orthogonal projection on affine subsets is reviewed in §E.4.

2.1.1 Vectorized matrix inner product

Euclidean space $\mathbb{R}^n$ comes equipped with a linear vector inner product

$$\langle y\,,z\rangle \triangleq y^T z \tag{14}$$

Two vectors are *orthogonal* (*perpendicular*) to one another if and only if their inner product vanishes;

$$y \perp z \;\Leftrightarrow\; \langle y\,,z\rangle = 0 \tag{15}$$

An inner product defines a *norm*

$$\|y\|_2 \triangleq \sqrt{y^T y}\;, \qquad \|y\|_2 = 0 \;\Leftrightarrow\; y = 0 \tag{16}$$

When orthogonal vectors each have unit norm, then they are *orthonormal.* For linear operations on vectors represented by real matrices, the *adjoint operation* is transposition and defined for matrix operator A by [38, §3.10]

$$\langle Ay\,,z\rangle = \langle y\,,A^T z\rangle \tag{17}$$

The vector inner product for matrices is calculated just as it is for vectors by first transforming a matrix in $\mathbb{R}^{p\times k}$ to a vector in $\mathbb{R}^{pk}$ by concatenating its columns in the natural order. For lack of a better term, we shall call that linear bijective transformation *vectorization.* For example, the vectorization of $Y = [y_1\; y_2 \cdots\, y_k] \in \mathbb{R}^{p\times k}$ [40] [41] is

$$\operatorname{vec} Y \triangleq \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix} \in \mathbb{R}^{pk} \tag{18}$$

Then the vectorized-matrix inner product is the trace of the matrix inner product; for $Z \in \mathbb{R}^{p\times k}$, [1, §2.6.1] [29, §0.3.1] [42, §8] [43, §2.2]

$$\langle Y\,,\,Z\rangle \triangleq \operatorname{tr}(Y^T Z) \;=\; \operatorname{vec}(Y)^T \operatorname{vec} Z \tag{19}$$

where

$$\operatorname{tr}(Y^T Z) = \operatorname{tr}(Z Y^T) = \operatorname{tr}(Y Z^T) = \operatorname{tr}(Z^T Y) = \mathbf{1}^T (Y \circ Z)\mathbf{1} \tag{20}$$

and where $\circ$ denotes the Hadamard product[2.7] of matrices [28] [44, §1.1.4]. The adjoint operation can therefore be defined in like manner:

$$\langle AY\,,\, Z\rangle = \langle Y\,,\, A^T Z\rangle \tag{21}$$

For example, take any element $\mathcal{C}_1$ from a matrix-valued set in $\mathbb{R}^{p\times k}$, and consider any particular dimensionally compatible real vectors v and w. Then the vector inner product of $\mathcal{C}_1$ with vw^T is

$$\langle vw^T, \mathcal{C}_1\rangle \;=\; v^T\mathcal{C}_1 w \;=\; \operatorname{tr}(wv^T\mathcal{C}_1) \;=\; \mathbf{1}^T\big((vw^T)\circ \mathcal{C}_1\big)\,\mathbf{1} \tag{22}$$

Example. *Application of the image theorem.* Suppose the set $\mathcal{C}\subseteq\mathbb{R}^{p\times k}$ is convex. Then for any particular vectors $v\in\mathbb{R}^p$ and $w\in\mathbb{R}^k$, the set of vector inner products

$$\mathcal{Y} \triangleq v^T\mathcal{C}w \;=\; \langle vw^T, \mathcal{C}\rangle \subseteq \mathbb{R} \tag{23}$$

is convex. This result is a consequence of the *image theorem.* Yet it is easy to show directly that a convex combination of inner products from $\mathcal{Y}$ remains an element of $\mathcal{Y}$.[2.8] □

More generally, vw^T in (23) may be replaced with any particular matrix $Z\in\mathbb{R}^{p\times k}$ while convexity of the set $\langle Z\,,\,\mathcal{C}\rangle\subseteq\mathbb{R}$ persists. Further, replacing v and w with any particular respective matrices U and W of dimension compatible with convex set $\mathcal{C}$, the set $U^T\mathcal{C}W$ is convex by the *image theorem* because it is a linear mapping of $\mathcal{C}$.

[2.7] The Hadamard product is a simple entry-wise product of corresponding entries from two matrices of like size; *id est*, not necessarily square.

[2.8] To verify that, take any two elements $\mathcal{C}_1$ and $\mathcal{C}_2$ from the convex matrix-valued set $\mathcal{C}$, and then form the vector inner products (23) that are two elements of $\mathcal{Y}$ by definition. Now make a convex combination of those inner products; *videlicet*, for $0\leq\mu\leq 1$,

$$\mu\,\langle vw^T, \mathcal{C}_1\rangle \;+\; (1-\mu)\,\langle vw^T, \mathcal{C}_2\rangle \;=\; \langle vw^T, \mu\,\mathcal{C}_1 + (1-\mu)\mathcal{C}_2\rangle \tag{24}$$

The two sides are equivalent by linearity of the inner product. The right-hand side remains a vector inner product of vw^T with an element $\mu\,\mathcal{C}_1+(1-\mu)\mathcal{C}_2$ from the convex set $\mathcal{C}$; hence belongs to $\mathcal{Y}$. Since that holds true for any two elements from $\mathcal{Y}$, then it must be a convex set. ♦

2.1.1.1 Frobenius'

When $Z = Y \in \mathbb{R}^{p\times k}$ in (19), *Frobenius' norm* is resultant;

$$\begin{aligned}\|Y\|_{\mathrm F}^2 \;&=\; \|\operatorname{vec} Y\|_2^2 \;=\; \langle Y\,,\,Y\rangle \;=\; \operatorname{tr}(Y^TY) \;=\; \delta(YY^T)^T\mathbf{1}\\ &=\; \sum_{i,j} Y_{ij}^2 \;=\; \sum_i \lambda(Y^TY)_i \;=\; \sum_i \sigma(Y)_i^2\end{aligned} \tag{25}$$

where $\lambda(Y^TY)_i$ is the i^{th} eigenvalue of Y^TY, and $\sigma(Y)_i$ the i^{th} singular value of Y. Were Y a normal matrix (§A.5.2), then $\sigma(Y) = |\lambda(Y)|$ [45, §8.1] thus

$$\|Y\|_{\mathrm F}^2 \;=\; \sum_i \lambda(Y)_i^2 \;=\; \|\lambda(Y)\|_2^2 \tag{26}$$

The converse (26) $\Rightarrow$ normal Y also holds. [28, §2.5.4] Because the metrics

$$\|\operatorname{vec} X - \operatorname{vec} Y\|_2 = \|X-Y\|_{\mathrm F} \tag{27}$$

are equivalent and because vectorization (18) is a linear bijective map, then vector space $\mathbb{R}^{p\times k}$ is *isometrically isomorphic* with vector space $\mathbb{R}^{pk}$ in the Euclidean sense and vec is an isometric isomorphism on $\mathbb{R}^{p\times k}$ (but not on the vector space that is the range or nullspace associated with a particular matrix (§2.4, *e.g.*, p.217)).[2.9] Because of this Euclidean structure, all the known results from convex analysis in Euclidean space $\mathbb{R}^n$ carry over directly to the space of real matrices $\mathbb{R}^{p\times k}$.

The Frobenius norm is *orthogonally invariant*; meaning, for $X, Y \in \mathbb{R}^{p\times k}$ and compatible orthonormal matrix U and orthogonal matrix Q,

$$\|U(X-Y)Q\|_{\mathrm F} = \|X-Y\|_{\mathrm F} \tag{28}$$

[2.9] An isometric isomorphism of a vector space is a linear bijective mapping T (one-to-one and onto [38, App.A1.2]) that preserves distance; *id est*, for all $x, y \in \operatorname{dom} T$,

$$\|Tx - Ty\| = \|x - y\|$$

Unitary linear operator $Q : \mathbb{R}^n \to \mathbb{R}^n$ representing orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ (§B.5), for example, is an isometric isomorphism. Yet isometric operator $T : \mathbb{R}^{\mathbf 2} \to \mathbb{R}^{\mathbf 3}$ representing

$$T = \begin{bmatrix} 1 & 0\\ 0 & 1\\ 0 & 0\end{bmatrix}$$

is injective on $\mathbb{R}^{\mathbf 2}$ but not a surjective map [38, §1.6] to $\mathbb{R}^{\mathbf 3}$.

2.1.2 Symmetric matrices

Definition. *Symmetric subspace.* Define a subspace of $\mathbb{R}^{M\times M}$: the convex set of all symmetric $M\times M$ matrices;

$$\mathbb{S}^M \triangleq \left\{A\in\mathbb{R}^{M\times M} \mid A=A^T\right\} \subseteq \mathbb{R}^{M\times M} \tag{29}$$

This subspace comprising symmetric matrices $\mathbb{S}^M$ is *isomorphic* [38, §2.8-8, §3.2-2][2.10] [46] with the vector space $\mathbb{R}^{M(M+1)/2}$ whose dimension is the number of free variables in a symmetric $M\times M$ matrix. The *orthogonal complement* [26] [37] of $\mathbb{S}^M$ is

$$\mathbb{S}^{M\perp} \triangleq \left\{A\in\mathbb{R}^{M\times M} \mid A=-A^T\right\} \subset \mathbb{R}^{M\times M} \tag{30}$$

the subspace of all *antisymmetric* matrices in $\mathbb{R}^{M\times M}$; *id est*,

$$\mathbb{S}^M \oplus \mathbb{S}^{M\perp} = \mathbb{R}^{M\times M} \tag{31}$$

$\triangle$

All antisymmetric matrices are hollow by definition (have $\mathbf{0}$ main-diagonal). Any square matrix $A\in\mathbb{R}^{M\times M}$ can be written as the sum of its symmetric and antisymmetric parts: respectively,

$$A = \frac{1}{2}(A+A^T) + \frac{1}{2}(A-A^T) \tag{32}$$

The symmetric part is orthogonal in $\mathbb{R}^{M^2}$ to the antisymmetric part; *videlicet*,

$$\operatorname{tr}\big((A^T+A)(A-A^T)\big) = 0 \tag{33}$$

In the ambient space of real matrices, the antisymmetric subspace can be described

$$\mathbb{S}^{M\perp} \triangleq \left\{\frac{1}{2}(A-A^T) \mid A\in\mathbb{R}^{M\times M}\right\} \subset \mathbb{R}^{M\times M} \tag{34}$$

because any matrix in $\mathbb{S}^M$ is orthogonal to any matrix in $\mathbb{S}^{M\perp}$. Further confined to the ambient subspace of symmetric matrices, because of antisymmetry, $\mathbb{S}^{M\perp}$ would become trivial.

[2.10] An isomorphism of a vector space is a transformation equivalent to a linear bijective mapping. The image and inverse image under the transformation operator are then called isomorphic vector spaces.

2.1.2.1 Isomorphism on symmetric subspace

When a matrix is symmetric in $\mathbb{S}^M$, we may still employ the vectorization transformation (18) to $\mathbb{R}^{M^2}$; vec, an isometric isomorphism. We might instead choose to realize in the lower-dimensional subspace $\mathbb{R}^{M(M+1)/2}$ by ignoring redundant entries (below the main diagonal) during transformation. Such a realization would remain isomorphic but not isometric. Lack of isometry is a spatial distortion due now to disparity in metric between $\mathbb{R}^{M^2}$ and $\mathbb{R}^{M(M+1)/2}$. To realize isometrically in $\mathbb{R}^{M(M+1)/2}$, we must make a correction: For $Y=[Y_{ij}]\in\mathbb{S}^M$ we introduce the symmetric vectorization

$$\operatorname{svec} Y \triangleq \begin{bmatrix} Y_{11} \\ \sqrt{2}Y_{12} \\ Y_{22} \\ \sqrt{2}Y_{13} \\ \sqrt{2}Y_{23} \\ Y_{33} \\ \vdots \\ Y_{MM} \end{bmatrix} \in \mathbb{R}^{M(M+1)/2} \tag{35}$$

where all entries off the main diagonal have been scaled. Now for $Z\in\mathbb{S}^M$,

$$\langle Y\,,\,Z\rangle \;\triangleq\; \operatorname{tr}(Y^TZ) \;=\; \operatorname{vec}(Y)^T\operatorname{vec} Z \;=\; \operatorname{svec}(Y)^T\operatorname{svec} Z \tag{36}$$

Then because the metrics become equivalent

$$\|\operatorname{svec} X-\operatorname{svec} Y\|_2=\|X-Y\|_{\mathrm F} \tag{37}$$

whenever $X\in\mathbb{S}^M$, and because symmetric vectorization (35) is a linear bijective mapping, svec is an isometric isomorphism on the symmetric matrix subspace; in other words, $\mathbb{S}^M$ is isometrically isomorphic with $\mathbb{R}^{M(M+1)/2}$ in the Euclidean sense under the transformation svec.

The set of all symmetric matrices $\mathbb{S}^M$ forms a proper subspace in $\mathbb{R}^{M\times M}$, so for it there exists a standard orthonormal basis in isometrically isomorphic $\mathbb{R}^{M(M+1)/2}$;

$$\{E_{ij}\in\mathbb{S}^M\} = \left\{\begin{array}{ll} e_i e_i^T\,, & i=j=1\ldots M \\ \frac{1}{\sqrt{2}}\left(e_i e_j^T + e_j e_i^T\right), & 1\leq i<j\leq M \end{array}\right\} \tag{38}$$

where $M(M+1)/2$ standard basis matrices E_{ij} are formed from the standard basis vectors $e_i \in \mathbb{R}^M$. Thus we have a basic *orthogonal expansion* for $Y \in \mathbb{S}^M$,

$$Y = \sum_{j=1}^{M}\sum_{i=1}^{j}\langle E_{ij}\,, Y\rangle\, E_{ij} \tag{39}$$

whose coefficients

$$\langle E_{ij}\,, Y\rangle \;=\; \begin{cases} Y_{ii}\,, & i=1\ldots M \\ Y_{ij}\sqrt{2}\,, & 1\leq i<j\leq M \end{cases} \tag{40}$$

correspond to entries of the symmetric vectorization (35).

2.1.2.2 Symmetric hollow matrices

Definition. *Symmetric hollow subspace.* [47] Define a subspace of $\mathbb{R}^{M\times M}$: the convex set of all symmetric $M\times M$ matrices having $\mathbf{0}$ main-diagonal;

$$\mathbb{S}_{\mathbf{0}}^M \triangleq \left\{A \in \mathbb{S}^M \mid \delta(A) = \mathbf{0}\right\} \subset \mathbb{R}^{M\times M} \tag{41}$$

where the main diagonal of $A\in\mathbb{R}^{M\times M}$ is denoted (§A.1)

$$\delta(A) \in \mathbb{R}^M \tag{42}$$

This subspace comprising symmetric hollow matrices is isomorphic with subspace $\mathbb{R}^{M(M-1)/2}$. The orthogonal complement of $\mathbb{S}_{\mathbf{0}}^M$ is

$$\mathbb{S}_{\mathbf{0}}^{M\perp} \triangleq \left\{A\in\mathbb{R}^{M\times M} \mid A = -A^T + 2\delta^2(A)\right\} \subseteq \mathbb{R}^{M\times M} \tag{43}$$

the subspace of all *antisymmetric antihollow* matrices in $\mathbb{R}^{M\times M}$; *id est*,

$$\mathbb{S}_{\mathbf{0}}^M \oplus \mathbb{S}_{\mathbf{0}}^{M\perp} \;=\; \mathbb{R}^{M\times M} \tag{44}$$

Yet defined instead as a proper subspace of $\mathbb{S}^M$,

$$\mathbb{S}_{\mathbf{0}}^M \triangleq \left\{A \in \mathbb{S}^M \mid \delta(A) = \mathbf{0}\right\} \subset \mathbb{S}^M \tag{45}$$

the orthogonal complement $\mathbb{S}_{\mathbf{0}}^{M\perp}$ of $\mathbb{S}_{\mathbf{0}}^M$ in ambient $\mathbb{S}^M$

$$\mathbb{S}_{\mathbf{0}}^{M\perp} \triangleq \left\{A\in\mathbb{S}^M \mid A = \delta^2(A)\right\} \subseteq \mathbb{S}^M \tag{46}$$

is simply the set of all diagonal matrices; *id est*,

$$\mathbb{S}_{\mathbf{0}}^{M} \oplus \mathbb{S}_{\mathbf{0}}^{M\perp} = \mathbb{S}^{M} \tag{47}$$

$\triangle$

Any matrix $A\in\mathbb{R}^{M\times M}$ can be written as the sum of its symmetric hollow and antisymmetric antihollow parts: respectively,

$$A = \left(\frac{1}{2}(A+A^T) - \delta^2(A)\right) \;+\; \left(\frac{1}{2}(A-A^T) + \delta^2(A)\right) \tag{48}$$

The symmetric hollow part is orthogonal in $\mathbb{R}^{M^{\mathbf{2}}}$ to the antisymmetric antihollow part; *videlicet*,

$$\operatorname{tr}\!\left(\left(\frac{1}{2}(A+A^T) - \delta^2(A)\right)\!\left(\frac{1}{2}(A-A^T) + \delta^2(A)\right)\right) = 0 \tag{49}$$

In the ambient space of real matrices, the antisymmetric antihollow subspace is described

$$\mathbb{S}_{\mathbf{0}}^{M\perp} \triangleq \left\{\frac{1}{2}(A-A^T) + \delta^2(A) \mid A\in\mathbb{R}^{M\times M}\right\} \subseteq \mathbb{R}^{M\times M} \tag{50}$$

because any matrix in $\mathbb{S}_{\mathbf{0}}^{M}$ is orthogonal to any matrix in $\mathbb{S}_{\mathbf{0}}^{M\perp}$. Yet in the ambient space of symmetric matrices $\mathbb{S}^M$, the antihollow subspace is nontrivial;

$$\mathbb{S}_{\mathbf{0}}^{M\perp} \triangleq \left\{\delta^2(A) \mid A\in\mathbb{S}^M\right\} \;=\; \left\{\delta(u) \mid u\in\mathbb{R}^M\right\} \subseteq \mathbb{S}^M \tag{51}$$

In anticipation of their utility with Euclidean distance matrices (EDMs) in §4, we introduce the linear bijective vectorization dvec that is the natural analogue to symmetric matrix vectorization svec (35) for symmetric hollow matrices: For $Y=[Y_{ij}]\in\mathbb{S}_{\mathbf{0}}^{M}$,

$$\operatorname{dvec} Y \;\triangleq\; \sqrt{2}\begin{bmatrix} Y_{12}\\ Y_{13}\\ Y_{23}\\ Y_{14}\\ Y_{24}\\ Y_{34}\\ \vdots\\ Y_{M-1,M}\end{bmatrix} \in \mathbb{R}^{M(M-1)/2} \tag{52}$$

Like before, dvec is an isometric isomorphism on the symmetric hollow subspace.

The set of all symmetric hollow matrices $\mathbb{S}_{\mathbf{0}}^M$ forms a proper subspace in $\mathbb{R}^{M\times M}$, so for it there must be a standard orthonormal basis in isometrically isomorphic $\mathbb{R}^{M(M-1)/2}$;

$$\{E_{ij}\in\mathbb{S}_{\mathbf{0}}^M\} \;=\; \left\{\frac{1}{\sqrt{2}}\big(e_i e_j^T + e_j e_i^T\big)\,,\quad 1\leq i<j\leq M\right\} \tag{53}$$

where $M(M-1)/2$ standard basis matrices E_{ij} are formed from the standard basis vectors $e_i\in\mathbb{R}^M$.

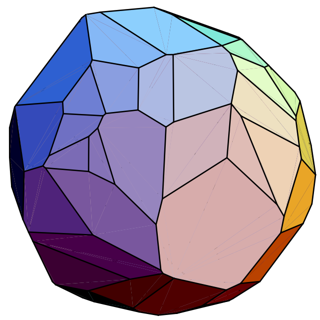


Figure 2.2: Convex hull of a random list of points in $\mathbb{R}^3$. Some points from that generating list reside in the interior of this convex polyhedron. [48, *Convex Polyhedron*] (Avis-Fukuda-Mizukoshi)

2.2 Hulls

2.2.1 Affine dimension, affine hull

Ascribe the points in a list $\{x_\ell \in \mathbb{R}^n,\ \ell = 1 \ldots N\}$ to the columns of matrix X ;

$$X = [\, x_1 \ \cdots \ x_N \,] \in \mathbb{R}^{n\times N} \tag{54}$$

The affine dimension of any nonempty list (or set) in $\mathbb{R}^n$ is the dimension of the smallest affine set (empty set, point, line, plane, hyperplane (§2.3.2), subspace, $\mathbb{R}^n$) that contains it. Affine dimension is the same as the dimension of the subspace parallel to that affine set. [30, §1] [29, §A.2.1] In particular, we define the affine dimension r of the N-point list X as the dimension of the smallest affine set in Euclidean space $\mathbb{R}^n$ that contains X ; r is a lower bound sometimes called the *embedding dimension* [47] [49]:

$$r \triangleq \dim \operatorname{aff} X \tag{55}$$

That affine set in which the points are embedded is unique and called the *affine hull* [1, §2.1.2] [31, §2.1];

$$\mathcal{A} \triangleq \operatorname{aff}\{x_\ell\,,\ \ell = 1 \ldots N\} \ = \ \operatorname{aff} X \ = \ \{Xa \mid a^T\mathbf{1} = 1\} \ \subseteq \ \mathbb{R}^n \tag{56}$$

The subspace of all symmetric matrices $\mathbb{S}^m$, for example, is the affine hull of the cone of positive semidefinite matrices; (§2.6.6)

$$\operatorname{aff} \mathbb{S}^m_+ = \mathbb{S}^m \tag{57}$$

Given some arbitrary set $\mathcal{C}$ and any $x \in \mathcal{C}$,

$$\operatorname{aff}\mathcal{C} = x + \operatorname{aff}(\mathcal{C} - x) \tag{58}$$

where $\operatorname{aff}(\mathcal{C}-x)$ is a subspace. Affine transformations preserve affine hulls. Given any affine mapping T, [30, p.8]

$$\operatorname{aff}(T\mathcal{C}) = T(\operatorname{aff}\mathcal{C}) \tag{59}$$

We analogize *affine subset* to subspace,[2.11] defining it to be any nonempty affine set that is a subset of $\mathbb{R}^n$ and parallel to a subspace. All affine sets are convex.

2.2.2 Convex hull

The *convex hull* [29, §A.1.4] [1, §2.1.4] [30] of any *bounded*[2.12] list (or set) of N points $X \in \mathbb{R}^{n\times N}$ forms a unique *convex polyhedron* (§2.7.0.0.1) whose vertices constitute some subset of that list;

$$\mathcal{P} \;\triangleq\; \operatorname{conv}\{x_\ell\,,\ \ell=1\ldots N\} \;=\; \operatorname{conv}X \;=\; \{Xa \mid a^T\mathbf{1} = 1,\ a \succeq 0\} \;\subseteq\; \mathbb{R}^n \tag{60}$$

The union of the relative interior and relative boundary of the polyhedron comprise the convex hull $\mathcal{P}$, the smallest closed convex set that contains the list X; *e.g.*, Figure **2.2**. Given $\mathcal{P}$, the *generating list* $\{x_\ell\}$ is not unique.

Given some arbitrary set $\mathcal{C}$,

$$\operatorname{conv}\mathcal{C} \;\subseteq\; \operatorname{aff}\mathcal{C} \;=\; \operatorname{aff}\overline{\mathcal{C}} \;=\; \operatorname{aff}\operatorname{conv}\mathcal{C} \tag{61}$$

2.2.2.1 Comparison with respect to $\mathbb{R}^N_+$

The notation $a \succeq 0$ means vector a belongs to the nonnegative orthant $\mathbb{R}^N_+$, whereas $a \succeq b$ denotes comparison of vector a to vector b on $\mathbb{R}^N$ with respect to the nonnegative orthant; *id est*, $a \succeq b$ means $a-b$ belongs to the nonnegative orthant. In particular, $a \succeq b \;\Leftrightarrow\; a_i \succeq b_i \;\; \forall i$. (198)

[2.11] The popular term *affine subspace* is an oxymoron.

[2.12] A set in $\mathbb{R}^n$ is bounded if and only if it can be contained in a Euclidean ball having finite radius. [50, §2.2] (*confer* §4.7.3.0.1)

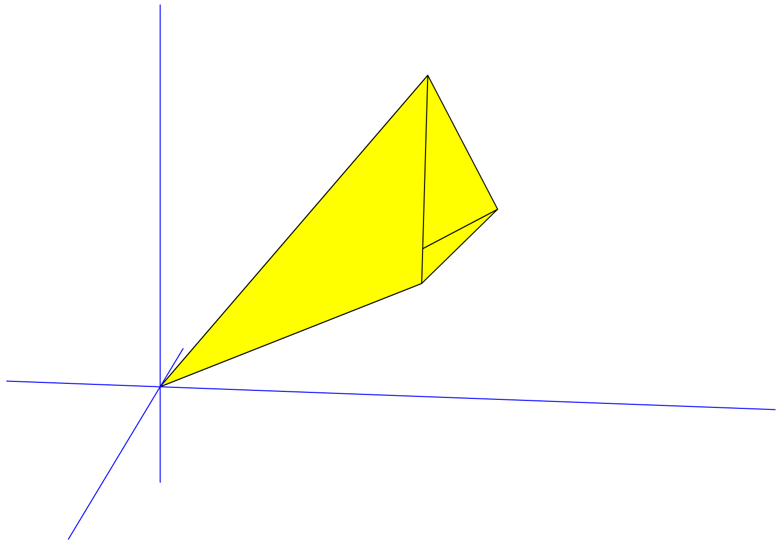


Figure 2.3: A simplicial cone (§2.7.3.0.1) in $\mathbb{R}^{\mathbf{3}}$ whose boundary is drawn truncated; constructed using $A \in \mathbb{R}^{\mathbf{3}\times\mathbf{3}}$ and $C = \mathbf{0}$ in (159). By the most fundamental definition of a cone (§2.6.1), the entire boundary can be constructed from an aggregate of rays emanating exclusively from the origin. The extreme directions are the directions of the three edges (§2.5); they are conically and linearly independent for this cone. Because this set is polyhedral, the exposed directions are in one-to-one correspondence with the extreme directions; there are only three.

2.2.2.1.1 Example. *Convex hull of outer product.* [51, §3] [52, §2.4]

$$\operatorname{conv}\left\{XX^T \mid X \in \mathbb{R}^{n\times k},\ X^TX = I\right\} = \{A \in \mathbb{S}^n \mid I \succeq A \succeq 0\,,\ \langle I\,,A\rangle = k\} \tag{62}$$

□

2.2.3 Conic hull

In terms of a finite-length point list (or set) arranged columnar in $X \in \mathbb{R}^{n\times N}$ (54), its conic hull is expressed

$$\mathcal{K} \triangleq \operatorname{cone}\{x_\ell\,,\ \ell = 1\ldots N\} = \operatorname{cone} X = \{Xa \mid a \succeq 0\} \subseteq \mathbb{R}^n \tag{63}$$

The conic hull of any list forms a *polyhedral cone* [29, §A.4.3] (§2.7.1; *e.g.*, Figure **2.3**); the smallest closed convex cone that contains the list.

Given some arbitrary set $\mathcal{C}$, it is apparent

$$\operatorname{conv}\mathcal{C} \subseteq \operatorname{cone}\mathcal{C} \tag{64}$$

2.2.3.1 Vertex-description

The constraints in (56), (60), and (63) respectively define an affine, convex, and conic combination of elements from the set or list. Whenever a Euclidean object can be described as some hull or span of a set of points, then that representation is loosely called a *vertex-description.*

2.3 Halfspace, Hyperplane

A two-dimensional affine set is called a *plane.* An $(n-1)$-dimensional affine set in $\mathbb{R}^n$ is called a hyperplane. [30] [29] Every hyperplane partially bounds a halfspace (which is convex but not affine).

2.3.1 Halfspaces $\mathcal{H}_+$ and $\mathcal{H}_-$

Euclidean space $\mathbb{R}^n$ is partitioned into two halfspaces by any hyperplane $\partial\mathcal{H}$; *id est*, $\mathcal{H}_- + \mathcal{H}_+ = \mathbb{R}^n$. The resulting (closed convex) halfspaces, both partially bounded by $\partial\mathcal{H}$, may be described

$$\mathcal{H}_- = \{y \mid a^T y \leq b\} = \{y \mid a^T(y - y_p) \leq 0\} \subset \mathbb{R}^n \tag{65}$$
$$\mathcal{H}_+ = \{y \mid a^T y \geq b\} = \{y \mid a^T(y - y_p) \geq 0\} \subset \mathbb{R}^n \tag{66}$$

where nonzero vector $a \in \mathbb{R}^n$ is an *outward-normal* to the hyperplane partially bounding $\mathcal{H}_-$ while an *inward-normal* with respect to $\mathcal{H}_+$. Visualization is easier if we say $b = a^T y_p \in \mathbb{R}$. Then for any vector $y - y_p$ that makes an obtuse angle with normal a , y will lie in the halfspace $\mathcal{H}_-$ on one side (shaded in Figure **2.4**) of the hyperplane, while acute angles denote y in $\mathcal{H}_+$ on the other side.

An equivalent more intuitive representation of a halfspace comes about when we consider all the points in $\mathbb{R}^n$ closer to point d than to point c or equidistant, in the Euclidean sense; from Figure **2.4**,

$$\mathcal{H}_- = \{y \mid \|y - \mathrm{d}\| \leq \|y - \mathrm{c}\|\} \tag{67}$$

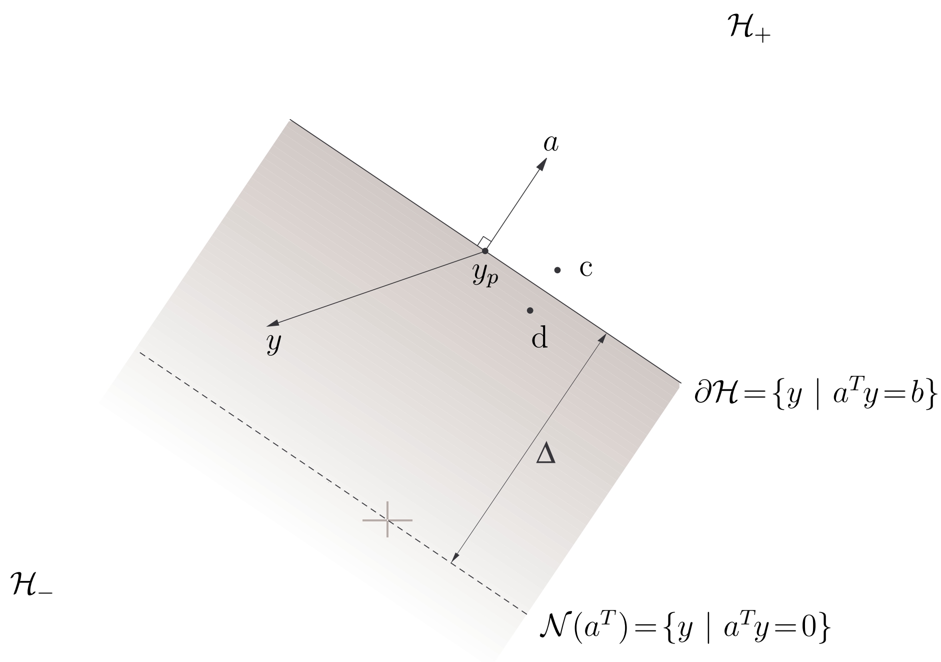


Figure 2.4: Hyperplane illustrated $\partial\mathcal{H}$ is a line partially bounding halfspaces $\mathcal{H}_- = \{y \mid a^Ty \leq b\}$ and $\mathcal{H}_+ = \{y \mid a^Ty \geq b\}$ in $\mathbb{R}^2$. Shaded is a rectangular piece of semi-infinite $\mathcal{H}_-$ with respect to which vector a is outward-normal to bounding hyperplane; vector a is inward-normal with respect to $\mathcal{H}_+$. In this particular instance, $\mathcal{H}_-$ contains nullspace $\mathcal{N}(a^T)$ (dashed line through origin) because $b > 0$. Hyperplane, halfspace, and nullspace are each drawn truncated. Points c and d are equidistant from hyperplane, and vector $\mathrm{c} - \mathrm{d}$ is normal to it. Δ is distance from origin to hyperplane.

This representation, in terms of proximity, is resolved with the more conventional representation of a halfspace (65) by squaring both sides of the inequality in (67);

$$\mathcal{H}_- = \left\{ y \mid (\mathrm{c}-\mathrm{d})^T y \leq \frac{\|\mathrm{c}\|^2 - \|\mathrm{d}\|^2}{2} \right\} = \left\{ y \mid (\mathrm{c}-\mathrm{d})^T \left(y - \frac{\mathrm{c}+\mathrm{d}}{2} \right) \leq 0 \right\} \tag{68}$$

A halfspace may be represented just as well using a matrix variable Y. For $A, Y \in \mathbb{R}^{m\times n}$, and $b = \langle A, Y_p\rangle \in \mathbb{R}$, (§2.1.1)

$$\mathcal{H}_- = \{Y \in \mathbb{R}^{mn} \mid \langle A, Y\rangle \leq b\} = \{Y \in \mathbb{R}^{mn} \mid \langle A, Y - Y_p\rangle \leq 0\} \tag{69}$$
$$\mathcal{H}_+ = \{Y \in \mathbb{R}^{mn} \mid \langle A, Y\rangle \geq b\} = \{Y \in \mathbb{R}^{mn} \mid \langle A, Y - Y_p\rangle \geq 0\} \tag{70}$$

2.3.1.1 PRINCIPLE 1: Halfspace-description of convex sets

The most fundamental principle in convex geometry follows from the *geometric Hahn-Banach theorem* [37, §5.12] [53, §1] that guarantees any closed convex set to be an intersection of halfspaces.

2.3.1.1.1 Theorem. *Halfspaces.* [1, §2.3.1] [30, §18] [29, §A.4.2(b)] [33, §2.4] A closed convex set in $\mathbb{R}^n$ is equivalent to the intersection of all halfspaces that contain it. ⋄

The intersection of multiple halfspaces may be represented using a matrix constant A;

$$\bigcap_i \mathcal{H}_{i-} = \{y \mid A^T y \preceq b\} = \{y \mid A^T(y - y_p) \preceq 0\} \tag{71}$$
$$\bigcap_i \mathcal{H}_{i+} = \{y \mid A^T y \succeq b\} = \{y \mid A^T(y - y_p) \succeq 0\} \tag{72}$$

where b is now a vector, and the i^{th} column of A is normal to a hyperplane $\partial\mathcal{H}_i$ partially bounding $\mathcal{H}_i$. By the *halfspaces theorem*, intersections like this can describe interesting convex Euclidean objects such as polyhedra and cones, giving rise to the term *halfspace-description.*

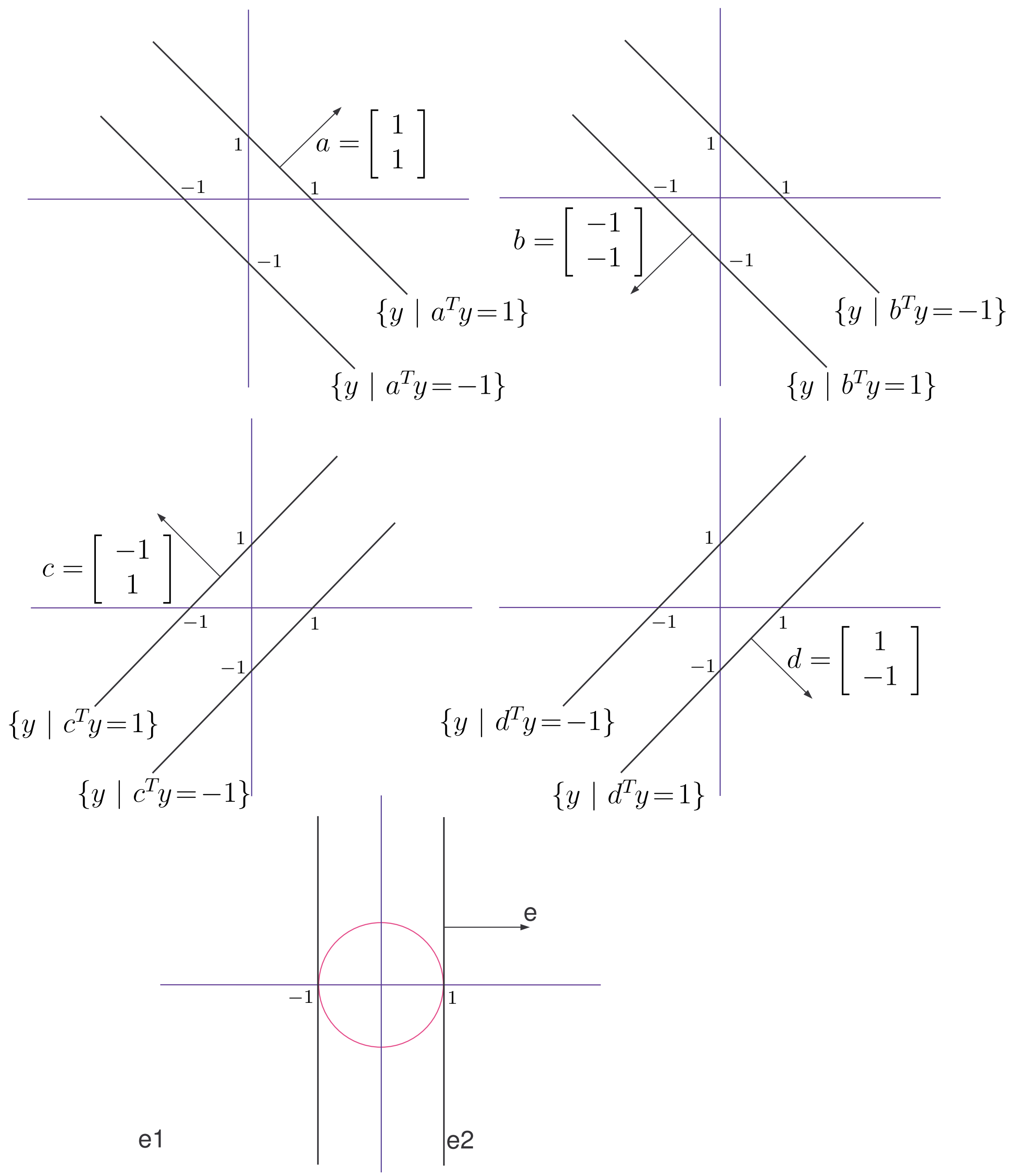


Figure 2.5: Hyperplanes in $\mathbb{R}^2$ (truncated). Hyperplane movement in direction of normal increases inner product. This simple visual concept can be exploited to attain the analytic solution of some linear programs; *e.g.*, [1, exer.4.8-4.20]

2.3.2 Hyperplane $\partial\mathcal{H}$ representations

Every hyperplane $\partial\mathcal{H}$ is an affine set parallel to an $(n-1)$-dimensional subspace of $\mathbb{R}^n$; it is itself a subspace if and only if it contains the origin.

$$\dim \partial\mathcal{H} = n-1 \tag{73}$$

Every hyperplane can be described as the intersection of complementary halfspaces; [30, §19]

$$\partial\mathcal{H} \;=\; \mathcal{H}_- \cap \mathcal{H}_+ \;=\; \{y \mid a^T y \preceq b\,,\; a^T y \succeq b\} \;=\; \{y \mid a^T y = b\} \tag{74}$$

a halfspace-description. Assuming normal $a \in \mathbb{R}^n$ to be nonzero, then any hyperplane in $\mathbb{R}^n$ can be described as the solution set to the vector equation $a^T y = b$, illustrated in Figure **2.4** and Figure **2.5** for $\mathbb{R}^{\mathbf{2}}$;

$$\partial\mathcal{H} \triangleq \{y \mid a^T y = b\} = \{y \mid a^T(y - y_p) = 0\} = \{Z\xi + y_p \mid \xi \in \mathbb{R}^{n-1}\} \subset \mathbb{R}^n \tag{75}$$

All solutions y constituting the hyperplane are offset from the nullspace of a^T by the same constant vector $y_p \in \mathbb{R}^n$ that is any particular solution to $a^T y = b$; *id est*,

$$y = Z\xi + y_p \tag{76}$$

where the columns of $Z \in \mathbb{R}^{n\times n-1}$ constitute a basis for the nullspace $\mathcal{N}(a^T)$.[2.13]

Conversely, given any point y_p in $\mathbb{R}^n$, the unique hyperplane containing it having normal a is the affine set $\partial\mathcal{H}$ (75) where b equals $a^T y_p$ and $\mathcal{R}(Z) = \mathcal{N}(a^T)$. The hyperplane dimension is apparent from the dimensions of Z; the hyperplane is parallel to the span of its columns.

2.3.2.1 Distance from origin to hyperplane

Given the (shortest) distance $\Delta \in \mathbb{R}_+$ from the origin to a hyperplane having normal vector a, we can find its representation $\partial\mathcal{H}$ by dropping a perpendicular. The point thus found is the orthogonal projection of the origin on $\partial\mathcal{H}$ (§E.5.0.1.5), equal to $a\Delta/\|a\|$ if the origin is known *a priori* to belong to

[2.13] We will later find this expression of y in terms of nullspace of a^T (more generally, of matrix A^T) to be a useful device for eliminating affine equality constraints, much as we did here.

halfspace $\mathcal{H}_-$ (Figure **2.4**), or to $-a\Delta/\|a\|$ if the origin belongs to halfspace $\mathcal{H}_+$; *id est*, when $\mathcal{H}_- \ni \mathbf{0}$

$$\partial\mathcal{H} \;=\; \left\{y \mid a^T(y - a\Delta/\|a\|) = 0\right\} \;=\; \left\{y \mid a^T y = \|a\|\Delta\right\} \tag{77}$$

or when $\mathcal{H}_+ \ni \mathbf{0}$

$$\partial\mathcal{H} \;=\; \left\{y \mid a^T(y + a\Delta/\|a\|) = 0\right\} \;=\; \left\{y \mid a^T y = -\|a\|\Delta\right\} \tag{78}$$

Knowledge of only distance Δ and normal a thus introduces ambiguity into the hyperplane representation.

2.3.2.2 Matrix variable

Hyperplanes may be represented equally well using matrix variables instead. For $A\,, Y \in \mathbb{R}^{m\times n}$, and $b = \langle A\,, Y_p\rangle \in \mathbb{R}$, (§2.1.1)

$$\partial\mathcal{H} \;=\; \{Y \mid \langle A\,, Y\rangle = b\} \;=\; \{Y \mid \langle A\,, Y - Y_p\rangle = 0\} \subset \mathbb{R}^{mn} \tag{79}$$

Vector a is normal to the hyperplane illustrated in Figure **2.4**. Likewise in the case of matrix variables, for nonzero A we have

$$A \;\perp\; \partial\mathcal{H} \;\text{ in } \mathbb{R}^{mn} \tag{80}$$

2.3.2.3 Vertex-description of hyperplane

A hyperplane may be described as the affine hull of a *minimal set* of points $\{x_\ell\}$ arranged columnar in a matrix $X \in \mathbb{R}^{n\times n}$ (54):

$$\begin{aligned}
\partial\mathcal{H} &= \operatorname{aff}\{x_\ell \in \mathbb{R}^n\} \mid \ell = 1 \ldots n\,,\;\; \dim\operatorname{aff}\{x_\ell\} = n-1\\
&= \operatorname{aff} X \;\mid\; \dim\operatorname{aff} X = n-1\\
&= x_1 + \mathcal{R}\{x_\ell - x_1\} \mid \ell = 2 \ldots n\,,\;\; \dim\mathcal{R}\{x_\ell - x_1\} = n-1\\
&= x_1 + \mathcal{R}(X - x_1\mathbf{1}^T) \;\mid\; \dim\mathcal{R}(X - x_1\mathbf{1}^T) \,=\, n-1
\end{aligned} \tag{81}$$

2.3.2.3.1 Affine independence, minimal set. For affine sets, a minimal set of points constituting a vertex-description is an *affinely independent* (a.i.) descriptive set and *vice versa*; $\{x_\ell\,,\ \ell = 1 \ldots n\}$ is affinely independent if and only if $\{x_\ell - x_1\,,\ \ell = 2 \ldots n\}$ is *linearly independent* (l.i.). [29, §A.1.3] [54, §3] We deduce

$$\text{l.i.} \;\Rightarrow\; \text{a.i.} \tag{82}$$

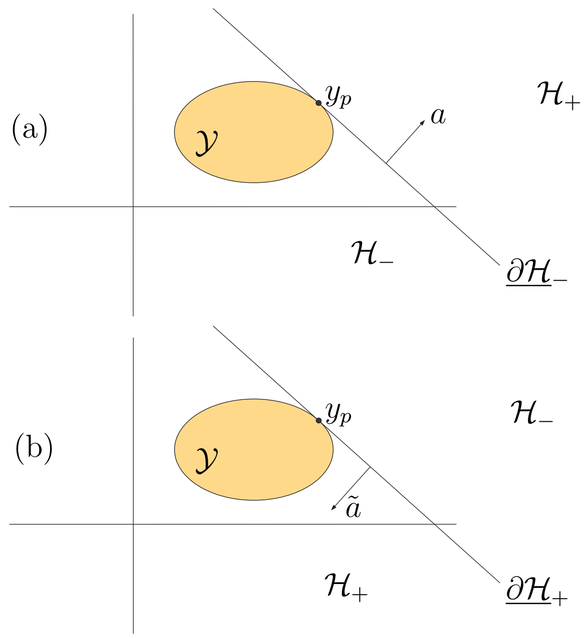


Figure 2.6: **(a)** Hyperplane $\underline{\partial\mathcal{H}_-}$ supporting closed set $\mathcal{Y}\in\mathbb{R}^{\mathbf{2}}$. **(b)** $\underline{\partial\mathcal{H}_+}$ unconventionally supporting $\mathcal{Y}$. Tradition [29] [30] recognizes only positive normal polarity in support function as in (84); *id est*, normal a figure (a).

2.3.2.3.2 Vertex-description of halfspace. Logically consequent to hyperplane definition (81) comes a new representation of a halfspace

$$\begin{aligned}\mathcal{H} &= \bigcup_{\zeta\geq 0} \zeta\, x_1 + \mathcal{R}\{x_\ell - x_1\} \mid \ell=2\ldots n\,,\;\; \dim\mathcal{R}\{x_\ell - x_1\}=n-1 \\ &= \quad \{\zeta\, x_1 + \mathcal{R}\{x_\ell - x_1\} \mid \ell=2\ldots n\,,\;\; \dim\mathcal{R}\{x_\ell - x_1\}=n-1,\;\zeta\geq 0\}\end{aligned} \tag{83}$$

that is a union of parallel hyperplanes. Were x_1 normal to $\mathcal{R}\{x_\ell - x_1\}$, then this halfspace could be designated $\mathcal{H}_+$ by our convention; $\mathcal{H}_-$ would correspond with $\zeta\leq 0$.

2.3.2.4 PRINCIPLE 2: Supporting hyperplane

The second most fundamental principle of convex geometry also follows from the *geometric Hahn-Banach theorem* [37, §5.12] [53, §1] that guarantees existence of at least one hyperplane in $\mathbb{R}^n$ supporting a convex set (having nonempty interior)[2.14] at each point on its boundary.

2.3.2.4.1 Definition. *Supporting hyperplane* $\underline{\partial\mathcal{H}}$. The partial boundary $\partial\mathcal{H}$ of a closed halfspace containing arbitrary set $\mathcal{Y}$ is called a supporting hyperplane $\underline{\partial\mathcal{H}}$ to $\mathcal{Y}$ when it contains at least one point of $\overline{\mathcal{Y}}$. [30, §11] Specifically, given normal $a\neq\mathbf{0}$ (belonging to $\mathcal{H}_+$ by definition), the supporting hyperplane to $\mathcal{Y}$ at $y_p\in\partial\mathcal{Y}$ [*sic*] is

$$\begin{aligned}\underline{\partial\mathcal{H}_-} &= \left\{y \mid a^T(y-y_p)=0\,,\quad y_p\in\overline{\mathcal{Y}}\,,\quad a^T(z-y_p)\leq 0\ \ \forall z\in\overline{\mathcal{Y}}\right\}\\ &= \left\{y \mid a^Ty=\sup\{a^Tz \mid z\in\mathcal{Y}\}\right\}\end{aligned}\tag{84}$$

where normal a and set $\mathcal{Y}$ reside in opposite halfspaces. (Figure **2.6**(a)) The real function $\sigma_{\mathcal{Y}}(a)\triangleq\sup\{a^Tz \mid z\in\mathcal{Y}\}$ is called the *support function* of $\mathcal{Y}$.

An equivalent but non-traditional representation is obtained by reversing the polarity of normal a; (1166)

$$\begin{aligned}\underline{\partial\mathcal{H}_+} &= \left\{y \mid \tilde{a}^T(y-y_p)=0\,,\quad y_p\in\overline{\mathcal{Y}}\,,\quad \tilde{a}^T(z-y_p)\geq 0\ \ \forall z\in\overline{\mathcal{Y}}\right\}\\ &= \left\{y \mid \tilde{a}^Ty=-\inf\{\tilde{a}^Tz \mid z\in\mathcal{Y}\}=\sup\{-\tilde{a}^Tz \mid z\in\mathcal{Y}\}\right\}\end{aligned}\tag{85}$$

where normal $\tilde{a}$ and set $\mathcal{Y}$ now reside in $\mathcal{H}_+$. (Figure **2.6**(b))

When the supporting hyperplane contains only a single point of $\overline{\mathcal{Y}}$, that hyperplane is termed *strictly supporting* (and termed *tangent* to $\mathcal{Y}$ if the supporting hyperplane is unique there [30, §18, p.169]). △

There is no geometric difference[2.15] between supporting hyperplane $\underline{\partial\mathcal{H}_+}$ or $\underline{\partial\mathcal{H}_-}$ and an ordinary hyperplane $\partial\mathcal{H}$ coincident with them.

2.3.2.5 PRINCIPLE 3: Separating hyperplane

The third most fundamental principle of convex geometry again follows from the *geometric Hahn-Banach theorem* [37, §5.12] [53, §1] that guarantees existence of a hyperplane separating two nonempty convex sets in $\mathbb{R}^n$ whose relative interiors are nonintersecting. *Separation* intuitively means each set belongs to a halfspace on an opposing side of the hyperplane. There are two cases of interest:

[2.14] It is customary to speak of a hyperplane supporting set $\mathcal{C}$ but not containing $\mathcal{C}$. [30, p.100]

[2.15] If vector-normal polarity is unimportant, we may instead represent a supporting hyperplane by $\underline{\partial\mathcal{H}}$.

1) If the two sets intersect only at their relative boundaries, then there exists a separating hyperplane $\underline{\partial\mathcal{H}}$ containing the intersection but containing no points relatively interior to either set. If at least one of the two sets is open, conversely, then the existence of a separating hyperplane implies the two sets are nonintersecting. [1, §2.5.1]

2) A *strictly separating hyperplane* $\partial\mathcal{H}$ intersects the closure of neither set; its existence is guaranteed when the intersection of the closures is empty and at least one set is bounded. [29, §A.4.1]

2.4 Subspace representations

There are two common forms of expression for subspaces, both coming from elementary linear algebra: *range form* and *nullspace form*; `a.k.a.`, vertex-description and halfspace-description.

The fundamental vector subspaces associated with a matrix $A\in\mathbb{R}^{m\times n}$ [26, §3.1] are ordinarily related

$$\mathcal{R}(A^T)\perp\mathcal{N}(A)\,,\qquad \mathcal{N}(A^T)\perp\mathcal{R}(A) \tag{86}$$

and of dimension:

$$\dim\mathcal{R}(A^T) \;=\; \dim\mathcal{R}(A) \;=\; \operatorname{rank}A \;\leq\; \min\{m\,,n\} \tag{87}$$

$$\dim\mathcal{N}(A) = n-\operatorname{rank}A\,,\qquad \dim\mathcal{N}(A^T) = m-\operatorname{rank}A \tag{88}$$

From these four fundamental subspaces, the rowspace and range identify one form of subspace description (range form or vertex-description (§2.2.3.1)), respectively,

$$\mathcal{R}(A^T) \triangleq \{A^Ty \mid y\in\mathbb{R}^m\} \;=\; \{x\in\mathbb{R}^n \mid A^Ty=x\,,\; y\in\mathcal{R}(A)\} \tag{89}$$

$$\mathcal{R}(A) \triangleq \{Ax \mid x\in\mathbb{R}^n\} \;=\; \{y\in\mathbb{R}^m \mid Ax=y\,,\; x\in\mathcal{R}(A^T)\} \tag{90}$$

while the nullspaces identify the second common form (nullspace form or halfspace-description (74)),

$$\mathcal{N}(A) \triangleq \{x\in\mathbb{R}^n \mid Ax=\mathbf{0}\} \tag{91}$$

$$\mathcal{N}(A^T) \triangleq \{y\in\mathbb{R}^m \mid A^Ty=\mathbf{0}\} \tag{92}$$

The range forms (89) (90) are realized as the respective span of the column vectors in matrices A^T and A.

The nullspace form (91) or (92) is the solution set to a linear equation similar to hyperplane definition (75). Yet because matrix A generally has multiple rows, halfspace-description $\mathcal{N}(A)$ is actually the intersection of as many hyperplanes through the origin; for (91), each row of A is normal to a hyperplane while for (92), each row of A^T is a normal.

2.4.1 Subspace or affine set...

Any particular vector subspace $\mathcal{R}_p$ can be described as $\mathcal{N}(A)$ the nullspace of some matrix A or as $\mathcal{R}(B)$ the range of some matrix B.

More generally, we have the choice of expressing an $n-m$-dimensional affine subset in $\mathbb{R}^n$ as the intersection of m hyperplanes, or as the offset span of $n-m$ vectors:

2.4.1.1 as hyperplane intersection

Any affine subset $\mathcal{A}$ of dimension $n-m$ can be described as an intersection of m hyperplanes in $\mathbb{R}^n$; given fat *full-rank* (rank $=\min\{m,n\}$) matrix

$$A \triangleq \begin{bmatrix} a_1^T \\ \vdots \\ a_m^T \end{bmatrix} \in \mathbb{R}^{m\times n} \tag{93}$$

and vector $b\in\mathbb{R}^m$,

$$\mathcal{A} \triangleq \{x\in\mathbb{R}^n \mid Ax=b\} = \bigcap_{i=1}^{m} \left\{x \mid a_i^T x=b_i\right\} \tag{94}$$

a halfspace-description. (74)

For example: The intersection of any two independent hyperplanes in $\mathbb{R}^{\mathbf{3}}$ is a line, whereas three independent hyperplanes intersect at a point. In $\mathbb{R}^{\mathbf{4}}$, the intersection of two independent hyperplanes is a plane, whereas three hyperplanes intersect at a line, four at a point, and so on.

From the result in §2.3.2.3, any affine subset $\mathcal{A}$ therefore also has a vertex-description.

2.4.1.2 as span of nullspace basis

Alternatively, we may compute a basis for the nullspace of matrix A and then equivalently express the affine subset as its range plus an offset: Define

$$Z \triangleq \text{basis}\,\mathcal{N}(A) \in \mathbb{R}^{n\times n-m} \tag{95}$$

so that $AZ=\mathbf{0}$. Then we have the vertex-description,

$$\mathcal{A} = \left\{Z\xi + x_p \mid \xi \in \mathbb{R}^{n-m}\right\} \subseteq \mathbb{R}^n \tag{96}$$

the offset span of $n-m$ column vectors, where x_p is any particular solution to $Ax=b$.

2.4.2 Intersection of subspaces

The intersection of nullspaces associated with two matrices $A\in\mathbb{R}^{m\times n}$ and $B\in\mathbb{R}^{k\times n}$ can be expressed most simply as

$$\mathcal{N}(A)\cap\mathcal{N}(B) \;=\; \mathcal{N}\left(\begin{bmatrix} A \\ B \end{bmatrix}\right) \;\triangleq\; \{x\in\mathbb{R}^n \mid \begin{bmatrix} A \\ B \end{bmatrix} x = \mathbf{0}\} \tag{97}$$

the nullspace of their row-wise concatenation.

Suppose the columns of a matrix Z constitute a basis for $\mathcal{N}(A)$ while the columns of a matrix W constitute a basis for $\mathcal{N}(BZ)$. Then [44, §12.4.2]

$$\mathcal{N}(A)\cap\mathcal{N}(B) = \mathcal{R}(ZW) \tag{98}$$

If each basis is orthonormal, then the columns of ZW constitute an orthonormal basis for the intersection.

In the particular circumstance A and B are each positive semidefinite [55, §6], or in the circumstance A and B are two linearly independent dyads (§B.1.1), then

$$\mathcal{N}(A)\cap\mathcal{N}(B) = \mathcal{N}(A+B)\,, \quad \left\{\begin{array}{l} A\,,B\in\mathbb{S}_+^M \\ \quad\textbf{or} \\ A+B = u_1v_1^T + u_2v_2^T \quad \text{(l.i.)} \end{array}\right. \tag{99}$$

2.5 Extreme, Exposed

Definition. *Extreme point.* An extreme point x_ε of a convex set $\mathcal{C}$ is a point, belonging to its closure $\overline{\mathcal{C}}$ [33, §3.3], that is not expressible as a convex combination of points in $\overline{\mathcal{C}}$ distinct from x_ε ; *id est*, for $x_\varepsilon \in \overline{\mathcal{C}}$ and all $x_1, x_2 \in \overline{\mathcal{C}} \backslash x_\varepsilon$,

$$\mu x_1 + (1-\mu)x_2 \neq x_\varepsilon\,, \quad \mu \in [0,1] \tag{100}$$

$\triangle$

In other words, x_ε is an extreme point of $\mathcal{C}$ if and only if x_ε is not a point relatively interior to any line segment in $\overline{\mathcal{C}}$. [35, §2.10]

The set consisting of a single point $\mathcal{C} = \{x_\varepsilon\}$ is itself an extreme point.

Theorem. *Extreme existence.* [30, §18.5.3] [23, §II.3.5] A nonempty closed convex set containing no lines has at least one extreme point. $\diamond$

Definition. *Face, edge.* [29, §A.2.3]

- A *face* $\mathcal{F}$ of convex set $\mathcal{C}$ is a convex subset $\mathcal{F} \subseteq \overline{\mathcal{C}}$ such that every closed line segment $\overline{x_1 x_2}$ in $\overline{\mathcal{C}}$, having an interior-point $x \in \operatorname{rel\,int} \overline{x_1 x_2}$ in $\mathcal{F}$, has both endpoints in $\mathcal{F}$. The zero-dimensional faces of $\mathcal{C}$ constitute its extreme points. The empty set and $\overline{\mathcal{C}}$ itself are conventional faces of $\mathcal{C}$. [30, §18]
- All faces $\mathcal{F}$ are extreme sets by definition; *id est*, for $\mathcal{F} \subseteq \overline{\mathcal{C}}$ and all $x_1, x_2 \in \overline{\mathcal{C}} \backslash \mathcal{F}$,

$$\mu x_1 + (1-\mu)x_2 \notin \mathcal{F}\,, \quad \mu \in [0,1] \tag{101}$$

- A one-dimensional face of a convex set is called an *edge.*

$\triangle$

The dimension of a face is the penultimate number of affinely independent points (§2.3.2.3.1) belonging to it;

$$\dim \mathcal{F} = \sup_\rho \dim\{x_2 - x_1\,,\ x_3 - x_1\,,\ \ldots\ x_\rho - x_1 \mid x_i \in \mathcal{F}\,,\ i=1\ldots\rho\} \tag{102}$$

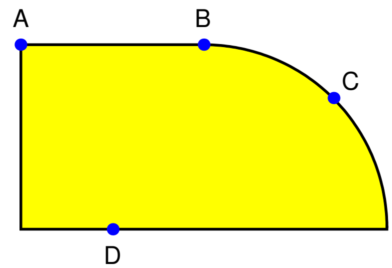


Figure 2.7: Closed convex set in $\mathbb{R}^2$. Point A is exposed hence extreme. Point B is extreme but not an exposed point. Point C is exposed and extreme. Point D is neither an exposed or extreme point although it belongs to a one-dimensional exposed face. [29, §A.2.4] [31, §3.6] Closed face $\overline{\mathrm{AB}}$ is exposed; a facet. The arc is not a conventional face, yet it is composed entirely of extreme points. The union of rotations of this entire set about its vertical edge produces another set in three dimensions having no edges; the same is false for rotation about the horizontal edge.

The point of intersection in $\overline{\mathcal{C}}$ with a strictly supporting hyperplane identifies an extreme point, but not *vice versa.* The nonempty intersection of any supporting hyperplane with $\overline{\mathcal{C}}$ identifies a face, in general, but not *vice versa.* To acquire a converse, the concept *exposed face* requires introduction:

2.5.1 Exposure

2.5.1.0.1 Definition. *Exposed face, exposed point, vertex, facet.* [29, §A.2.3, A.2.4]

- $\mathcal{F}$ is an *exposed face* of an n-dimensional convex set $\mathcal{C}$ iff there is a supporting hyperplane $\underline{\partial\mathcal{H}}$ to $\overline{\mathcal{C}}$ such that

$$\mathcal{F} = \overline{\mathcal{C}} \cap \underline{\partial\mathcal{H}} \tag{103}$$

  Only faces of dimension -1 through $n-1$ can be exposed by a hyperplane.

- An *exposed point*, the definition of *vertex*, is equivalent to a zero-dimensional exposed face; the point of intersection with a strictly supporting hyperplane.

- A *facet* is an $(n-1)$-dimensional exposed face of an n-dimensional convex set $\mathcal{C}$; in one-to-one correspondence with the $(n-1)$-dimensional faces.[2.16]

- $\overline{\{\text{exposed points}\}} = \{\text{extreme points}\}$
  $\{\text{exposed faces}\} \subseteq \{\text{faces}\}$ $\triangle$

2.5.1.1 Density of exposed points

For any closed convex set $\mathcal{C}$, its exposed points constitute a *dense* subset of its extreme points; [30, §18] [56] [31, §3.6, p.115] dense in the sense [48] that closure of that subset yields the set of extreme points.

For the convex set illustrated in Figure **2.7**, point B cannot be exposed because it relatively bounds both the facet $\overline{\mathrm{AB}}$ and the closed quarter circle, each bounding the set. Since B is not relatively interior to any line segment in the set, then B is an extreme point by definition. Point B may be regarded as the limit of some sequence of exposed points beginning at C .

2.5.1.2 Face transitivity and algebra

Faces enjoy a transitive relationship. If $\mathcal{F}_1$ is a face (an extreme set) of $\mathcal{F}_2$ which, in turn, is a face of $\mathcal{F}_3$, then it is always true that $\mathcal{F}_1$ is a face of $\mathcal{F}_3$. [30, §18] [57, def.115/6, p.358] For example, any extreme point of $\mathcal{F}_2$ is an extreme point of $\mathcal{F}_3$. (The parallel statement for exposed faces is false.) Yet it is erroneous to presume that a face, of dimension 1 or more, consists entirely of extreme points, nor is a face of dimension 2 or more entirely composed of edges, and so on.

For the polyhedron in $\mathbb{R}^3$ from Figure **2.2**, for example, the nonempty faces exposed by a hyperplane are the vertices, edges, and facets; there are no more. The zero-, one-, and two-dimensional faces are in one-to-one correspondence with the exposed faces in that example.

Define the smallest face $\mathcal{F}$ of a convex set $\mathcal{C}$ containing some element G :

$$\mathcal{F}(\mathcal{C} \ni G) \tag{104}$$

[2.16] This coincidence occurs simply because the facet's dimension is the same as the dimension of the supporting hyperplane exposing it.

An affine set has no faces except itself and the empty set. The smallest face of the intersection of $\mathcal{C}$ with an affine set $\mathcal{A}$ is [52, §2.4]

$$\mathcal{F}\big((\mathcal{C}\cap\mathcal{A})\ni G\big) = \mathcal{F}(\mathcal{C}\ni G)\cap\mathcal{A} \tag{105}$$

2.5.1.3 Boundary

The classical definition of *boundary* of a set $\mathcal{C}$ presumes nonempty interior:

$$\partial\mathcal{C} = \overline{\mathcal{C}} \setminus \operatorname{int}\mathcal{C} \tag{5}$$

More suitable for the study of convex sets is the relative boundary [29, §A.2.1.2]

$$\operatorname{rel}\partial\mathcal{C} = \overline{\mathcal{C}} \setminus \operatorname{rel\,int}\mathcal{C} \tag{106}$$

which is conventionally equivalent to:

2.5.1.3.1 Definition. *Conventional boundary of convex set.* [29, §C.3.1] The relative boundary $\partial\mathcal{C}$ of a nonempty convex set $\mathcal{C}$ is the union of all the exposed faces of $\overline{\mathcal{C}}$. △

Equivalence of these two definitions comes about because it is conventionally presumed that any supporting hyperplane, central to the definition of exposure, does not contain $\mathcal{C}$. [30, p.100]

A bounded convex polyhedron (§2.7.0.0.1) having nonempty interior, for example, in $\mathbb{R}$ has a boundary constructed from two points, in $\mathbb{R}^2$ from at least three line segments, in $\mathbb{R}^3$ from convex polygons, while a convex *polychoron* (a bounded polyhedron in $\mathbb{R}^4$ [48]) has a boundary constructed from three-dimensional convex polyhedra.

By Definition 2.5.1.3.1, an affine set has no relative boundary. Analogous to the result (105) for faces of a convex set $\mathcal{C}$ intersecting an affine set $\mathcal{A}$,

$$\operatorname{rel}\partial(\mathcal{C}\cap\mathcal{A}) = \operatorname{rel}\partial(\mathcal{C})\cap\mathcal{A} \tag{107}$$

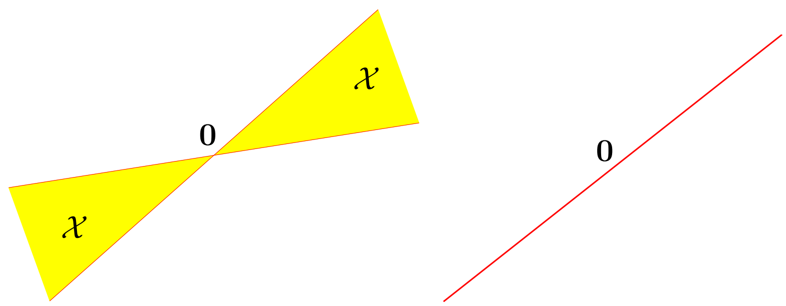
(a)  (b)

Figure 2.8: **(a)** Two-dimensional non-convex cone drawn truncated. Boundary of this cone is itself a cone. [37, §2.4] **(b)** This convex cone (drawn truncated) is a line through the origin in any dimension.

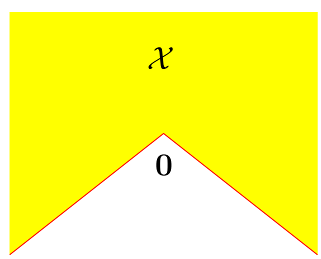


Figure 2.9: Truncated non-convex cone in $\mathbb{R}^2$. Boundary is also a cone. [37, §2.4]

2.6 Cones

Definition. *Ray.* The one-dimensional set

$$\{\zeta\Gamma + B \mid \zeta \geq 0\,,\ \Gamma \neq \mathbf{0}\} \subset \mathbb{R}^n \tag{108}$$

defines a *half-line* called a *ray* in *direction* $\Gamma \in \mathbb{R}^n$ having *base* $B \in \mathbb{R}^n$. When $B = \mathbf{0}$, a ray is the conic hull of direction Γ; hence a convex cone.

△

The conventional boundary of a single ray, base $\mathbf{0}$, in any dimension is the origin because that is the union of all exposed faces not containing the entire set.

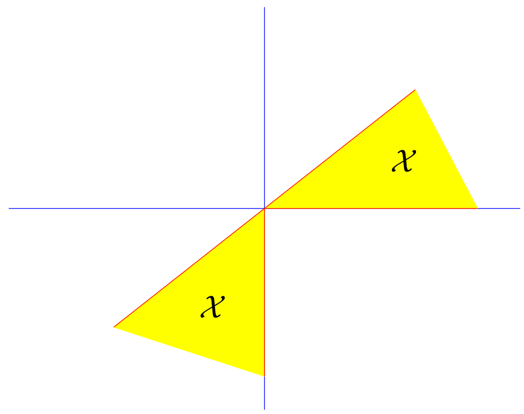


Figure 2.10: Truncated non-convex cone $\mathcal{X}=\{x\in\mathbb{R}^{\mathbf{2}} \mid x_1\geq x_2\,,\ x_1 x_2\geq 0\}$. Boundary is also a cone. [37, §2.4] Cartesian axes drawn for reference.

2.6.1 Cone

A set $\mathcal{X}$ is called, simply, *cone* if and only if

$$\Gamma\in\mathcal{X} \;\Rightarrow\; \zeta\Gamma\in\mathcal{X} \;\text{ for all }\; \zeta\geq 0 \tag{109}$$

An example of such a cone is the union of two opposing quadrants; *e.g.*, $\mathcal{X}=\left\{x\in\mathbb{R}^{\mathbf{2}} \mid x_1 x_2\geq 0\right\}$ which is not convex. [32, §2.5] Similar examples are shown in Figure **2.8** and Figure **2.10**.

Not all cones are necessarily convex, but they can all be defined by an aggregate of rays emanating exclusively from the origin.

Hence all cones contain the origin and are unbounded, excepting the simplest cone $\{\mathbf{0}\}$. The empty set $\emptyset$ is not a cone, but [31, §2.1]

$$\operatorname{cone}\emptyset \triangleq \{\mathbf{0}\} \tag{110}$$

2.6.2 Convex cone

We call the set $\mathcal{K}\subseteq\mathbb{R}^M$ a *convex cone* iff

$$\Gamma_1\,,\Gamma_2\in\mathcal{K} \;\Rightarrow\; \zeta\Gamma_1+\xi\Gamma_2\in\mathcal{K} \;\text{ for all }\; \zeta\,,\xi\geq 0 \tag{111}$$

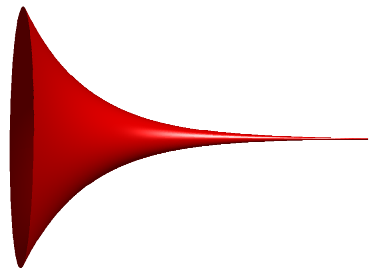


Figure 2.11: Not a cone, ironically, the three-dimensional *flared horn* (with or without its interior) resembling the mathematical symbol $\succ$ denoting cone membership and partial order.

Obvious from this definition, $\zeta\,\Gamma_1 \in \mathcal{K}$ and $\xi\,\Gamma_2 \in \mathcal{K}$ for all $\zeta\,,\xi \geq 0$. The set $\mathcal{K}$ is convex since, for any particular $\zeta\,,\xi \geq 0$,

$$\mu\,\zeta\,\Gamma_1 \,+\, (1-\mu)\,\xi\,\Gamma_2 \in \mathcal{K} \quad \forall\,\mu \in [0,1] \tag{112}$$

because $\mu\,\zeta\,,(1-\mu)\,\xi \geq 0$.

Obviously,

$$\{\mathcal{X}\} \supset \{\mathcal{K}\} \tag{113}$$

the set of all convex cones is a proper subset of all cones. The set of convex cones is a narrower but more familiar class of cone, any member of which can be equivalently described as the intersection of a possibly (but not necessarily) infinite number of hyperplanes (through the origin) and halfspaces whose bounding hyperplanes pass through the origin; a halfspace-description (§2.3). The interior of a convex cone is possibly empty.

Familiar examples of convex cones include an unbounded ice-cream cone (`a.k.a.` second-order, quadratic, or Lorentz cone [1, exmp.2.3&2.25]) united with its interior,

$$\mathcal{K}_\ell = \left\{ \begin{bmatrix} x \\ t \end{bmatrix} \in \mathbb{R}^n \times \mathbb{R} \mid \|x\|_2 \leq t \right\} \tag{114}$$

and any polyhedral cone (§2.7.1); *e.g.*, any orthant generated by the Cartesian axes (§2.1.0.7.1). Esoteric examples of convex cones include the point at the origin, any line through the origin, any ray having the origin as base such as the nonnegative real line $\mathbb{R}_+$ in subspace $\mathbb{R}$, any halfspace partially bounded by a hyperplane through the origin, the positive semidefinite cone $\mathbb{S}_+^M$ (120), the cone of Euclidean distance matrices $\mathbb{EDM}^N$ (335) (§5), any subspace, and $\mathbb{R}^n$.

More Euclidean objects are cones, it seems, than are not. (*confer* Figure **2.8** - Figure **2.11**)

Theorem. *Cone intersection.* [30, §2, §19] The intersection of an arbitrary collection of convex cones is a convex cone. The intersection of a finite number of polyhedral cones (§2.7.1, Figure **2.16**, p.71) is polyhedral. $\diamond$

The property *pointedness* is associated with a convex cone.

2.6.2.0.1 Definition. *Pointed convex cone.* (*confer* §2.7.2.1.1)
A convex cone $\mathcal{K}$ is *pointed* iff it contains no line. Equivalently, $\mathcal{K}$ is not pointed iff there exists any nonzero direction $\Gamma \in \overline{\mathcal{K}}$ such that $-\Gamma \in \overline{\mathcal{K}}$. [1, §2.4.1] If the origin is an extreme point of $\overline{\mathcal{K}}$ or, equivalently, if

$$\overline{\mathcal{K}} \cap -\overline{\mathcal{K}} = \{\mathbf{0}\} \tag{115}$$

then $\mathcal{K}$ is pointed, and *vice versa.* [31, §2.10] $\triangle$

Thus the simplest convex cone $\mathcal{K} = \{\mathbf{0}\} \subseteq \mathbb{R}^n$ is pointed by convention, but has empty interior.

If closed convex $\mathcal{K}$ is not pointed, then it has no extreme point. Yet a pointed closed convex cone has only one extreme point; it resides at the origin. [33, §3.3]

From the *cone intersection theorem* it follows that an intersection of convex cones is pointed if at least one of the cones is.

2.6.2.0.2 Definition. *Proper cone*: [1, §2.4.1] A cone that is

- convex
- closed
- pointed
- and has nonempty interior. $\triangle$

Examples of proper cones are the positive semidefinite cone $\mathbb{S}_+^M$ in the ambient space of symmetric matrices (§2.6.6), the nonnegative real line $\mathbb{R}_+$ in vector space $\mathbb{R}$, and any orthant in $\mathbb{R}^n$.

2.6.3 Cone boundary

Every hyperplane supporting a convex cone contains the origin. [29, §A.4.2] Because any supporting hyperplane to a convex cone must therefore be itself a cone, then from the *cone intersection theorem* it follows:

2.6.3.0.1 Lemma. *Cone faces.* [23, §II.8]
Each nonempty exposed face of a convex cone is a convex cone. ⋄

2.6.3.0.2 Theorem. *Proper-cone boundary.* Suppose a nonzero point Γ lies on the boundary $\partial\mathcal{K}$ of proper cone $\mathcal{K}$ in $\mathbb{R}^n$. Then it follows that the ray $\{\zeta\Gamma \mid \zeta \geq 0\}$ also belongs to $\partial\mathcal{K}$. ⋄

Proof. By virtue of its propriety, a proper cone guarantees the existence of a strictly supporting hyperplane at the origin. [30, Cor.11.7.3][2.17] Hence the origin belongs to the boundary of $\mathcal{K}$ because it is the zero-dimensional exposed face. The origin belongs to the ray through Γ, and the ray belongs to $\mathcal{K}$ by definition (109). By the *cone faces lemma*, each and every nonempty exposed face must include the origin. Hence the closed line segment $\overline{\mathbf{0}\Gamma}$ must lie in an exposed face of $\mathcal{K}$ because both endpoints do by Definition 2.5.1.3.1. That means there exists a supporting hyperplane $\partial\underline{\mathcal{H}}$ to $\mathcal{K}$ containing $\overline{\mathbf{0}\Gamma}$. So the ray through Γ belongs both to $\mathcal{K}$ and to $\partial\underline{\mathcal{H}}$. $\partial\underline{\mathcal{H}}$ must therefore expose a face of $\mathcal{K}$ that contains the ray; *id est*,

$$\{\zeta\Gamma \mid \zeta \geq 0\} \subseteq \mathcal{K} \cap \partial\underline{\mathcal{H}} \subset \partial\mathcal{K} \tag{116}$$

♦

Proper cone $\{\mathbf{0}\}$ in $\mathbb{R}^{\mathbf{0}}$ has no boundary (106) because $\operatorname{rel\,int}\{\mathbf{0}\} = \{\mathbf{0}\}$. (4)

The boundary of any proper cone in $\mathbb{R}$ is the origin.

The boundary of any proper cone whose dimension exceeds 1 can be constructed entirely from an aggregate of rays emanating exclusively from the origin.

[2.17] Rockafellar's corollary yields a supporting hyperplane at the origin to any convex cone in $\mathbb{R}^n$ not equal to $\mathbb{R}^n$.

2.6.4 Extreme direction

The property *extreme direction* arises naturally in connection with the pointed closed convex cone $\mathcal{K} \subset \mathbb{R}^n$, being analogous to extreme point. [30, §18, p.162][2.18] An extreme direction Γ_ε of pointed $\mathcal{K}$ corresponds to an edge that is a ray emanating from the origin.[2.19] Nonzero direction Γ_ε in pointed $\mathcal{K}$ is extreme if and only if,

$$\zeta_1\Gamma_1+\zeta_2\Gamma_2 \neq \Gamma_\varepsilon \quad \forall\, \zeta_1\,,\zeta_2 \geq 0\,, \quad \forall\, \Gamma_1\,,\Gamma_2 \in \mathcal{K}\backslash\{\zeta\Gamma_\varepsilon\!\in\mathcal{K} \mid \zeta\geq 0\} \tag{117}$$

In words, an extreme direction in a pointed closed convex cone is the direction of a ray that cannot be expressed as a conic combination of directions of rays in the cone distinct from the extreme ray.

By (64), extreme direction Γ_ε is not a point relatively interior to any line segment in $\mathcal{K}\backslash\{\zeta\Gamma_\varepsilon \in \mathcal{K} \mid \zeta \geq 0\}$. An extreme *direction* is unique, but its vector representation Γ_ε is not because any positive scaling of it produces another vector in the same (extreme) direction. Thus, by analogy, the corresponding extreme ray $\{\zeta\Gamma_\varepsilon \mid \zeta \geq 0\}$ is not a ray relatively interior to any *plane segment*[2.20] in $\mathcal{K}$.

The extreme directions of the positive semidefinite cone (§2.6.6), for example, comprise the set of all symmetric rank-one matrices $\{zz^T\!\in\mathbb{S}^M \mid \|z\|=1\}$. [55, §6] [58, §III]

If closed convex $\mathcal{K}$ is not pointed, then it has no extreme directions and no vertex. [55, §1] Conversely, pointed closed convex $\mathcal{K}$ is the convex hull of its extreme directions and vertex. [30, §18, p.167] That is the practical utility of extreme direction; to facilitate construction of polyhedral sets, apparent from the *extremes theorem*:

2.6.4.0.1 Theorem (Klee). *Extremes.* [31, §3.6] [30, §18, p.166] (*confer* §2.2.2, §2.7.2) Any closed convex set containing no lines can be expressed as the convex hull of all its extreme points and directions.

◇

[2.18] Indeed, Rockafellar suggests the mnemonic "extreme point at infinity".

[2.19] An edge of a convex cone is not necessarily a ray. A convex cone may contain an edge that is a line; *e.g.*, a wedge-shaped polyhedral cone ($\mathcal{K}^*$ in Figure **2.21**, p.108).

[2.20] A planar fragment; in this context, a planar cone.

It follows that any element of a convex set containing no lines may be expressed as a linear combination of its extreme elements; *e.g.*, Example 2.6.6.3.2.

2.6.4.1 Generators

When the *extremes theorem* applies, the extreme points and directions are termed *generators* of a convex set. An arbitrary collection of generators for a convex set includes its extreme elements as a subset; the set of all extreme elements of a convex set is a minimal set of generators for that set. More generally, generators for a convex set comprise any collection of points and directions whose convex hull constructs the set.

When the convex set under scrutiny is a pointed closed convex cone, conic combination of the generators during its construction is implicit:

Example. *Application of extremes theorem.* Given an extreme point at the origin and N extreme directions, denoting the i^{th} extreme direction by $\Gamma_i \in \mathbb{R}^n$, then the convex hull is (60)

$$\begin{aligned}\mathcal{P} &= \left\{[\mathbf{0}\;\;\Gamma_1\;\;\Gamma_2\cdots\Gamma_N]\,a\,\zeta \mid a^T\mathbf{1}=1,\; a\succeq 0,\; \zeta\geq 0\right\}\\ &= \left\{[\Gamma_1\;\;\Gamma_2\cdots\Gamma_N]\,a\,\zeta \mid a^T\mathbf{1}\leq 1,\; a\succeq 0,\; \zeta\geq 0\right\}\\ &= \left\{[\Gamma_1\;\;\Gamma_2\cdots\Gamma_N]\,b \mid b\succeq 0\right\}\subset\mathbb{R}^n\end{aligned} \tag{118}$$

a closed convex set that is simply a conic hull like (63). □

2.6.5 Exposed direction

Definition. *Exposed direction, exposed point of a pointed convex cone.* [30, §18] (*confer* §2.5.1.0.1)

- When a convex cone has a vertex, an exposed point, it resides at the origin; there can be only one.
- In the closure of a pointed convex cone, an *exposed direction* is the direction of a one-dimensional exposed face that is a ray emanating from the origin.
- $\overline{\{\text{exposed directions}\}} = \{\text{extreme directions}\}$ △

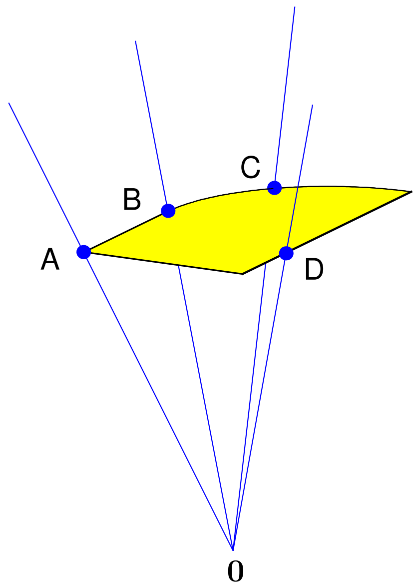


Figure 2.12: Four rays on boundary of conic hull of closed convex set from Figure **2.7** lifted to $\mathbb{R}^3$. Properties of extreme points carry over to extreme directions. [30, §18] Ray through point A is exposed hence extreme. Extreme direction B on cone boundary is not an exposed direction, although it belongs to the exposed face $\text{cone}\{A\,,B\}$. Extreme ray through C is exposed. Point D is neither an exposed or extreme direction although it belongs to a two-dimensional exposed face of the conic hull.

It follows from Lemma 2.6.3.0.1 for any pointed closed convex cone, there is one-to-one correspondence of one-dimensional exposed faces with exposed directions; *id est*, there is no one-dimensional exposed face that is not a ray base $\mathbf{0}$.

The pointed closed convex cone $\mathbb{EDM}^2$, for example, is a ray in isomorphic $\mathbb{R}$ whose relative boundary (§2.5.1.3.1) is the origin. The conventionally exposed directions of $\mathbb{EDM}^2$ constitute the empty set $\emptyset \subset \{\text{extreme direction}\}$.

2.6.5.1 Connection between boundary and extremes

2.6.5.1.1 Theorem. *Exposed.* [30, §18.7] (*confer* §2.6.4.0.1)
Any closed convex set $\mathcal{C}$ containing no lines can be expressed as the closure of the convex hull of all its exposed points and directions. $\diamond$

From Theorem 2.6.4.0.1,

$$\begin{aligned}
\operatorname{rel}\partial\mathcal{C} &= \overline{\mathcal{C}} \setminus \operatorname{rel}\operatorname{int}\mathcal{C} && (106)\\
&= \overline{\operatorname{conv}\{\text{exposed points and directions}\}} \setminus \operatorname{rel}\operatorname{int}\mathcal{C} && (119)\\
&= \operatorname{conv}\{\text{extreme points and directions}\} \setminus \operatorname{rel}\operatorname{int}\mathcal{C}
\end{aligned}$$

Thus each and every extreme point and direction of a convex set containing no lines (a set that is not a half-line) resides on its relative boundary because extreme points and directions do not belong to the relative interior by definition.

The relationship between extreme sets and the relative boundary actually goes deeper: Any face $\mathcal{F}$ of convex set $\mathcal{C}$ (that is not $\mathcal{C}$ itself) belongs to $\operatorname{rel}\partial\mathcal{C}$, so $\dim\mathcal{F} < \dim\mathcal{C}$. [30, §18.1.3]

2.6.5.1.2 Converse caveat

Yet this result does not mean each and every extreme point and direction is necessarily exposed, as might be erroneously inferred from the *conventional boundary definition* (§2.5.1.3.1); although it does mean each and every extreme point and direction belongs to some exposed face.

Arbitrary points residing on the relative boundary of a convex set are not necessarily exposed or extreme points. Similarly, the direction of an arbitrary ray, base $\mathbf{0}$, on the boundary of a convex cone is not necessarily an exposed or extreme direction. For the convex cone illustrated in Figure **2.3**, for example, there are three two-dimensional exposed faces constituting the entire boundary, each composed of an infinity of rays. Yet there are only three exposed directions.

Neither is an extreme direction on the boundary of a pointed convex cone necessarily an exposed direction. Lift the two-dimensional set in Figure **2.7**, for example, into three dimensions such that no two points in the set are collinear with the origin. Then its conic hull can have an extreme direction B on the boundary that is not an exposed direction, illustrated in Figure **2.12**.

2.6.6 Positive semidefinite (PSD) cone

Definition. *Positive semidefinite (PSD) cone.* The set of all symmetric positive semidefinite matrices of particular dimension M is called the *positive semidefinite cone*:

$$\begin{aligned}\mathbb{S}_+^M &\triangleq \left\{A \in \mathbb{S}^M \mid A \succeq 0\right\}\\ &= \left\{A \in \mathbb{S}^M \mid y^T\!A y \geq 0\,,\ \ \|y\| = 1\right\}\\ &= \bigcap_{\|y\|=1} \left\{A \in \mathbb{S}^M \mid \langle yy^T, A\rangle \geq 0\right\}\end{aligned} \tag{120}$$

formed by the intersection of an infinite number of halfspaces (§2.3.1.1) in variable A,[2.21] each halfspace having partial boundary containing the origin in isometrically isomorphic $\mathbb{R}^{M(M+1)/2}$. It is a unique immutable proper cone in the ambient space of symmetric matrices $\mathbb{S}^M$.

The positive definite (full-rank) matrices comprise the cone interior,[2.22]

$$\operatorname{int} \mathbb{S}_+^M = \left\{A \in \mathbb{S}^M \mid A \succ 0\right\} \tag{121}$$

while all singular positive semidefinite matrices (having at least one 0 eigenvalue) reside on the cone boundary (*e.g.*, Figure **2.13**); (§A.7.4)

$$\begin{aligned}\partial\mathbb{S}_+^M &= \left\{A \in \mathbb{S}_+^M \mid \langle zz^T, A\rangle = 0 \ \text{ for any } \|z\| = 1\right\}\\ &= \left\{A \in \mathbb{S}^M \mid \ \min\{\lambda(A)_i\,,\ i = 1 \ldots M\} = 0\right\}\end{aligned} \tag{122}$$

where $\lambda(A) \in \mathbb{R}^M$ holds the eigenvalues of A. The only symmetric positive semidefinite matrix having M 0-eigenvalues resides at the origin. (§A.7.2.0.1) △

[2.21] In higher dimensions, this cone is non-polyhedral because it is the intersection of an infinite number of halfspaces whose partial boundaries have independent normals yy^T. Because $y^T\!A\,y = y^T\!A^T y$, matrix A is almost always assumed symmetric. (§A.2.1)

[2.22] The remaining inequalities in (120) also become strict for membership to the cone interior.

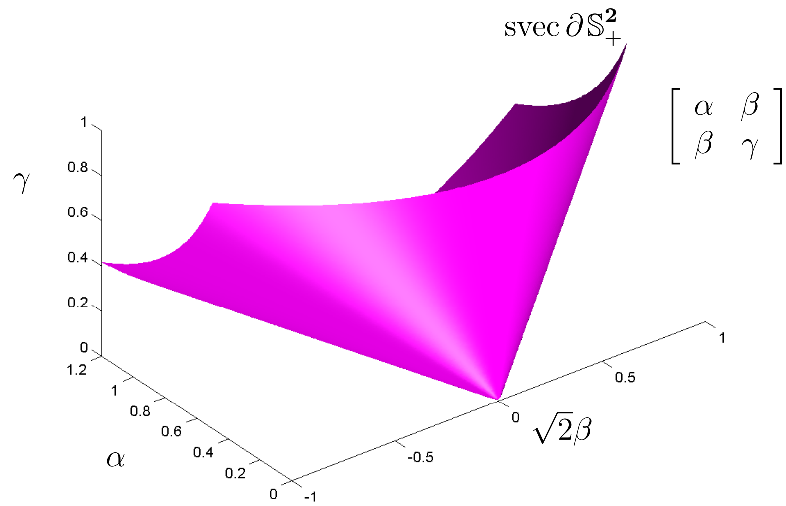


Figure 2.13: Truncated boundary of PSD cone in $\mathbb{S}^2$ plotted in isometrically isomorphic $\mathbb{R}^3$ (via svec, (35)); courtesy, Alexandre W. d'Aspremont. Plotted is 0-contour of minimum eigenvalue (122). Entire boundary can be constructed from an aggregate of rays (§2.6) emanating exclusively from the origin, $\left\{\zeta\,[\,z_1^2 \;\; \sqrt{2}z_1 z_2 \;\; z_2^2\,]^T \mid \|z\|=1\,,\; \zeta\geq 0\right\}$. In this dimension, each and every ray on boundary is an extreme direction, but that is not the case in any higher dimension (*confer* Figure **2.3**). (In any dimension, an extreme direction is a symmetric dyad; yy^T.) PSD cone geometry is not as simple in higher dimensions [23, §II.12], although for real matrices it is self-dual (199) in ambient space of symmetric matrices. [58, §II] PSD cone has no two-dimensional faces in any dimension, and its only extreme point resides at the origin.

2.6.6.1 Membership

Observe the notation $A \succeq 0$; meaning,[2.23] matrix A is symmetric and belongs to the positive semidefinite cone in the subspace of symmetric matrices, whereas $A \succ 0$ denotes membership to that cone's interior. (§2.8.2)

2.6.6.2 PSD cone is convex

The set of all positive semidefinite matrices forms a convex cone in the ambient space of symmetric matrices because any pair satisfies definition (111); [28, §7.1] *videlicet*, for all $\zeta_1, \zeta_2 \geq 0$ and each and every $A_1, A_2 \in \mathbb{S}^M$,

$$\zeta_1 A_1 + \zeta_2 A_2 \succeq 0 \;\Leftarrow\; A_1 \succeq 0\,,\; A_2 \succeq 0 \tag{123}$$

a fact easily verified by the definitive test for positive semidefiniteness of a symmetric matrix (§A):

$$A \succeq 0 \Leftrightarrow x^T\! A\, x \geq 0 \;\text{ for each and every } \|x\| = 1\,; \tag{124}$$

id est, for $A_1, A_2 \succeq 0$ and each and every $\zeta_1, \zeta_2 \geq 0$,

$$\zeta_1\, x^T\! A_1\, x + \zeta_2\, x^T\! A_2\, x \geq 0 \quad \text{for each and every normalized } x \in \mathbb{R}^M. \tag{125}$$

The convex cone $\mathbb{S}^M_+$ is more easily visualized in the isomorphic vector space $\mathbb{R}^{M(M+1)/2}$ whose dimension is the number of free variables in a symmetric $M{\times}M$ matrix. When $M=2$ the PSD cone is semi-infinite in expanse in $\mathbb{R}^{\mathbf{3}}$, having boundary illustrated in Figure **2.13**. When $M=3$ the PSD cone is six-dimensional, and so on.

2.6.6.3 Faces of PSD cone and their dimension *versus* rank

Each and every face of the positive semidefinite cone, having dimension less than that of the cone, is exposed. [59, §6] [24, §2.3.4] Because each and every face of the positive semidefinite cone contains the origin (§2.6.3.0.1), each face belongs to a subspace of the same dimension.

[2.23] For matrices, the notation $A \succeq B$ denotes comparison on $\mathbb{S}^M$ with respect to the positive semidefinite cone; *id est*, $A \succeq B \Leftrightarrow A - B \in \mathbb{S}^M_+$, a generalization of comparison on the real line. The symbol $\geq$ is reserved for scalar comparison on the real line $\mathbb{R}$ with respect to the nonnegative real line $\mathbb{R}_+$ as in $a^T y \geq b$, while $a \succeq b$ denotes comparison of vectors on $\mathbb{R}^M$ with respect to the nonnegative orthant $\mathbb{R}^M_+$.

Given positive semidefinite matrix $A\in\mathbb{S}_+^M$, define $\mathcal{F}\big(\mathbb{S}_+^M\ni A\big)$ as the smallest face of $\mathbb{S}_+^M$ containing A . Then, [50, §31.5.3] [52, §2.4]

$$\mathcal{F}\big(\mathbb{S}_+^M\ni A\big)=\{X\in\mathbb{S}_+^M \mid \mathcal{N}(X)\supseteq\mathcal{N}(A)\} \tag{126}$$

which is isomorphic with the convex cone $\mathbb{S}_+^{\operatorname{rank}A}$. Thus the dimension of the smallest face containing given matrix A is

$$\dim\mathcal{F}\big(\mathbb{S}_+^M\ni A\big)=\operatorname{rank}(A)\big(\operatorname{rank}(A)+1\big)/2 \tag{127}$$

in isomorphic $\mathbb{R}^{M(M+1)/2}$, and each and every face of $\mathbb{S}_+^M$ is isomorphic with a positive semidefinite cone of dimension $\leq M(M+1)/2$. Observe not all dimensions are represented, and the only zero-dimensional face is the origin. The PSD cone has no facets, for example.

For the positive semidefinite cone in isometrically isomorphic $\mathbb{R}^{\mathbf{3}}$ depicted in Figure **2.13**, for example, rank 2 matrices belong to the interior of the face having dimension 3 (the entire closed cone), while rank 1 matrices belong to the relative interior of a face having dimension 1 (the boundary constitutes all the one-dimensional faces, in this dimension, which are rays emanating from the origin), and the only rank 0 matrix is the point at the origin (the zero-dimensional face).

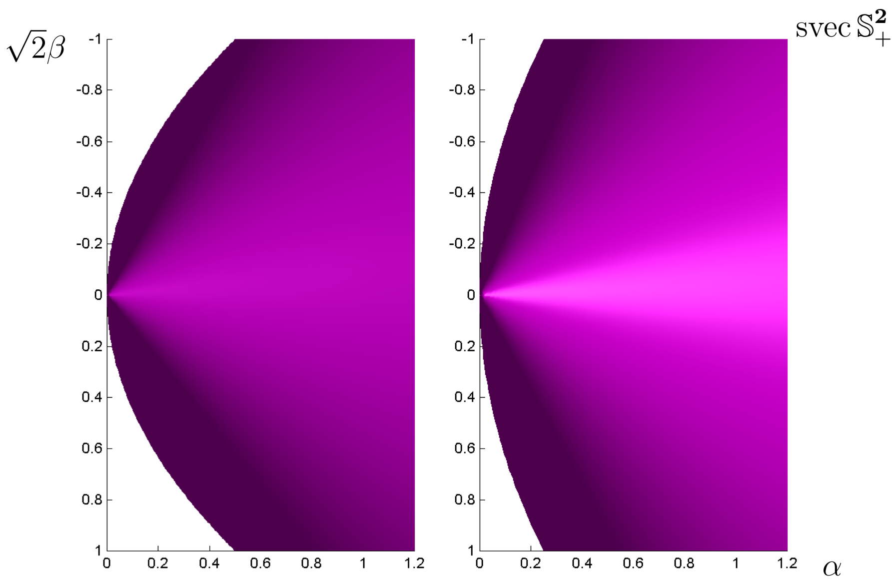
2.6.6.3.1 Extreme directions of the PSD cone

Because the positive semidefinite cone is pointed (§2.6.2.0.1), there is a one-to-one correspondence of one-dimensional faces with extreme directions in any dimension M ; *id est*, from the mentioned one-to-one correspondence of extreme and exposed faces for $\mathbb{S}_+^M$ and the *cone faces lemma* (§2.6.3.0.1) it follows there is no one-dimensional face of the PSD cone that is not a ray emanating from the origin. Symmetric dyads, therefore, constitute the set of all extreme directions.

Each and every extreme direction yy^T makes the same angle with the identity matrix in isomorphic $\mathbb{R}^{M(M+1)/2}$, dependent only on dimension; *videlicet*, [49, p.162]

$$\measuredangle=\arccos\frac{\langle yy^T,\, I\rangle}{\|yy^T\|_{\mathrm{F}}\,\|I\|_{\mathrm{F}}}=\arccos\left(\frac{1}{\sqrt{M}}\right)\quad\forall\,y\in\mathbb{R}^M \tag{128}$$

(a)



(b)

$$\begin{bmatrix} \alpha & \beta \\ \beta & \gamma \end{bmatrix}$$

Figure 2.14: **(a)** Projection of the PSD cone $\mathbb{S}^{\mathbf{2}}_+$, truncated above $\gamma = 1$, on $\alpha\beta$-plane in isometrically isomorphic $\mathbb{R}^{\mathbf{3}}$. View is from above with respect to Figure **2.13**. **(b)** Truncated above $\gamma = 2$. From these plots we may infer, for example, the line $\left\{[\,0 \quad 1/\sqrt{2} \quad \gamma\,]^T \mid \gamma \in \mathbb{R}\right\}$ intercepts the PSD cone at some large value of γ ; in fact, $\gamma = \infty$.

2.6.6.3.2 Example. *Positive semidefinite matrix from extreme directions.* Diagonalizability (§A.5) of symmetric matrices yields the following results:

Any symmetric positive semidefinite matrix (845) can be written in the form

$$A = \sum_i \lambda_i z_i z_i^T = \sum_i a_i a_i^T \succeq 0\,, \qquad \lambda \succeq 0 \tag{129}$$

a conic combination of extreme directions ($z_i z_i^T$ or $a_i a_i^T$), where λ is a vector of eigenvalues.

If we limit consideration to all symmetric positive semidefinite matrices bounded such that $\operatorname{tr} A = 1$, then any matrix from that set may be expressed as a convex combination of extreme directions;

$$A = \sum_i \lambda_i z_i z_i^T\,, \qquad \mathbf{1}^T\lambda = 1\,, \quad \lambda \succeq 0 \tag{130}$$

□

2.6.6.3.3 Example. *Sets from the PSD cone.* The set

$$\mathcal{C} = \{X \in \mathbb{S}^n \times x \in \mathbb{R}^n \mid X \succeq xx^T\} \tag{131}$$

is convex because it has a Schur form; (§A.4)

$$X - xx^T \succeq 0 \quad \Leftrightarrow \quad f(X,x) \triangleq \begin{bmatrix} X & x \\ x^T & 1 \end{bmatrix} \succeq 0 \tag{132}$$

Set $\mathcal{C}$ is the inverse image (§2.1.0.10.2) of $\mathbb{S}_+^{n+1}$ under the affine mapping f. The set $\{X \in \mathbb{S}^n \times x \in \mathbb{R}^n \mid X \preceq xx^T\}$ is not convex, in contrast, having no Schur form. Yet for fixed $x = x_p$, the set

$$\{X \in \mathbb{S}^n \mid X \preceq x_p x_p^T\} \tag{133}$$

is simply the negative semidefinite cone shifted to $x_p x_p^T$. □

2.6.6.3.4 Example. *Inverse image of the PSD cone.* Now consider finding the set of all matrices $X \in \mathbb{S}^N$ satisfying

$$AX + B \succeq 0 \tag{134}$$

given $A\,, B \in \mathbb{S}^N$. Define the set

$$\mathcal{X} \triangleq \{X \mid AX + B \succeq 0\} \subseteq \mathbb{S}^N \tag{135}$$

which is the inverse image of the positive semidefinite cone under the affine transformation $g(X) \triangleq AX+B$. Set $\mathcal{X}$ must therefore be convex by Theorem 2.1.0.10.2.

Yet we would like a less amorphous characterization of this set, so instead we consider its vectorization (18) which is easier to visualize:

$$\operatorname{vec} g(X) \;=\; \operatorname{vec}(AX) + \operatorname{vec} B \;=\; (I \otimes A)\operatorname{vec} X + \operatorname{vec} B \tag{136}$$

where

$$I \otimes A \triangleq Q\Lambda Q^T \in \mathbb{S}^{N^2} \tag{137}$$

is a block-diagonal matrix formed by Kronecker product (§A.1 no.16, §D.1.2.1). Assign

$$\begin{aligned} x &\triangleq \operatorname{vec} X \in \mathbb{R}^{N^2} \\ b &\triangleq \operatorname{vec} B \in \mathbb{R}^{N^2} \end{aligned} \tag{138}$$

then make the equivalent problem: Find

$$\operatorname{vec}\mathcal{X} = \{x \in \mathbb{R}^{N^2} \mid (I \otimes A)x + b \in \mathcal{K}\} \tag{139}$$

where

$$\mathcal{K} \triangleq \operatorname{vec}\mathbb{S}_+^N \tag{140}$$

is a proper cone isometrically isomorphic with the positive semidefinite cone in the subspace of symmetric matrices; the vectorization of every element of $\mathbb{S}_+^N$. Utilizing the diagonalization (137),

$$\begin{aligned} \operatorname{vec}\mathcal{X} &= \{x \mid \Lambda Q^T x \in Q^T(\mathcal{K} - b)\} \\ &= \{x \mid \Phi Q^T x \in \Lambda^\dagger Q^T(\mathcal{K} - b)\} \subseteq \mathbb{R}^{N^2} \end{aligned} \tag{141}$$

where

$$\Phi \triangleq \Lambda^\dagger \Lambda \tag{142}$$

is a diagonal projection matrix whose entries are either 1 or 0 (§E.3). We have the complementary sum

$$\Phi Q^T x + (I - \Phi)Q^T x = Q^T x \tag{143}$$

So, adding $(I-\Phi)Q^T x$ to both sides of the membership within (141) admits

$$\begin{aligned} \operatorname{vec}\mathcal{X} &= \{x \in \mathbb{R}^{N^2} \mid Q^T x \in \Lambda^\dagger Q^T(\mathcal{K} - b) + (I - \Phi)Q^T x\} \\ &= \{x \mid Q^T x \in \Phi\big(\Lambda^\dagger Q^T(\mathcal{K} - b)\big) \oplus (I - \Phi)\mathbb{R}^{N^2}\} \\ &= \{x \in Q\Lambda^\dagger Q^T(\mathcal{K} - b) \oplus Q(I - \Phi)\mathbb{R}^{N^2}\} \\ &= (I \otimes A)^\dagger(\mathcal{K} - b) \;\oplus\; \mathcal{N}(I \otimes A) \end{aligned} \tag{144}$$

where we used the facts: linear function $Q^T x$ in x is a bijection on $\mathbb{R}^{N^2}$, and $\Phi\Lambda^\dagger = \Lambda^\dagger$.

In words, set $\operatorname{vec}\mathcal{X}$ is the vector sum of the translated PSD cone (mapped linearly onto the rowspace of $I\otimes A$ (§E)) and the nullspace of $I\otimes A$ (synthesis of facts from §A.6.3 and §A.7.2.0.1). Should $I\otimes A$ have no nullspace, then $\operatorname{vec}\mathcal{X} = (I\otimes A)^{-1}(\mathcal{K} - b)$ which is the expected result. □

2.6.6.4 Barvinok's proposition

The following theory quantifies the rank of a positive semidefinite matrix whose rank is the least of all matrices belonging to the intersection of the PSD cone with an affine subset; it is a least upper bound on rank:

2.6.6.4.1 Proposition. *Affine intersection with PSD cone.*
[23, §II.13] [60, §2.2] Consider finding a matrix $G\in\mathbb{S}^N$ satisfying

$$G \succeq 0\,, \qquad \langle A_j\,,\, G\rangle = b_j\;, \quad j=1\ldots m \tag{145}$$

given nonzero linearly independent $A_j\in\mathbb{S}^N$ and real b_j. Define the affine subset

$$\mathcal{A} \triangleq \{G \mid \langle A_j\,,\,G\rangle = b_j\;,\; j=1\ldots m\} \subseteq \mathbb{S}^N \tag{146}$$

If the feasible set $\mathcal{A}\cap\mathbb{S}^N_+$ is nonempty, then there exists a matrix $G\in\mathcal{A}\cap\mathbb{S}^N_+$ such that given a number of equalities m,

$$\operatorname{rank}G\,(\operatorname{rank}G+1)/2 \le m \tag{147}$$

whence the least upper bound

$$\operatorname{rank}G \le \left\lfloor \frac{\sqrt{8m+1}-1}{2} \right\rfloor \tag{148}$$

or given desired rank instead, equivalently,

$$m < (\operatorname{rank}G+1)(\operatorname{rank}G+2)/2 \tag{149}$$

An extreme point of $\mathcal{A}\cap\mathbb{S}^N_+$ satisfies (148) and (149). A matrix $G = X^T X$ is an extreme point if and only if the dimension of the smallest face of $\mathcal{A}\cap\mathbb{S}^N_+$ containing G is 0; [52, §2.4] *id est*, iff

$$\dim\mathcal{F}\big((\mathcal{A}\cap\mathbb{S}^N_+)\ni G\big) = \operatorname{rank}(G)\big(\operatorname{rank}(G)+1\big)/2 - \operatorname{rank}\big[\operatorname{svec}XA_1X^T\;\; \operatorname{svec}XA_2X^T \cdots\; \operatorname{svec}XA_mX^T\big] \tag{150}$$

equals 0 in isomorphic $\mathbb{R}^{N(N+1)/2}$.

Now the feasible set $\mathcal{A}\cap\mathbb{S}_+^N$ is assumed bounded: Assume a given nonzero least upper bound ρ on rank, a number of equalities

$$m=(\rho+1)(\rho+2)/2 \tag{151}$$

and matrix dimension $N\geq\rho+2\geq 3$. If the feasible set is nonempty and bounded, then there exists a matrix $G\in\mathcal{A}\cap\mathbb{S}_+^N$ such that

$$\operatorname{rank} G\leq\rho \tag{152}$$

This represents a tightening of the least upper bound; a reduction by exactly 1 of the bound provided by (148) given the same specified number of equalities; *id est*,

$$\operatorname{rank} G\leq\frac{\sqrt{8m+1}-1}{2}-1 \tag{153}$$

$\diamond$

When the feasible set $\mathcal{A}\cap\mathbb{S}_+^N$ is known *a priori* to consist of only a single point, then Barvinok's proposition provides the greatest upper bound on its rank. The feasible set can be a single nonzero point only if the number of linearly independent hyperplanes m constituting $\mathcal{A}$ satisfies[2.24]

$$N(N+1)/2-1\leq m\leq N(N+1)/2 \tag{154}$$

2.6.7 Conic independence (c.i.)

In contrast to extreme direction, the property *conically independent direction* is more generally applicable, inclusive of all closed convex cones (not only pointed closed convex cones). Similar to the definition for linear independence, arbitrary given directions $\{\Gamma_i\in\mathbb{R}^n,\ i=1\ldots N\}$ are *conically independent* if and only if, for all $\zeta_i\geq 0$,

$$\Gamma_i\,\zeta_i+\cdots+\Gamma_j\,\zeta_j-\Gamma_\ell\,\zeta_\ell=\mathbf{0}\,,\qquad i\neq\cdots\neq j\neq\ell=1\ldots N \tag{155}$$

has only the trivial solution; in words, iff no direction from the given set can be expressed as a conic combination of those remaining. (Figure **2.15**,

[2.24] $N(N+1)/2-1$ independent hyperplanes in $\mathbb{R}^{N(N+1)/2}$ can make a line tangent to $\operatorname{svec}\partial\mathbb{S}_+^N$ at a point because all one-dimensional faces of $\mathbb{S}_+^N$ are exposed. Because a pointed convex cone has only one vertex, the origin, there can be no intersection of $\operatorname{svec}\partial\mathbb{S}_+^N$ with any higher-dimensional affine subset $\mathcal{A}$ that will make a nonzero point.

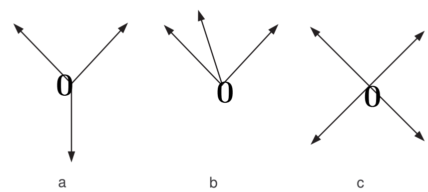


Figure 2.15: Vectors in $\mathbb{R}^2$: **(a)** conically independent, **(b)** conically dependent. Neither example exhibits linear independence.

for example. A Matlab implementation of test (155) is given in §F.2.) It is evident that linear independence (l.i.) of N directions implies their conic independence;

- l.i. $\Rightarrow$ c.i.

Arranging any set of generators for a particular convex cone in a matrix columnar,

$$X \triangleq [\,\Gamma_1 \;\; \Gamma_2 \;\cdots\; \Gamma_N\,] \in \mathbb{R}^{n\times N} \tag{156}$$

then the relationship l.i.$\Rightarrow$c.i. implies the number of l.i. generators in the columns of X cannot exceed the number of c.i. generators. Denoting by k the number of conically independent generators contained in X, we have the most fundamental rank inequality for convex cones

$$\dim \operatorname{aff} \mathcal{K} \;=\; \dim \operatorname{aff}[\,\mathbf{0}\;\; X\,] \;=\; \operatorname{rank} X \leq k \leq N \tag{157}$$

Whereas N directions in n dimensions can no longer be linearly independent once N exceeds n, conic independence remains possible:

2.6.7.1 Table: Maximum number conically independent directions

n	$\sup k$ (pointed)	$\sup k$ (not pointed)
0	0	0
1	1	2
2	2	4
3	∞	∞
$\vdots$	$\vdots$	$\vdots$

Assuming veracity of this table, there is an apparent vastness between two and three dimensions. Conic independence is certainly one convex idea that cannot be completely explained by a two-dimensional picture. [23, p.vii] From this table it is also evident that dimension of Euclidean space cannot exceed the number of conically independent directions possible;

- $n \leq \sup k$

We suspect the number of conically independent columns (rows) of X to be the same for $X^{\dagger T}$.

- The columns (rows) of X are c.i. $\Leftrightarrow$ the columns (rows) of $X^{\dagger T}$ are c.i.

Proof. Pending.

2.6.7.2 Pointed closed convex $\mathcal{K}$ and conic independence

The following bullets can be derived from definitions (117) and (155) in conjunction with the *extremes theorem* (§2.6.4.0.1):

The set of all extreme directions from a pointed closed convex cone $\mathcal{K} \subset \mathbb{R}^n$ is not necessarily a linearly independent set, yet it must be a conically independent set; (compare Figure **2.3**, p.35, with Figure **2.16**(a))

- extreme directions $\Rightarrow$ c.i.

Yet any collection of n or fewer extreme directions from pointed closed convex cone $\mathcal{K}$ must be linearly independent;

- $\leq n$ extreme directions $\Rightarrow$ l.i.

Conversely, when a conically independent set of directions from pointed closed convex cone $\mathcal{K}$ is known *a priori* to comprise generators, then all directions from that set must be extreme directions of the cone;

- c.i. generators of pointed closed convex $\mathcal{K} \Rightarrow$ extreme directions

Barker & Carlson [55, §1] call the extreme directions a *minimal generating set.* A minimal set of generators is therefore a conically independent set of generators, and *vice versa* for a pointed closed convex cone.[2.25]

[2.25] The converse does not hold for a non-pointed closed convex cone as Table **2.6.7.1** implies.

(a)

(b)

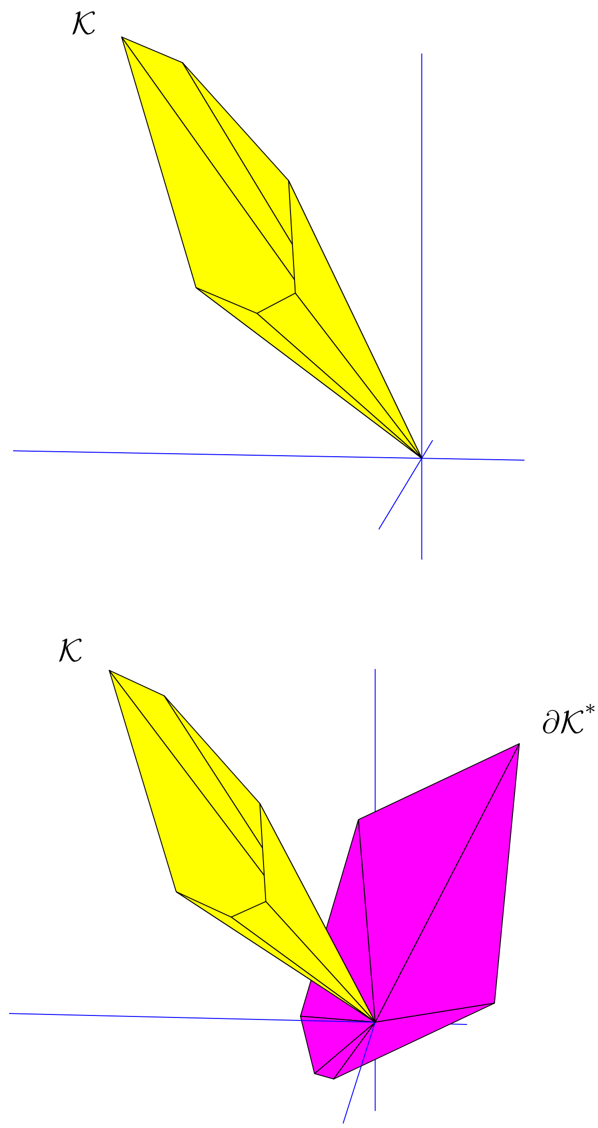


Figure 2.16: **(a)** A pointed polyhedral cone (drawn truncated) in $\mathbb{R}^{\mathbf{3}}$ having six facets. The extreme directions, corresponding to six edges emanating from the origin, are generators for this cone; not linearly independent but they must be conically independent. **(b)** The boundary of dual cone $\mathcal{K}^*$ (drawn truncated) is now added to the drawing of same $\mathcal{K}$. $\mathcal{K}^*$ is polyhedral, proper, and has the same number of extreme directions as $\mathcal{K}$ has facets.

2.6.8 When extreme means exposed

For any convex polyhedral set in $\mathbb{R}^n$ having nonempty interior, the distinction between the terms *extreme* and *exposed* vanishes [31, §2.4] [50, §2.2] for faces of all dimensions except n ; their meanings become equivalent as we saw in Figure **2.2** (discussed in §2.5.1.2). In other words, each and every face of any polyhedral set (except the set itself) can be exposed by a hyperplane, and *vice versa*; *e.g.*, Figure **2.3**.

Lewis [59, §6] [24, §2.3.4] claims nonempty extreme proper subsets and the exposed subsets coincide for $\mathbb{S}_+^n$; *id est*, each and every face of the positive semidefinite cone, whose dimension is less than the dimension of the cone, is exposed. A more general discussion of cones having this property can be found in [61]; *e.g.*, the Lorentz cone (114) [62, §II.A].

2.7 Convex polyhedra

Every polyhedron, such as the convex hull (60) of a bounded list X , can be expressed as the solution set of a finite system of linear equalities and inequalities, and *vice versa.* [50, §2.2]

2.7.0.0.1 Definition. *Convex polyhedra, halfspace-description.* [1, §2.2.4] A convex polyhedron is the intersection of a finite number of halfspaces and hyperplanes;

$$\mathcal{P} = \{y \mid Ay \succeq b\,,\; Cy = d\} \subseteq \mathbb{R}^n \tag{158}$$

where the coefficients A and C generally denote matrices. Each row of C is a vector normal to a hyperplane, while each row of A is a vector inward-normal to a hyperplane partially bounding a halfspace. △

By the *halfspaces theorem* in §2.3.1.1.1, a polyhedron thus described is a closed convex set having possibly empty interior; *e.g.*, Figure **2.2**. Convex polyhedra[2.26] are finite-dimensional comprising all affine sets (§2.2.1), polyhedral cones, line segments, rays, halfspaces, convex polygons, *solids* [57, def.104/6, p.343], polychora, *polytopes*,[2.27] *etcetera.*

[2.26]We consider only convex polyhedra throughout, but acknowledge the existence of concave polyhedra. [48, *Kepler-Poinsot Solid*]

[2.27]Some authors distinguish bounded polyhedra via the designation *polytope.* [50, §2.2]

It follows from definition (158) by exposure that each face of a convex polyhedron is a convex polyhedron.

The projection of any polyhedron on a subspace remains a polyhedron. More generally, the image of a polyhedron under any linear transformation is a polyhedron. [23, §I.9]

When b and d in (158) are $\mathbf{0}$, the resultant is a polyhedral cone. The set of all polyhedral cones is a subset of convex cones:

2.7.1 Polyhedral cone

From §2.6, the number of hyperplanes and halfspaces constituting a convex cone is possibly but not necessarily infinite. When the number is finite, the convex cone is termed *polyhedral.* That is the primary distinguishing feature between the set of all convex cones and polyhedra; all polyhedra, including polyhedral cones, are *finitely generated* [30, §19]. We distinguish polyhedral cones in the set of all convex cones for this very reason.

Definition. *Polyhedral cone, halfspace-description.*[2.28] (*confer* (165))
A polyhedral cone is the intersection of a finite number of halfspaces and hyperplanes about the origin;

$$\begin{aligned}
\mathcal{K} &= \{y \mid Ay \succeq 0\,,\ Cy = \mathbf{0}\} \subseteq \mathbb{R}^n & \text{(a)}\\
&= \{y \mid Ay \succeq 0\,,\ Cy \succeq 0\,,\ Cy \preceq 0\} & \text{(b)}\\
&= \left\{ y \mid \begin{bmatrix} A \\ C \\ -C \end{bmatrix} y \succeq 0 \right\} & \text{(c)}
\end{aligned} \qquad (159)$$

where coefficients A and C generally denote matrices of finite dimension. Each row of C is a vector normal to a hyperplane containing the origin, while each row of A is a vector inward-normal to a hyperplane containing the origin and partially bounding a halfspace. △

A polyhedral cone thus defined is closed, convex, possibly has empty interior, and only a finite number of generators (§2.6.4.1), and *vice versa.* (Minkowski/Weyl) [31, §2.8]

[2.28] Rockafellar [30, §19] proposes affine sets be handled via complementary pairs of affine inequalities; *e.g.*, $Cy \succeq d$ and $Cy \preceq d$.

From the definition it follows that any single hyperplane through the origin, or any halfspace partially bounded by a hyperplane through the origin is a polyhedral cone. The most familiar example of polyhedral cone is any quadrant (or orthant, §2.1.0.7.1) generated by the Cartesian axes. Esoteric examples of polyhedral cone include the point at the origin, any line through the origin, any ray having the origin as base such as the nonnegative real line $\mathbb{R}_+$ in subspace $\mathbb{R}$, polyhedral variations of the proper Lorentz cone (*confer* (114)), (for $\ell = 1$ or ∞)

$$\mathcal{K}_\ell \triangleq \left\{ \begin{bmatrix} x \\ t \end{bmatrix} \in \mathbb{R}^n \times \mathbb{R} \mid \|x\|_\ell \leq t \right\} \tag{160}$$

any subspace, and $\mathbb{R}^n$. More examples are illustrated in Figure **2.16** and Figure **2.3**.

2.7.2 Vertices of convex polyhedra

By definition, a vertex (§2.5.1.0.1) always lies on the relative boundary of a convex polyhedron. [57, def.115/6, p.358] In Figure **2.2**, each vertex of the polyhedron is located at the intersection of three or more facets, and every edge belongs to precisely two facets [23, §VI.1, p.252]. In Figure **2.3**, the only vertex of that polyhedral cone lies at the origin.

The set of all polyhedral cones is clearly a subset of convex polyhedra and a subset of convex cones. Not all convex polyhedra are bounded, evidently, neither can they all be described by the convex hull of a bounded set of points as we defined it in (60). Hence we propose a universal vertex-description of polyhedra in terms of that same finite-length list X (54):

Definition. *Convex polyhedra, vertex-description.* (*confer* §2.6.4.0.1) Denote the truncated a-vector,

$$a_{i:\ell} = \begin{bmatrix} a_i \\ \vdots \\ a_\ell \end{bmatrix} \tag{161}$$

By discriminating a suitable finite-length generating list (or set) arranged columnar in $X \in \mathbb{R}^{n \times N}$, then any particular polyhedron may be described,

$$\mathcal{P} = \left\{ Xa \mid a_{1:k}^T \mathbf{1} = 1\,,\; a_{m:N} \succeq 0\,,\; \{1 \ldots k\} \cup \{m \ldots N\} = \{1 \ldots N\} \right\} \tag{162}$$

where $0 \leq k \leq N$ and $1 \leq m \leq N+1$. Setting $k=0$ eliminates the affine equality constraint. Setting $m = N+1$ eliminates the inequality. $\triangle$

The coefficient indices in (162) may or may not be overlapping, but all the coefficients are assumed constrained. From (56), (60), and (63), we summarize how the constraints may be applied;

$$\left.\begin{array}{lcl} \text{affine sets} & \longrightarrow & a_{1:k}^T\mathbf{1} = 1 \\ \text{polyhedral cones} & \longrightarrow & a_{m:N} \succeq 0 \end{array}\right\} \longleftarrow \text{convex hull } (m \leq k) \tag{163}$$

It is always possible to describe a convex hull in the region of overlapping indices because, for $1 \leq m \leq k \leq N$,

$$\{a_{m:k} \mid a_{m:k}^T\mathbf{1} = 1,\ a_{m:k} \succeq 0\} \subseteq \{a_{m:k} \mid a_{1:k}^T\mathbf{1} = 1,\ a_{m:N} \succeq 0\} \tag{164}$$

Members of a generating list are not necessarily vertices of the corresponding polyhedron; certainly true for (60) and (162), some subset of list members reside in the polyhedron's relative interior. Conversely, when boundedness (60) applies, the convex hull of the vertices is a polyhedron identical to the convex hull of the generating list.

2.7.2.1 Vertex-description of polyhedral cone

Given closed convex cone $\mathcal{K}$ in a subspace of $\mathbb{R}^n$ having any set of generators for it arranged in a matrix $X \in \mathbb{R}^{n\times N}$ as in (156), then that cone is described setting $m=1$ and $k=0$ in vertex-description (162):

$$\mathcal{K} = \operatorname{cone}(X) = \{Xa \mid a \succeq 0\} \subseteq \mathbb{R}^n \tag{165}$$

a conic hull, like (63), of N generators.

2.7.2.1.1 Pointedness. [31, §2.10] Assuming all generators constituting the columns of $X \in \mathbb{R}^{n\times N}$ are nonzero, $\mathcal{K}$ is pointed (§2.6.2.0.1) if and only if there is no nonzero $a \succeq 0$ that solves $Xa = \mathbf{0}$; *id est*, iff $\mathcal{N}(X) \cap \mathbb{R}_+^N = \mathbf{0}$. (If $\operatorname{rank} X = n$, then the *dual cone* $\mathcal{K}^*$ is pointed. (176))

A polyhedral proper cone in $\mathbb{R}^n$ must have at least n generators that are linearly independent, or be the intersection of at least n halfspaces whose partial boundaries have normals that are linearly independent. Otherwise, the cone will contain at least one line and there can be no vertex; *id est*, the cone cannot otherwise be pointed.

For any pointed polyhedral cone, there is a one-to-one correspondence of one-dimensional faces with extreme directions.

Examples of pointed closed convex cones $\mathcal{K}$ are not limited to polyhedral cones: the origin, any $\mathbf{0}$-based ray in a subspace, any two-dimensional V-shaped cone in a subspace, the Lorentz (ice-cream) cone (including the interior) and its polyhedral variations, the cone of Euclidean distance matrices $\mathbb{EDM}^N$ in $\mathbb{S}^N_{\mathbf{0}}$, the proper cones: $\mathbb{S}^M_+$ in ambient $\mathbb{S}^M$, any orthant in $\mathbb{R}^n$ or $\mathbb{R}^{m\times n}$; *e.g.*, the nonnegative real line $\mathbb{R}_+$ in vector space $\mathbb{R}$.

2.7.3 Unit simplex

A peculiar convex subset of the nonnegative orthant having halfspace-description

$$\mathcal{S} \triangleq \{s \mid s \succeq 0\,,\ \mathbf{1}^T s \leq 1\} \subseteq \mathbb{R}^n_+ \tag{166}$$

is a unique bounded convex polyhedron called *unit simplex* (Figure **2.17**) having nonempty interior, $n+1$ vertices, and dimension [1, §2.2.4]

$$\dim \mathcal{S} \,=\, n \tag{167}$$

The origin supplies one vertex while heads of the *standard basis* [28] [26] $\{e_i\,,\ i=1\ldots n\}$ in $\mathbb{R}^n$ constitute those remaining;[2.29] thus its vertex-description:

$$\begin{aligned} \mathcal{S} &= \operatorname{conv}\{\mathbf{0},\ \{e_i\,,\ i=1\ldots n\}\} \\ &= \left\{[\,\mathbf{0}\ \ e_1\ \ e_2\ \cdots\ e_n\,]\,a \mid a^T\mathbf{1} = 1\,,\ a \succeq 0\right\} \end{aligned} \tag{168}$$

The unit simplex comes from a class of general polyhedra called *simplex*, having vertex-description: [63] [30] [32] [50]

$$\operatorname{conv}\{x_\ell \in \mathbb{R}^n\} \mid \ell = 1\ldots k+1\,,\ \ \dim \operatorname{aff}\{x_\ell\} = k\,,\ n \geq k \tag{169}$$

So defined, a simplex is a closed bounded convex set having possibly empty interior.

[2.29] In $\mathbb{R}^{\mathbf{0}}$ the unit simplex is the point at the origin, in $\mathbb{R}$ the unit simplex is the line segment $[0,1]$, in $\mathbb{R}^{\mathbf{2}}$ it is a triangle and its relative interior, in $\mathbb{R}^{\mathbf{3}}$ it is the convex hull of a tetrahedron (Figure **2.17**), in $\mathbb{R}^{\mathbf{4}}$ it is the convex hull of a pentatope [48], and so on.

2.7.3.0.1 Definition. *Simplicial cone.* A polyhedral proper (§2.6.2.0.2) cone $\mathcal{K}$ in $\mathbb{R}^n$ is called *simplicial* iff $\mathcal{K}$ has exactly n extreme directions; [62, §II.A] equivalently, iff proper $\mathcal{K}$ has exactly n linearly independent generators contained in any given set of generators. △

There are an infinite variety of simplicial cones in $\mathbb{R}^n$; *e.g.*, Figure **2.3**, Figure **2.18**, Figure **2.24**. Any orthant is simplicial.

2.7.4 Converting between descriptions

Conversion between halfspace-descriptions (158) (159) and equivalent vertex-descriptions (60) (162) is nontrivial, in general, [64] [50, §2.2] but the conversion is easy for simplices. [1, §2.2] Nonetheless, we tacitly assume the two descriptions to be equivalent. [30, §19, thm.19.1] We explore conversions in §2.8.2.1 and §2.9:

2.8 Dual cone, generalized inequality, biorthogonal expansion

These three concepts, dual cone, generalized inequality, and biorthogonal expansion, are inextricably melded; meaning, it is difficult to completely discuss one without mentioning the others. Knowledge of the dual cone is crucial to efficient methods for projection on convex cones (§E.8.1.0.1) such as might occur in schemes for rank minimization (§7). The dual cone is critical in tests for convergence in contemporary primal/dual methods for numerical solution of conic problems. [4] [6, §4.5]

One way to think of a pointed closed convex cone is as a new kind of coordinate system whose basis is generally nonorthogonal; a conic system very much like the Cartesian system whose analogous cone is the nonnegative orthant. The generalized inequality $\succeq_{\mathcal{K}}$ is a formalized means to determine membership to any pointed closed convex cone, while the biorthogonal expansion is simply a formulation for determining coordinates in any pointed conic system. When the underlying cone is the nonnegative orthant, then these three concepts come into alignment with the familiar Cartesian prototype.

2.8.1 Dual cone

For any cone $\mathcal{K}$ (convex or not), the dual cone [1, §2.6.1]

$$\mathcal{K}^* = \{y \in \mathbb{R}^n \mid \langle y\,, x\rangle \geq 0 \;\text{ for all }\; x \in \mathcal{K}\} \tag{170}$$

is a unique cone[2.30] that is always closed and convex because it is an intersection of halfspaces (*halfspaces theorem*, §2.3.1.1.1) whose partial boundaries each contain the origin, each having inward-normal x belonging to $\mathcal{K}$; *e.g.*, Figure **2.19**(a).

When cone $\mathcal{K}$ is convex, the dual cone $\mathcal{K}^*$ is the union of each and every vector y inward-normal to a hyperplane supporting or containing $\mathcal{K}$; *e.g.*, Figure **2.19**(b). When $\mathcal{K}$ is represented by a halfspace description such as (159), for example, where

$$A \triangleq \begin{bmatrix} a_1^T \\ \vdots \\ a_m^T \end{bmatrix} \in \mathbb{R}^{m\times n}\,, \qquad C \triangleq \begin{bmatrix} c_1^T \\ \vdots \\ c_k^T \end{bmatrix} \in \mathbb{R}^{k\times n} \tag{171}$$

then the dual cone can be represented as the conic hull

$$\mathcal{K}^* = \operatorname{cone}\{a_1\,, \ldots\,, a_m\;, \pm c_1\,, \ldots\,, \pm c_k\} \tag{172}$$

a vertex-description, because each and every conic combination of normals from the halfspace description of $\mathcal{K}$ yields another inward-normal to a hyperplane supporting or containing $\mathcal{K}$.

As defined, dual cone $\mathcal{K}^*$ exists even when the affine hull of the original cone is a proper subspace; *id est*, even when the original cone has empty interior. Rockafellar formulates the dimension of $\mathcal{K}$ and $\mathcal{K}^*$. [30, §14][2.31]

To further motivate our understanding of the dual cone, consider the ease with which convergence can be observed in the following optimization problem (p):

Example. *Dual problem.* Essentially, duality theory concerns the representation of a given optimization problem as half a *minimax problem*

[2.30] The dual cone is the negative of the *polar cone* defined by some authors; $\mathcal{K}^* = -\mathcal{K}^\circ$. [29] [30] [65] [23] [31]

[2.31] His monumental work *Convex Analysis* has not one figure or illustration. See [23, §II.16] for a good illustration of Rockafellar's *recession cone* [33].

$(\inf_x \sup_y f(x,y))$ [30, §36] [1, §5.4] whose *saddle-value* [66] exists. [34, p.3] Consider primal conic problem (p) and its corresponding dual problem (d): [67, §3.3.1] [52, §2.1] for matrix constant C,

$$\begin{array}{llllllll} & \underset{x}{\text{minimize}} & \alpha^T x & & \underset{y,z}{\text{maximize}} & \beta^T z & & \\ \text{(p)} & \text{subject to} & x \in \mathcal{K} & & \text{subject to} & y \in \mathcal{K}^* & \text{(d)} & (173) \\ & & Cx = \beta & & & C^T z + y = \alpha & & \end{array}$$

Observe the dual problem is also conic, and its *objective*[2.32] never exceeds that of the primal;

$$\begin{aligned} \alpha^T x &\geq \beta^T z \\ x^T(C^T z + y) &\geq (Cx)^T z \\ x^T y &\geq 0 \end{aligned} \tag{174}$$

which is true by definition (170). Under the sufficient condition that (p) is convex and satisfies *Slater's condition*,[2.33] then each problem (p) and (d) achieves the same optimal value of its objective and so (p) and (d) are together equivalent to the minimax problem

$$\begin{array}{ll} \underset{x,y,z}{\text{minimize}} & \alpha^T x - \beta^T z \\ \text{subject to} & x \in \mathcal{K}, \quad y \in \mathcal{K}^* \\ & Cx = \beta, \quad C^T z + y = \alpha \end{array} \tag{175}$$

Each problem (p) and (d) is called a *strong dual* to the other because the *duality gap* is 0; the optimal value of the objective in the minimax problem (175) is always the saddle-value 0 (regardless of the particular convex cone $\mathcal{K}$ and other problem parameters). [69, §3.2] □

2.8.1.1 Key properties of dual cone

- For any cone, $(-\mathcal{K})^* = -\mathcal{K}^*$
- For any cones $\mathcal{K}_1$ and $\mathcal{K}_2$, $\mathcal{K}_1 \subseteq \mathcal{K}_2 \Rightarrow \mathcal{K}_1^* \supseteq \mathcal{K}_2^*$ [31, §2.7]

[2.32] The objective is the function that is argument to minimization or maximization.

[2.33] In this context, (p) is convex if $\mathcal{K}$ is a convex cone. *Slater's condition* is satisfied whenever any primal strictly feasible point exists; *id est*, for any point feasible with the affine equality (or affine inequality) constraint functions and relatively interior to $\mathcal{K}$. If $\mathcal{K}$ is polyhedral, then *Slater's condition* is satisfied when any feasible point exists. [1, §5.2] [4, §1.3.8] [65, p.325] [68, p.485]

- (Symmetry) When $\mathcal{K}$ is any convex cone, the dual of the dual cone is the closure of the original cone; $\mathcal{K}^{**} = \overline{\mathcal{K}}$. When $\mathcal{K}$ is closed and convex, then the dual of the dual cone is the original cone; $\mathcal{K}^{**} = \mathcal{K}$. [30, §14]

- If any cone $\mathcal{K}$ has nonempty interior, then $\mathcal{K}^*$ is pointed;

$$\mathcal{K} \text{ nonempty interior } \Rightarrow \mathcal{K}^* \text{ pointed} \tag{176}$$

  Conversely, if the closure of any convex cone $\mathcal{K}$ is pointed, then $\mathcal{K}^*$ has nonempty interior;

$$\overline{\mathcal{K}} \text{ pointed } \Rightarrow \mathcal{K}^* \text{ nonempty interior} \tag{177}$$

- [30, §16.4.2] [70, §4.6] For convex cones $\mathcal{K}_1$ and $\mathcal{K}_2$ (dual vector-sum)

$$(\mathcal{K}_1 + \mathcal{K}_2)^* = \mathcal{K}_1^* \cap \mathcal{K}_2^* \tag{178}$$

  For closed convex cones $\mathcal{K}_1$ and $\mathcal{K}_2$

$$(\mathcal{K}_1 \cap \mathcal{K}_2)^* = \overline{\mathcal{K}_1^* + \mathcal{K}_2^*} \tag{179}$$

  (closure of vector sum of duals).[2.34]

- $\mathcal{K}$ is proper if and only if $\mathcal{K}^*$ is proper.

- $\mathcal{K}$ is polyhedral if and only if $\mathcal{K}^*$ is polyhedral. [31, §2.8]

- $\mathcal{K}$ is simplicial if and only if $\mathcal{K}^*$ is simplicial. (§2.9.2.1)

- $\mathcal{K} \boxplus -\mathcal{K}^* = \mathbb{R}^n \Rightarrow \mathcal{K}$ is closed convex [31, thm.2.7.7] (p.447)

- $\mathcal{K} \boxplus -\mathcal{K}^* = \mathbb{R}^n \Leftarrow \mathcal{K}$ is polyhedral [31, §2.8.7]

[2.34] These parallel the analogous results for subspaces $\mathcal{R}_1, \mathcal{R}_2 \subseteq \mathbb{R}^n$, [70, §4.6]

$$\begin{aligned}(\mathcal{R}_1 + \mathcal{R}_2)^\perp &= \mathcal{R}_1^\perp \cap \mathcal{R}_2^\perp \\ (\mathcal{R}_1 \cap \mathcal{R}_2)^\perp &= \overline{\mathcal{R}_1^\perp + \mathcal{R}_2^\perp}\end{aligned}$$

$\mathcal{R}^{\perp\perp} = \mathcal{R}$ for any subspace $\mathcal{R}$.

2.8.1.1.1 Examples of dual cone

When cone $\mathcal{K}$ is a halfspace in $\mathbb{R}^n$ with $n>0$ (Figure **2.20** for example), the dual cone $\mathcal{K}^*$ is a ray (base $\mathbf{0}$) belonging to that halfspace but orthogonal to its bounding hyperplane (that contains the origin), and *vice versa.*

When $\mathcal{K}$ is a subspace, $\mathcal{K}^*$ is its orthogonal complement, and *vice versa.* (§E.8.1.1)

When $\mathcal{K}$ is $\mathbb{R}^n$, $\mathcal{K}^*$ is the point at the origin, and *vice versa.*

When convex cone $\mathcal{K}$ is a closed halfplane in $\mathbb{R}^{\mathbf{3}}$ (Figure **2.22**), it is neither pointed or of nonempty interior; hence, the dual cone $\mathcal{K}^*$ can be neither of nonempty interior or pointed.

When $\mathcal{K}$ is any particular orthant in $\mathbb{R}^n$, the dual cone is identical; *id est*, $\mathcal{K}=\mathcal{K}^*$.

When $\mathcal{K}$ is any quadrant in subspace $\mathbb{R}^{\mathbf{2}}$, $\mathcal{K}^*$ is a wedge-shaped polyhedral cone in $\mathbb{R}^{\mathbf{3}}$; *e.g.*, for $\mathcal{K}$ equal to quadrant I, $\mathcal{K}^*$ is the union of two orthants: $\mathbb{R}^{\mathbf{3}}_+ + \mathbb{R}^{\mathbf{3}}_{\mathbf{3-}}$.

When $\mathcal{K}$ is a polyhedral variation of the Lorentz cone $\mathcal{K}_\ell$ (160), the dual is the polyhedral proper cone $\mathcal{K}_q$: for $\ell=1$ or ∞ ,

$$\mathcal{K}_q \;=\; \mathcal{K}_\ell^* \;=\; \left\{\begin{bmatrix} x \\ t \end{bmatrix} \in \mathbb{R}^n \times \mathbb{R} \mid \|x\|_q \leq t\right\} \tag{180}$$

where $\|x\|_q$ is the *dual norm* and $1/\ell + 1/q = 1$.

2.8.2 Abstractions of *Farkas' lemma*

2.8.2.0.1 Corollary. *Generalized inequality and membership relation.* [29, §A.4.2] Let $\mathcal{K}$ be any closed convex cone and $\mathcal{K}^*$ its dual, and let x and y belong to a vector space $\mathbb{R}^n$. Then

$$x \in \mathcal{K} \;\Leftrightarrow\; \langle y\,,x\rangle \geq 0 \;\text{ for all }\; y \in \mathcal{K}^* \tag{181}$$

which is a simple translation of the *Farkas lemma* as in [30, §22] to the language of convex cones, and a generalization of the well-known Cartesian fact

$$x \succeq 0 \;\Leftrightarrow\; \langle y\,,x\rangle \geq 0 \;\text{ for all }\; y \succeq 0 \tag{182}$$

for which implicitly $\mathcal{K} = \mathcal{K}^* = \mathbb{R}^n_+$ the nonnegative orthant. By closure we have symmetry:

$$y \in \mathcal{K}^* \;\Leftrightarrow\; \langle y\,,x\rangle \geq 0 \;\text{ for all }\; x \in \mathcal{K} \tag{183}$$

merely, a statement of fact by definition of the dual cone (170).

When $\mathcal{K}$ and $\mathcal{K}^*$ are pointed closed convex cones, *membership relation* (181) is often written as the *generalized inequality*

$$x \underset{\mathcal{K}}{\succeq} 0 \;\Leftrightarrow\; \langle y\,,x\rangle \geq 0 \;\text{ for all }\; y \underset{\mathcal{K}^*}{\succeq} 0 \tag{184}$$

meaning that the coordinates for *biorthogonal expansion* of x [43] can be nonnegative when x belongs to $\mathcal{K}$, and must be nonnegative when x belongs to simplicial $\mathcal{K}$.[2.35] By symmetry

$$y \underset{\mathcal{K}^*}{\succeq} 0 \;\Leftrightarrow\; \langle y\,,x\rangle \geq 0 \;\text{ for all }\; x \underset{\mathcal{K}}{\succeq} 0 \tag{185}$$

◇

When pointed closed convex $\mathcal{K}$ is clear from context, shorthand is prevalent:

$$\begin{aligned} x \succeq 0 \;&\Leftrightarrow\; x \in \mathcal{K} \\ x \succ 0 \;&\Leftrightarrow\; x \in \operatorname{rel}\operatorname{int}\mathcal{K} \end{aligned} \tag{186}$$

Strict versions are also useful; *e.g.*, for any closed convex cone $\mathcal{K}$ having nonempty interior,

$$\begin{aligned} x \in \operatorname{int}\mathcal{K} \;&\Leftrightarrow\; \langle y\,,x\rangle > 0 \;\text{ for all }\; y \in \mathcal{K}^*,\; y \neq 0 \\ x \in \mathcal{K},\; x \neq 0 \;&\Leftrightarrow\; \langle y\,,x\rangle > 0 \;\text{ for all }\; y \in \operatorname{int}\mathcal{K}^* \end{aligned} \tag{187}$$

By symmetry, we also have their duals.

2.8.2.0.2 Null certificate

If $x_p \notin \mathcal{K}$, the construction in Figure **2.19**(b) suggests there exists a hyperplane having inward-normal belonging to dual cone $\mathcal{K}^*$ separating x_p from $\mathcal{K}$; indeed, for closed convex cone $\mathcal{K}$,

$$x_p \notin \mathcal{K} \;\Leftrightarrow\; \exists\, y \in \mathcal{K}^* \;\ni\; \langle y\,,x_p\rangle < 0 \tag{188}$$

The existence of any one such y is a certificate of null membership.

[2.35] A simplicial cone $\mathcal{K}$ and its (simplicial) dual $\mathcal{K}^* \subset \mathbb{R}^n$ are polyhedral proper cones (*e.g.*, Figure **2.24**, p.111), but not the converse; *id est*, polyhedral proper cones are not necessarily simplicial.

2.8.2.1 Discretization

2.8.2.1.1 Dual halfspace-description. The halfspace-description of the corresponding dual cone is equally simple as vertex-description (165) for a closed convex cone: By definition (170),

$$\begin{aligned}\mathcal{K}^* &= \left\{y \in \mathbb{R}^n \mid z^T y \geq 0 \text{ for all } z \in \mathcal{K}\right\}\\ &= \left\{y \in \mathbb{R}^n \mid z^T y \geq 0 \text{ for all } z = Xa\,,\; a \succeq 0\right\}\\ &= \left\{y \in \mathbb{R}^n \mid a^T X^T y \geq 0\,,\; a \succeq 0\right\}\\ &= \left\{y \in \mathbb{R}^n \mid X^T y \succeq 0\right\}\end{aligned} \tag{189}$$

(*confer* (159)) that follows from the *generalized inequality and membership corollary* (182). The semi-infinity of tests specified by all $z \in \mathcal{K}$ has been reduced to a discrete set of generators constituting the columns of X; *id est*, the test has been discretized.

Whenever $\mathcal{K}$ is known to be closed and convex, then the converse must also hold; *id est*, given any set of generators for $\mathcal{K}^*$ arranged columnar in Y, then the consequent vertex-description of the dual cone connotes a halfspace-description for $\mathcal{K}$: [31, §2.8]

$$\mathcal{K}^* = \{Ya \mid a \succeq 0\} \;\Leftrightarrow\; \mathcal{K}^{**} = \mathcal{K} = \left\{y \mid Y^T y \succeq 0\right\} \tag{190}$$

2.8.2.1.2 First dual-cone formula. From these two results we deduce a general principle: From any given vertex-description of a convex cone $\mathcal{K}$, a halfspace-description of the dual cone $\mathcal{K}^*$ is immediate by matrix transposition. Various converses are just a little bit trickier. (§2.9)

We deduce further: For any polyhedral cone $\mathcal{K}$, the dual cone $\mathcal{K}^*$ is also polyhedral and $\mathcal{K}^{**} = \mathcal{K}$. [31, §2.8]

The *generalized inequality and membership corollary* is discretized in the following theorem [55, §1][2.36] that follows directly from (189) and (190):

2.8.2.1.3 Theorem. *Discrete membership.*
Given any discrete set of generators (§2.6.4.1) denoted by $\mathcal{G}(\mathcal{K})$ for closed convex cone $\mathcal{K}$, and denoted by $\mathcal{G}(\mathcal{K}^*)$ for its dual, let x and y belong to vector space $\mathbb{R}^n$. Then discretization of the *generalized inequality and membership corollary* is necessary and sufficient for certifying membership:

$$x \in \mathcal{K} \;\Leftrightarrow\; \langle \gamma^*, x\rangle \geq 0 \text{ for all } \gamma^* \in \mathcal{G}(\mathcal{K}^*) \tag{191}$$

[2.36] Barker & Carlson state the theorem only for the pointed closed convex case.

$$y \in \mathcal{K}^* \;\Leftrightarrow\; \langle \gamma\,,\, y\rangle \geq 0 \;\;\text{for all}\;\; \gamma \in \mathcal{G}(\mathcal{K}) \tag{192}$$

$\diamond$

2.8.2.1.4 Dual of pointed polyhedral cone

In a subspace of $\mathbb{R}^n$, now we consider a pointed polyhedral cone $\mathcal{K}$ given in terms of its extreme directions Γ_i arranged columnar in X ;

$$X = [\,\Gamma_1 \;\; \Gamma_2 \;\; \cdots \;\; \Gamma_N\,] \in \mathbb{R}^{n\times N} \tag{156}$$

The *extremes theorem* (§2.6.4.0.1) provides the vertex-description of a pointed polyhedral cone in terms of its finite number of extreme directions and its lone vertex at the origin:

Definition. *Pointed polyhedral cone, vertex-description encore.*
(*confer* (165) (118)) Given pointed polyhedral cone $\mathcal{K}$ in a subspace of $\mathbb{R}^n$, denoting its i^{th} extreme direction by $\Gamma_i \in \mathbb{R}^n$ arranged in a matrix X as in (156), then that cone may be described, (60) (166)

$$\begin{aligned}\mathcal{K} &= \left\{[\mathbf{0}\ \ X]\, a\,\zeta \mid a^T\mathbf{1} = 1,\ a \succeq 0,\ \zeta \geq 0\right\} \\ &= \left\{X a\,\zeta \mid a^T\mathbf{1} \leq 1,\ a \succeq 0,\ \zeta \geq 0\right\} \\ &= \left\{X b \mid b \succeq 0\right\} \subseteq \mathbb{R}^n\end{aligned} \tag{193}$$

that is simply a conic hull (like (63)) of a finite number N of directions.

$\triangle$

Whenever $\mathcal{K}$ is pointed, closed, and convex, the dual cone $\mathcal{K}^*$ has a halfspace-description in terms of the extreme directions Γ_i in $\mathcal{K}$:

$$\mathcal{K}^* = \left\{y \mid \gamma^T y \geq 0 \ \text{ for all }\ \gamma \in \{\Gamma_i\,,\ i=1\ldots N\} \subseteq \operatorname{rel}\partial\mathcal{K}\right\} \tag{194}$$

$$= \left\{y \mid X^T y \succeq 0\right\} \subseteq \mathbb{R}^n \tag{195}$$

because when $\{\Gamma_i\}$ constitutes any set of generators for $\mathcal{K}$, the discretization result (189) allows relaxation of the requirement $\forall\, x \in \mathcal{K}$ in (170) to $\forall\, \gamma \in \{\Gamma_i\}$ in (194) directly.[2.37] That dual cone so defined is unique, identical to (170), and has nonempty interior because $\mathcal{K}$ is assumed pointed; but $\mathcal{K}^*$ is not necessarily pointed unless $\mathcal{K}$ has nonempty interior (§2.8.1.1), and $\mathcal{K}^*$ is polyhedral whenever the number of generators N is finite.

2.8.2.2 Facet normal

We see from (195) that the conically independent generators of cone $\mathcal{K}$ (namely, the extreme directions of pointed closed convex $\mathcal{K}$ constituting the columns of X) each define an inward-normal to a hyperplane supporting $\mathcal{K}^*$ and exposing a dual facet when N is finite. Were $\mathcal{K}^*$ pointed and finitely generated, then by symmetry the dual statement would also hold; *id est*, the extreme directions of pointed $\mathcal{K}^*$ each define a hyperplane that supports $\mathcal{K}$ and exposes a facet.

We may conclude the extreme directions of polyhedral proper $\mathcal{K}$ are respectively orthogonal to the facets of $\mathcal{K}^*$; likewise, the extreme directions of polyhedral proper $\mathcal{K}^*$ are respectively orthogonal to the facets of $\mathcal{K}$.

[2.37] We learned from (189) that any discrete set of generators for $\mathcal{K}$ including its extreme directions can be used to make a halfspace-description of $\mathcal{K}^*$. The extreme directions constitute a minimal set of generators. Apply this result to Figure **2.23**, for example.

2.8.2.3 Pointed closed convex cone and partial order

A pointed closed convex cone $\mathcal{K}$ induces a *partial order* [48] on $\mathbb{R}^n$ or $\mathbb{R}^{m\times n}$ [55, §1], respectively defined by vector or matrix inequality;

$$x \preceq z \quad \Leftrightarrow \quad z - x \in \mathcal{K} \tag{196}$$

$$x \prec z \quad \Leftrightarrow \quad z - x \in \operatorname{rel int} \mathcal{K} \tag{197}$$

Strict inequality $x \succ 0$ means that coordinates for biorthogonal expansion of x can be positive when x belongs to $\mathcal{K}$, and must be positive whenever x belongs to simplicial $\mathcal{K}$.

From the *discrete membership theorem* it directly follows, for example,

$$x \preceq z \;\Leftrightarrow\; x_i \leq z_i \;\; \forall i \tag{198}$$

when comparison is with respect to the nonnegative orthant $\mathcal{K} = \mathbb{R}^n_+$.

Comparable points (illustrated in Figure **2.23**) and the *minimum element*[2.38] of some vector- or matrix-valued set are thus well defined. More properties of partial ordering: such as reflexivity ($x \preceq x$), antisymmetry ($x \preceq z\,,\; z \preceq x \Rightarrow x = z$), transitivity ($x \preceq y\,,\; y \preceq z \Rightarrow x \preceq z$), additivity ($x \preceq z\,,\; u \preceq v \Rightarrow x + u \preceq z + v$), strict properties, and preservation under nonnegative scaling or limiting operations are cataloged in [1, §2.4.1] with respect to proper cones.[2.39]

2.8.2.4 Dual PSD cone and generalized inequality

The *dual positive semidefinite cone* $\mathcal{K}^*$ is confined to $\mathbb{S}^M$ by convention;

$$\mathbb{S}^{M*}_+ \triangleq \{Y \in \mathbb{S}^M \mid \langle X, Y\rangle \geq 0 \;\text{ for all } X \in \mathbb{S}^M_+\} \;=\; \mathbb{S}^M_+ \tag{199}$$

The positive semidefinite cone is *self-dual* in the ambient space of symmetric matrices [71] [58, §II] [1, §2.6.1], $\mathcal{K} = \mathcal{K}^*$.

Generalized inequality with respect to the positive semidefinite cone in the ambient space of symmetric matrices can therefore be simply stated: (Fejér)

$$X \succeq 0 \;\Leftrightarrow\; \operatorname{tr}(Y^T X) \geq 0 \;\text{ for all } Y \succeq 0 \tag{200}$$

[2.38] We say $x \in \mathcal{C}$ is the (unique) minimum element of $\mathcal{C}$ with respect to $\mathcal{K}$ if and only if for each and every $z \in \mathcal{C}$ we have $x \preceq_{\mathcal{K}} z$; equivalently, iff $\mathcal{C} \subseteq x + \mathcal{K}$. [1, §2.6.3]

[2.39] We distinguish pointed closed convex cones here because the *generalized inequality and membership corollary* remains intact. [29, §A.4.2.7]

The trace is introduced because membership to this cone can be determined in the isometrically isomorphic Euclidean space $\mathbb{R}^{M^2}$ via (19). (§2.1.1.1) By the two interpretations in §2.8.1, matrix Y can be interpreted as inward-normal to a hyperplane supporting the positive semidefinite cone.

The fundamental statement of positive semidefiniteness, $y^T X y \geq 0 \;\forall y$ (§A.3.0.0.1), is a particular instance of this generalized inequality with respect to the positive semidefinite cone (200):

$$X \succeq 0 \;\;\Leftrightarrow\;\; \langle yy^T, X\rangle \geq 0 \;\; \forall\, yy^T(\succeq 0) \tag{201}$$

Discretization (§2.8.2.1.3) allows replacement of matrix Y with this minimal set of generators comprised of all the extreme directions.

2.8.2.4.1 Example. *Linear matrix inequality.*
Consider a peculiar vertex-description for a convex cone defined over the positive semidefinite cone (instead of the nonnegative orthant as in def.(63)): for $X \in \mathbb{S}^n$ given $A_j \in \mathbb{S}^n$, $j = 1 \ldots m$,

$$\begin{aligned}\mathcal{K} &= \left\{ \begin{bmatrix} \langle A_1\,,\,X\rangle \\ \vdots \\ \langle A_m\,,\,X\rangle \end{bmatrix} \mid X \succeq 0 \right\} \subseteq \mathbb{R}^m \\ &= \left\{ \begin{bmatrix} \mathrm{vec}(A_1)^T \\ \vdots \\ \mathrm{vec}(A_m)^T \end{bmatrix} \mathrm{vec}\, X \mid X \succeq 0 \right\} \\ &\triangleq \{A \;\mathrm{vec}\, X \mid X \succeq 0\}\end{aligned} \tag{202}$$

where $A \in \mathbb{R}^{m \times n^2}$, and vectorization vec is defined in (18). $\mathcal{K}$ is indeed a convex cone because by (111) (§2.6.2)

$$A \;\mathrm{vec}\, X_{p_1}\,,\, A \;\mathrm{vec}\, X_{p_2} \in \mathcal{K} \;\Rightarrow\; A(\zeta \;\mathrm{vec}\, X_{p_1} + \xi \;\mathrm{vec}\, X_{p_2}) \in \mathcal{K} \;\text{ for all }\; \zeta\,,\xi \geq 0 \tag{203}$$

since a nonnegatively weighted sum of positive semidefinite matrices must be positive semidefinite. (881) Now consider the dual cone:

$$\begin{aligned}\mathcal{K}^* &= \{y \mid \langle A \;\mathrm{vec}\, X\,,\, y\rangle \geq 0 \;\text{ for all }\; X \succeq 0\} \subseteq \mathbb{R}^m \\ &= \left\{y \mid \langle \mathrm{vec}\, X\,,\, A^T y\rangle \geq 0 \;\text{ for all }\; X \succeq 0\right\} \\ &= \left\{y \mid \mathrm{vec}^{-1}(A^T y) \succeq 0\right\}\end{aligned} \tag{204}$$

that follows from (200) and leads to an equally peculiar halfspace-description

$$\mathcal{K}^* = \{y \mid \sum_{j=1}^{m} y_j A_j \succeq 0\} \tag{205}$$

The summation inequality with respect to the positive semidefinite cone is known as a *linear matrix inequality.* [3] [5] [72] □

2.8.3 Biorthogonal expansion, by example

2.8.3.0.1 Example. *Relationship to dual polyhedral cone.*
The proper cone $\mathcal{K}$ illustrated in Figure **2.23** induces a partial order on $\mathbb{R}^2$. All points greater than x with respect to $\mathcal{K}$, for example, are contained in the translated cone $x+\mathcal{K}$. The extreme directions Γ_1 and Γ_2 of $\mathcal{K}$ do not make an orthogonal set; neither do extreme directions Γ_3 and Γ_4 of dual cone $\mathcal{K}^*$; rather, we have the *biorthogonality condition*, [43]

$$\begin{gathered}\Gamma_4^T\Gamma_1 = \Gamma_3^T\Gamma_2 = 0\\ \Gamma_3^T\Gamma_1 \neq 0\,, \quad \Gamma_4^T\Gamma_2 \neq 0\end{gathered} \tag{206}$$

The biorthogonal expansion of $x\in\mathcal{K}$ is then

$$x \;=\; \Gamma_1\,\frac{\Gamma_3^T x}{\Gamma_3^T\Gamma_1} \;+\; \Gamma_2\,\frac{\Gamma_4^T x}{\Gamma_4^T\Gamma_2} \tag{207}$$

where $\Gamma_3^T x/(\Gamma_3^T\Gamma_1)$ is the nonnegative coefficient of nonorthogonal projection (§E.6.1) of x on Γ_1 in the direction orthogonal to Γ_3, and where $\Gamma_4^T x/(\Gamma_4^T\Gamma_2)$ is the nonnegative coefficient of nonorthogonal projection of x on Γ_2 in the direction orthogonal to Γ_4; they are the coordinates in this nonorthogonal system. Those coefficients must be nonnegative $x\succeq_{\mathcal{K}} 0$ because $x\in\mathcal{K}$ (186) and $\mathcal{K}$ is simplicial.

If we ascribe the extreme directions of $\mathcal{K}$ to the columns of a matrix X,

$$X \triangleq [\,\Gamma_1 \;\; \Gamma_2\,] \tag{208}$$

then we find

$$X^{\dagger T} = \begin{bmatrix}\Gamma_3\dfrac{1}{\Gamma_3^T\Gamma_1} & \Gamma_4\dfrac{1}{\Gamma_4^T\Gamma_2}\end{bmatrix} \tag{209}$$

Therefore,

$$x = XX^{\dagger}x \tag{210}$$

is the biorthogonal expansion (207) (§E.0.1), and the biorthogonality condition (206) can be expressed succinctly (§E.1.1)[2.40]

$$X^\dagger X = I \tag{211}$$

The expansion $XX^\dagger w$ for any $w \in \mathbb{R}^2$ is unique if and only if the extreme directions of $\mathcal{K}$ are linearly independent; *id est*, iff X has no nullspace.

□

2.8.3.1 Pointed cones and biorthogonality

The biorthogonality condition (211) $X^\dagger X = I$ means Γ_1 and Γ_2 are linearly independent generators of $\mathcal{K}$. (§B.1.1.1) From §2.6.7 we know that means Γ_1 and Γ_2 must be extreme directions of $\mathcal{K}$.

A biorthogonal expansion is necessarily associated with a pointed closed convex cone, otherwise there can be no extreme directions (§2.6.4). We will address biorthogonal expansion with respect to a pointed polyhedral cone having empty interior in §2.9.1.

2.8.3.1.1 Example. *Expansions implied by diagonalization.*
When matrix $X \in \mathbb{R}^{M\times M}$ is diagonalizable,

$$X = S\Lambda S^{-1} = [\, s_1 \cdots s_M \,]\, \Lambda \begin{bmatrix} w_1^T \\ \vdots \\ w_M^T \end{bmatrix} = \sum_{i=1}^{M} \lambda_i\, s_i w_i^T \tag{913}$$

coordinates λ_i (contained in diagonal matrix Λ) for its biorthogonal expansion

$$X = SS^{-1}X = [\, s_1 \cdots s_M \,] \begin{bmatrix} w_1^T X \\ \vdots \\ w_M^T X \end{bmatrix} = \sum_{i=1}^{M} \lambda_i\, s_i w_i^T \tag{212}$$

depend upon the geometric relationship of X to its linearly independent eigenmatrices $s_i w_i^T$ (§A.5.1, §B.1.1) which are dyads constituted by right and left eigenvectors and are generators of some simplicial cone. When S is real and X belongs to that simplicial cone in $\mathbb{R}^{M\times M}$, for example, then the coefficients of expansion, the eigenvalues λ_i, must be nonnegative.

[2.40] Possibly confusing is the fact that formula $XX^\dagger x$ is simultaneously the orthogonal projection of x on $\mathcal{R}(X)$ (1202), and the sum of nonorthogonal projections of $x \in \mathcal{R}(X)$ on the range of each column of full-rank X skinny-or-square (§E.5.0.1.2).

When X is symmetric, its eigenmatrices are extreme directions of the positive semidefinite cone $\mathbb{S}_+^M$ (120) in the subspace of symmetric matrices, although X does not necessarily belong to that cone. The coordinates for biorthogonal expansion of $X = Q\Lambda Q^T$ are its eigenvalues; *id est*, for $X \in \mathbb{S}^M$,

$$X \;=\; QQ^TX \;=\; \sum_{i=1}^M q_i\, q_i^TX \;=\; \sum_{i=1}^M \lambda_i\, q_i q_i^T \;\in\; \mathbb{S}^M \tag{213}$$

is an orthogonal expansion with orthonormality condition $Q^TQ = I$ where λ_i is the i^{th} eigenvalue of X, q_i is the i^{th} corresponding eigenvector of X arranged columnar in orthogonal matrix

$$Q = [\, q_1 \;\; q_2 \;\cdots\; q_M\,] \in \mathbb{R}^{M\times M} \tag{214}$$

and eigenmatrix $q_iq_i^T$ is the i^{th} member of an orthonormal basis for $\mathbb{S}^M$ (1275) and is an extreme direction of $\mathbb{S}_+^M$.

Similarly, when X belongs to the positive semidefinite cone in the subspace of symmetric matrices, the coordinates for biorthogonal expansion of $X = Q\Lambda Q^T$ can be its nonnegative eigenvalues (845); *id est*, for $X \in \mathcal{K} = \mathbb{S}_+^M$,

$$X \;=\; QQ^TX \;=\; \sum_{i=1}^M q_i\, q_i^TX \;=\; \sum_{i=1}^M \lambda_i\, q_i q_i^T \;\in\; \mathbb{S}_+^M \tag{215}$$

is an orthogonal expansion where $\lambda_i \geq 0$ is the i^{th} eigenvalue of X. □

2.8.3.2 Self-dual cones and biorthogonality

Whenever a pointed closed convex cone is self-dual, $\mathcal{K} = \mathcal{K}^*$, an associated biorthogonal expansion can become an orthogonal expansion; *id est*, the biorthogonality condition $X^\dagger X = I$ can instead become the orthonormality condition $X^TX = I$. The biorthogonal expansion (212), for example, became the orthogonal expansions (213) and (215); *id est*, extreme directions of some simplicial cone and its dual became extreme directions of the positive semidefinite self-dual cone.

The most prominent examples of self-dual cones are the orthants, the positive semidefinite cone $\mathbb{S}_+^M$ in the ambient space of symmetric matrices (199), and the second-order (Lorentz) cone (114) [62, §II.A] [1, exmp.2.25].

2.8.3.2.1 Example. *Biorthogonal expansion respecting nonpositive orthant.* Suppose $x \in \mathcal{K}$ any orthant in $\mathbb{R}^n$.[2.41] Then the coordinates for biorthogonal expansion of x must be nonnegative; in fact, the absolute value of the Cartesian coordinates.

Suppose, in particular, x belongs to the nonpositive orthant $\mathcal{K} = \mathbb{R}^n_-$. Then the biorthogonal expansion becomes an orthogonal expansion and, for $x \in \mathbb{R}^n_-$

$$x = XX^Tx = \sum_{i=1}^n -e_i(-e_i^Tx) = \sum_{i=1}^n -e_i|e_i^Tx| \in \mathbb{R}^n_- \tag{216}$$

the coefficients of expansion are nonnegative. For this orthant $\mathcal{K}$ we have orthonormality condition $X^TX = I$ where $X = -I$, $e_i \in \mathbb{R}^n$ is a standard basis vector, and $-e_i$ is an extreme direction (§2.6.4) of $\mathcal{K}$.

Of course, this expansion $x = XX^Tx$ applies more broadly to domain $\mathbb{R}^n$, but then the coefficients belong to $\mathbb{R}$. □

[2.41] An orthant is simplicial and self-dual.

2.9 Formulae and algorithm finding dual cone

2.9.1 Biorthogonal expansion, derivation

Unique biorthogonal expansion with respect to polyhedral cone $\mathcal{K}$ depends upon existence of its linearly independent extreme directions; $\mathcal{K}$ must therefore be pointed, closed, and convex to uniquely represent any point in their span.

In this section, we consider nonempty pointed polyhedral cone $\mathcal{K}$ having possibly empty interior. Hence we restrict observation to that section of the dual cone $\mathcal{K}^*$ in the affine hull of $\mathcal{K}$ because we are interested in biorthogonal expansion of $x \in \operatorname{aff}\mathcal{K} = \operatorname{aff}\operatorname{cone}X$ for $X \in \mathbb{R}^{n\times N}$ as in (156); we seek a vertex-description for $\mathcal{K}^* \cap \operatorname{aff}\mathcal{K}$ in terms of a set of dual generators $\{\Gamma_i^*\} \subset \operatorname{aff}\mathcal{K}$ in the same finite quantity[2.42] as the extreme directions $\{\Gamma_i\}$ of

$$\mathcal{K} = \operatorname{cone}(X) = \{Xa \mid a \succeq 0\} \subseteq \mathbb{R}^n \tag{165}$$

arranged columnar in X :

$$X = [\,\Gamma_1 \;\; \Gamma_2 \;\cdots\; \Gamma_N\,] \in \mathbb{R}^{n\times N} \tag{156}$$

We assume the quantity of extreme directions N does not exceed the dimension n of the ambient vector space because, otherwise, the expansion could not be unique; *id est*, assume N linearly independent extreme directions, hence $N \leq n$ (X *skinny*[2.43] or square, full-rank).

2.9.1.1 $x \in \mathcal{K}$

Suppose x belongs to $\mathcal{K} \subseteq \mathbb{R}^n$. Then $x = Xa$ for some $a \succeq 0$. Vector a is unique only when $\{\Gamma_i\}$ is a linearly independent set.[2.44] Vector $a \in \mathbb{R}^N$ can take the form $a = Bx$ if $\mathcal{R}(B) = \mathbb{R}^N$. Then we require $Xa = XBx = x$ and $Bx = BXa = a$. The pseudoinverse $B = X^\dagger \in \mathbb{R}^{N\times n}$ (§E) is suitable when X is skinny-or-square and full-rank. In that case $\operatorname{rank}X = N$, and for all $c \succeq 0$ and $i = 1 \ldots N$,

$$a \succeq 0 \;\Leftrightarrow\; X^\dagger Xa \succeq 0 \;\Leftrightarrow\; a^T X^T X^{\dagger T} c \geq 0 \;\Leftrightarrow\; \Gamma_i^T X^{\dagger T} c \geq 0 \tag{217}$$

[2.42] When $\mathcal{K}$ is contained in a proper subspace of $\mathbb{R}^n$, the ordinary dual cone $\mathcal{K}^*$ will have more (conic) generators in any minimal set than $\mathcal{K}$ has extreme directions.

[2.43] "Skinny" meaning thin; more rows than columns.

[2.44] Conic independence alone (§2.6.7) is insufficient to guarantee uniqueness.

The penultimate inequality follows from the *generalized inequality and membership corollary*, while the last inequality is a consequence of that corollary's discretization (§2.8.2.1.3).[2.45] From (217) and (194) we deduce

$$\mathcal{K}^* \cap \operatorname{aff}\mathcal{K} \;=\; \operatorname{cone}(X^{\dagger T}) \;=\; \{X^{\dagger T}c \mid c \succeq 0\} \subseteq \mathbb{R}^n \tag{218}$$

is the vertex-description for that section of $\mathcal{K}^*$ in the affine hull of $\mathcal{K}$ because $\mathcal{R}(X^{\dagger T}) = \mathcal{R}(X)$ by definition of the pseudoinverse. From (176), we know $\mathcal{K}^* \cap \operatorname{aff}\mathcal{K}$ must be pointed if $\operatorname{rel\,int}\mathcal{K}$ is logically assumed nonempty with respect to $\operatorname{aff}\mathcal{K}$.

Conversely, suppose full-rank skinny-or-square matrix

$$X^{\dagger T} \triangleq \begin{bmatrix} \Gamma_1^* & \Gamma_2^* & \cdots & \Gamma_N^* \end{bmatrix} \in \mathbb{R}^{n\times N} \tag{219}$$

comprises the extreme directions $\{\Gamma_i^*\} \subset \operatorname{aff}\mathcal{K}$ of the dual cone section in the affine hull of $\mathcal{K}$.[2.46] From the *discrete membership theorem* and (179) we get a partial dual to (194); *id est*, assuming $x \in \operatorname{aff}\operatorname{cone}X$,

$$\begin{aligned} x \in \mathcal{K} \quad &\Leftrightarrow \quad \gamma^{*T}x \geq 0 \;\text{ for all }\; \gamma^* \in \left\{\Gamma_i^*\,,\; i=1\ldots N\right\} \subset \partial\mathcal{K}^* \cap \operatorname{aff}\mathcal{K} &(220)\\ &\Leftrightarrow \quad X^\dagger x \succeq 0 &(221)\end{aligned}$$

that leads to a partial halfspace-description,

$$\mathcal{K} \;=\; \left\{x \in \operatorname{aff}\operatorname{cone}X \mid X^\dagger x \succeq 0\right\} \tag{222}$$

[2.45]

$$\begin{aligned} a \succeq 0 \;\Leftrightarrow\; a^T X^T X^{\dagger T} c \geq 0 \quad \forall\,(c \succeq 0 \quad &\Leftrightarrow \quad a^T X^T X^{\dagger T} c \geq 0 \quad \forall\, a \succeq 0)\\ \forall\,(c \succeq 0 \quad &\Leftrightarrow \quad \Gamma_i^T X^{\dagger T} c \geq 0 \qquad \forall\, i\,) \end{aligned}$$

♦

Intuitively, any nonnegative vector a is a conic combination of the standard basis $\{e_i \in \mathbb{R}^N\}$; $a \succeq 0 \Leftrightarrow a_i e_i \succeq 0$ for all i. The last inequality in (217) is a consequence of the fact that $x = Xa$ may be any extreme direction of $\mathcal{K}$, in which case a is a standard basis vector; $a = e_i \succeq 0$. Theoretically, because $c \succeq 0$ defines a pointed polyhedral cone (in fact, the nonnegative orthant in $\mathbb{R}^N$), we can take (217) one step further by discretizing c:

$$a \succeq 0 \;\Leftrightarrow\; \Gamma_i^T \Gamma_j^* \geq 0 \;\text{ for } i,j=1\ldots N \;\Leftrightarrow\; X^\dagger X \geq \mathbf{0}$$

In words, $X^\dagger X$ must be a matrix whose entries are each nonnegative.

[2.46]When closed convex $\mathcal{K}$ has empty interior, $\mathcal{K}^*$ has no extreme directions.

For $\gamma^* = X^{\dagger T} e_i$, any $x = Xa$, and for all i we have $e_i^T X^\dagger X a = e_i^T a \geq 0$ only when $a \succeq 0$. Hence $x \in \mathcal{K}$.

When X is full-rank, then the unique biorthogonal expansion of $x \in \mathcal{K}$ becomes (210)

$$x = XX^\dagger x = \sum_{i=1}^{N} \Gamma_i \Gamma_i^{*T} x \tag{223}$$

whose coefficients must be nonnegative because $\mathcal{K}$ is relatively simplicial by assumption. Whenever X is full-rank, so is its pseudoinverse $X^\dagger$. (§E) In the present case, the columns of $X^{\dagger T}$ are linearly independent and generators of the dual cone $\mathcal{K}^* \cap \operatorname{aff} \mathcal{K}$; hence, the columns constitute its extreme directions. (§2.6.7) That section of the dual cone is itself a polyhedral cone (by (159) or the *cone intersection theorem*, §2.6.2) having the same number of extreme directions as $\mathcal{K}$.

2.9.1.2 $x \in \operatorname{aff} \mathcal{K}$

The extreme directions of $\mathcal{K}$ and $\mathcal{K}^* \cap \operatorname{aff} \mathcal{K}$ have a distinct relationship; because $X^\dagger X = I$, then for $i, j = 1 \ldots N$, $\Gamma_i^T \Gamma_i^* = 1$, while for $i \neq j$, $\Gamma_i^T \Gamma_j^* = 0$. Yet neither set of extreme directions, $\{\Gamma_i\}$ nor $\{\Gamma_i^*\}$, is necessarily orthogonal. This is the exact description of a biorthogonality condition, [43, §2.2.4] [28] implying each set of extreme directions is linearly independent. (§B.1.1.1)

The biorthogonal expansion therefore applies more broadly; meaning, for any $x \in \operatorname{aff} \mathcal{K}$, vector x can be uniquely expressed $x = Xb$ where $b \in \mathbb{R}^N$ because $\operatorname{aff} \mathcal{K}$ contains the origin. Thus, for any such $x \in \mathcal{R}(X)$ (*confer* §E.1.1), the biorthogonal expansion (223) becomes $x = XX^\dagger X b = Xb$.

2.9.2 Dual of pointed $\mathcal{K}$, X skinny-or-square full-rank

We wish to derive expressions for the convex cone and its ordinary dual under the same general assumptions: pointed polyhedral $\mathcal{K}$ denoted by its extreme directions arranged columnar in matrix X such that

$$\operatorname{rank}(X \in \mathbb{R}^{n \times N}) = N \triangleq \dim \operatorname{aff} \mathcal{K} \leq n \tag{224}$$

The vertex-description is given:

$$\mathcal{K} = \{Xa \mid a \succeq 0\} \subseteq \mathbb{R}^n \tag{225}$$

from which a halfspace-description for the dual cone follows directly:

$$\mathcal{K}^* = \{y \in \mathbb{R}^n \mid X^T y \succeq 0\} \tag{226}$$

By defining a matrix

$$X^\perp \triangleq \operatorname{basis} \mathcal{N}(X^T) \tag{227}$$

(a columnar basis for the orthogonal complement of $\mathcal{R}(X)$), we can say

$$\operatorname{aff} \operatorname{cone} X \;=\; \operatorname{aff} \mathcal{K} \;=\; \{x \mid X^{\perp T} x = \mathbf{0}\} \tag{228}$$

meaning $\mathcal{K}$ lies in a subspace, perhaps $\mathbb{R}^n$. Thus we have a halfspace-description

$$\mathcal{K} = \{x \in \mathbb{R}^n \mid X^\dagger x \succeq 0,\; X^{\perp T} x = \mathbf{0}\} \tag{229}$$

and from (179), a vertex-description[2.47]

$$\mathcal{K}^* = \{\, [\, X^{\dagger T} \;\; X^\perp \;\; -X^\perp\,] b \mid b \succeq 0 \,\} \subseteq \mathbb{R}^n \tag{230}$$

These results are summarized for a pointed polyhedral cone, having linearly independent generators, and its ordinary dual:

Cone Table 1	$\mathcal{K}$	$\mathcal{K}^*$
vertex-description	X	$X^{\dagger T},\ \pm X^\perp$
halfspace-description	$X^\dagger,\ X^{\perp T}$	X^T

2.9.2.0.1 Example. *Theorem of the alternative for linear inequality.*
A myriad of alternative systems of linear inequalities can now be explained in terms of polyhedral cones and their duals. Consider the polyhedral cone $\mathcal{K}$, for example, constrained to lie in a subspace of $\mathbb{R}^n$ specified by an intersection of hyperplanes through the origin $\{x \in \mathbb{R}^n \mid A^T x = \mathbf{0}\}$ where $A \in \mathbb{R}^{n \times m}$. Then from (183) we may write,

$$b - Ay \in \mathcal{K}^* \;\Leftrightarrow\; x^T(b - Ay) \geq 0 \qquad \forall\, x \in \mathcal{K} \tag{231}$$

$$A^T x = \mathbf{0}\,,\quad b - Ay \in \mathcal{K}^* \;\Rightarrow\; x^T b \geq 0 \qquad \forall\, x \in \mathcal{K} \tag{232}$$

[2.47] These descriptions are not unique. A vertex-description of the dual cone, for example, might use four conically independent generators for a plane (§2.6.7.1) when only three would suffice.

Conversely, suppose we are given the membership relation (231). (§2.8.2.0.1) Then because x^TAy is unbounded below over all $y\in\mathbb{R}^m$, $x^T(b-Ay)\geq 0$ implies $A^Tx=\mathbf{0}$; *id est*, $\mathcal{K}$ lies in a subspace: for $y\in\mathbb{R}^m$,

$$A^Tx=\mathbf{0}\,,\quad b-Ay\in\mathcal{K}^* \;\Leftarrow\; x^T(b-Ay)\geq 0 \qquad \forall\, x\in\mathcal{K} \tag{233}$$

In toto, for any $y\in\mathbb{R}^m$,

$$b-Ay\in\mathcal{K}^* \;\Leftrightarrow\; x^Tb\geq 0\,,\;\; A^Tx=\mathbf{0}\quad \forall\, x\in\mathcal{K} \tag{234}$$

From this, the alternative systems of inequalities for pointed polyhedral cones $\mathcal{K}$ and $\mathcal{K}^*$ [30, p.201]

$$\begin{array}{c} Ay \underset{\mathcal{K}^*}{\preceq} b \\[2ex] \text{exclusive or} \\[2ex] x^Tb<0\,,\quad A^Tx=\mathbf{0}\quad \forall\, x \underset{\mathcal{K}}{\succeq} 0 \end{array} \tag{235}$$

derived from (234) simply by taking the complementary sense of the inequality in x^Tb. These two systems are incompatible; only one is feasible.

By invoking a strict membership relation (187), we can construct a more exotic interdependency;

$$b-Ay \underset{\mathcal{K}^*}{\succ} 0 \;\Leftrightarrow\; x^Tb>0\,,\;\; A^Tx=\mathbf{0}\quad \forall\, x \underset{\mathcal{K}}{\succeq} 0\,,\;\; x\neq\mathbf{0} \tag{236}$$

From this, the alternative systems of inequalities [1, pp.50, 54, 262]

$$\begin{array}{c} Ay \underset{\mathcal{K}^*}{\prec} b \\[2ex] \text{exclusive or} \\[2ex] x^Tb\leq 0\,,\quad A^Tx=\mathbf{0}\quad \forall\, x \underset{\mathcal{K}}{\succeq} 0\,,\;\; x\neq\mathbf{0} \end{array} \tag{237}$$

derived from (236) taking the complementary sense of the inequality in x^Tb.

□

2.9.2.1 Simplicial case

When a convex cone is simplicial (§2.7.3), Cone Table **1** simplifies because then $\operatorname{aff}\operatorname{cone} X = \mathbb{R}^n$: For square X and assuming simplicial $\mathcal{K}$ such that

$$\operatorname{rank}(X \in \mathbb{R}^{n\times N}) \;=\; N \;\triangleq\; \dim\operatorname{aff}\mathcal{K} \;=\; n \tag{238}$$

we have

Cone Table S	$\mathcal{K}$	$\mathcal{K}^*$
vertex-description	X	$X^{\dagger T}$
halfspace-description	$X^\dagger$	X^T

For example, vertex-description (230) simplifies to

$$\mathcal{K}^* \;=\; \{X^{\dagger T} b \mid b \succeq 0\} \subset \mathbb{R}^n \tag{239}$$

Now, because $\dim\mathcal{R}(X) = \dim\mathcal{R}(X^{\dagger T})$, (§E) the dual cone $\mathcal{K}^*$ is simplicial whenever $\mathcal{K}$ is.

2.9.2.2 Ambient space = $\operatorname{aff}\mathcal{K}$

It is obvious by definition (170) of the ordinary dual cone $\mathcal{K}^*$ in ambient vector space $\mathcal{S}$ that its determination instead in ambient vector space $\mathcal{M} \subseteq \mathcal{S}$ is identical to its intersection with $\mathcal{M}$; *id est*, assuming cone $\mathcal{K} \subseteq \mathcal{M}$,

$$\mathcal{K}^* \text{ in ambient } \mathcal{M} \subseteq \mathcal{S} \;=\; \mathcal{K}^* \cap \mathcal{M} \tag{240}$$

because

$$\{y \in \mathcal{M} \mid \langle y\,, x\rangle \geq 0 \text{ for all } x \in \mathcal{K}\} \;=\; \{y \in \mathcal{S} \mid \langle y\,, x\rangle \geq 0 \text{ for all } x \in \mathcal{K}\} \,\cap\, \mathcal{M} \tag{241}$$

From this, a constrained and new membership relation (§2.8.2.0.1) for the ordinary dual cone $\mathcal{K}^* \subseteq \mathcal{S}$, assuming $x\,, y \in \mathcal{M}$ and $\mathcal{K} \subseteq \mathcal{M}$,

$$y \in \mathcal{K}^* \cap \mathcal{M} \;\Leftrightarrow\; \langle y\,, x\rangle \geq 0 \text{ for all } x \in \mathcal{K} \tag{242}$$

By closure in ambient $\mathcal{M}$ we have symmetry (§2.8.1.1):

$$x \in \mathcal{K} \;\Leftrightarrow\; \langle y\,, x\rangle \geq 0 \text{ for all } y \in \mathcal{K}^* \cap \mathcal{M} \tag{243}$$

This means membership determination in ambient $\mathcal{M}$ requires knowledge of the dual cone only in $\mathcal{M}$.

Assume now an ambient space $\mathcal{M}$ that is the affine hull of cone $\mathcal{K}$: Consider again a pointed polyhedral cone $\mathcal{K}$ denoted by its extreme directions arranged columnar in matrix X such that

$$\operatorname{rank}(X \in \mathbb{R}^{n\times N}) \;=\; N \triangleq \dim \operatorname{aff} \mathcal{K} \;\leq\; n \tag{224}$$

We want expressions for the convex cone and its dual in ambient $\mathcal{M} = \operatorname{aff} \mathcal{K}$:

Cone Table A	$\mathcal{K}$	$\mathcal{K}^* \cap \operatorname{aff} \mathcal{K}$
vertex-description	X	$X^{\dagger T}$
halfspace-description	$X^{\dagger}\,,\ X^{\perp T}$	$X^T,\ X^{\perp T}$

When $\dim \operatorname{aff} \mathcal{K} = n$, this table reduces to Cone Table **S**. These descriptions facilitate work in an ambient space that may be a proper subspace. The subspace of symmetric matrices $\mathbb{S}^N$, for example, often serves as ambient space.[2.48]

2.9.2.2.1 Example. *The monotone nonnegative cone.*
[1, exer.2.33] [73, §2] Simplicial cone (§2.7.3.0.1) $\mathcal{K}_{\mathcal{M}+}$ is the cone of all nonnegative vectors having their entries sorted in nonincreasing order:

$$\begin{aligned}\mathcal{K}_{\mathcal{M}+} &\triangleq \{x \mid x_1 \geq x_2 \geq \cdots \geq x_n \geq 0\} \subseteq \mathbb{R}^n_+\\ &= \{x \mid (e_i - e_{i+1})^T x \geq 0,\ i = 1 \ldots n{-}1,\ e_n^T x \geq 0\}\\ &= \{x \mid X^{\dagger} x \succeq 0\}\end{aligned} \tag{244}$$

a halfspace-description where e_i is the i^{th} standard basis vector, and where

$$X^{\dagger T} \triangleq [\, e_1{-}e_2 \quad e_2{-}e_3 \quad \cdots \quad e_n \,] \in \mathbb{R}^{n\times n} \tag{245}$$

(With $X^{\dagger}$ in hand, we might concisely scribe the remaining vertex and halfspace-descriptions from the tables for $\mathcal{K}_{\mathcal{M}+}$ and its dual. Instead we use generalized inequality in their derivation.) For any x and y, simple algebra demands

$$\begin{aligned}x^T y \;=\; \sum_{i=1}^n x_i\, y_i \;=\; &(x_1 - x_2)y_1 + (x_2 - x_3)(y_1 + y_2) + (x_3 - x_4)(y_1 + y_2 + y_3) + \cdots\\ &+ (x_{n-1} - x_n)(y_1 + \cdots + y_{n-1}) + x_n(y_1 + \cdots + y_n)\end{aligned} \tag{246}$$

[2.48] The dual cone of positive semidefinite matrices $\mathbb{S}^{N^*}_+ = \mathbb{S}^N_+$ remains in $\mathbb{S}^N$ by convention, whereas the ordinary dual cone would venture into $\mathbb{R}^{N\times N}$.

Because $x_i - x_{i+1} \geq 0 \;\; \forall i$ by assumption whenever $x \in \mathcal{K}_{\mathcal{M}+}$, we can employ generalized inequality (185) with respect to the self-dual nonnegative orthant $\mathbb{R}^n_+$ to find the halfspace-description of the dual cone $\mathcal{K}^*_{\mathcal{M}+}$. We can say $x^Ty \geq 0$ for all $X^\dagger x \succeq 0$ [*sic*] if and only if,

$$y_1 \geq 0\,, \quad y_1 + y_2 \geq 0\,, \quad \ldots\,, \quad y_1 + y_2 + \cdots + y_n \geq 0 \tag{247}$$

id est,

$$x^Ty \geq 0 \;\; \forall\, X^\dagger x \succeq 0 \quad \Leftrightarrow \quad X^Ty \succeq 0 \tag{248}$$

where

$$X = [\, e_1 \quad e_1 + e_2 \quad e_1 + e_2 + e_3 \quad \cdots \quad \mathbf{1}\,] \in \mathbb{R}^{n\times n} \tag{249}$$

Because $X^\dagger x \succeq 0$ connotes membership of x to pointed $\mathcal{K}_{\mathcal{M}+}$, then by (170) the dual cone we seek comprises all y for which (248) holds; thus its halfspace-description,

$$\mathcal{K}^*_{\mathcal{M}+} = \{y \underset{\mathcal{K}^*_{\mathcal{M}+}}{\succeq} 0\} = \{y \mid \sum_{i=1}^k y_i \geq 0\,,\; k = 1 \ldots n\} = \{y \mid X^Ty \succeq 0\} \subset \mathbb{R}^n \tag{250}$$

The monotone nonnegative cone and its dual are simplicial, illustrated for two Euclidean spaces in Figure **2.24**.

From §2.8.2.2, the extreme directions of proper $\mathcal{K}_{\mathcal{M}+}$ are respectively orthogonal to the facets of $\mathcal{K}^*_{\mathcal{M}+}$. Because $\mathcal{K}^*_{\mathcal{M}+}$ is simplicial, the inward-normals to its facets constitute the linearly independent rows of X^T by (250). Hence the vertex-description for $\mathcal{K}_{\mathcal{M}+}$ employs the columns of X in agreement with Cone Table **S** because $X^\dagger = X^{-1}$. Likewise, the extreme directions of proper $\mathcal{K}^*_{\mathcal{M}+}$ are respectively orthogonal to the facets of $\mathcal{K}_{\mathcal{M}+}$ whose inward-normals are contained in the rows of $X^\dagger$ by (244). So the vertex-description for $\mathcal{K}^*_{\mathcal{M}+}$ employs the columns of $X^{\dagger T}$. □

2.9.2.2.2 Example. *Monotone cone.* (Figure **2.25**) Of nonempty interior but not pointed, the monotone cone is polyhedral and defined by the halfspace-description

$$\mathcal{K}_{\mathcal{M}} \triangleq \{x \in \mathbb{R}^n \mid x_1 \geq x_2 \geq \cdots \geq x_n\} = \{x \in \mathbb{R}^n \mid X^{*T}x \succeq 0\} \tag{251}$$

Its dual is therefore pointed but of empty interior, having vertex-description

$$\mathcal{K}^*_{\mathcal{M}} = \{\, X^* b \triangleq [\, e_1 - e_2 \;\; e_2 - e_3 \;\; \cdots \;\; e_{n-1} - e_n \,]\, b \mid b \succeq 0 \,\} \subset \mathbb{R}^n \tag{252}$$

where the columns of X^* comprise the extreme directions of $\mathcal{K}_{\mathcal{M}}^*$. Because $\mathcal{K}_{\mathcal{M}}^*$ is pointed and satisfies

$$\operatorname{rank}(X^* \in \mathbb{R}^{n\times N}) \;=\; N \;\triangleq\; \dim\operatorname{aff}\mathcal{K}^* \;\leq\; n \tag{253}$$

where $N = n-1$, and because $\mathcal{K}_{\mathcal{M}}$ is closed and convex, we may adapt Cone Table **1** as follows:

Cone Table 1*	$\mathcal{K}^*$	$\mathcal{K}^{**} = \mathcal{K}$
vertex-description	X^*	$X^{*\dagger T}$, $\pm X^{*\perp}$
halfspace-description	$X^{*\dagger}$, $X^{*\perp T}$	X^{*T}

The vertex-description for $\mathcal{K}_{\mathcal{M}}$ is therefore

$$\mathcal{K}_{\mathcal{M}} = \{[\,X^{*\dagger T} \quad X^{*\perp} \quad -X^{*\perp}\,]a \mid a \succeq 0\} \subset \mathbb{R}^n \tag{254}$$

where $X^{*\perp} = \mathbf{1}$ and

$$X^{*\dagger} = \frac{1}{n}\begin{bmatrix} n-1 & -1 & -1 & \cdots & -1 & -1 & -1 \\ n-2 & n-2 & -2 & \ddots & \cdots & -2 & -2 \\ \vdots & n-3 & n-3 & \ddots & -(n-4) & \vdots & -3 \\ 3 & \vdots & n-4 & \ddots & -(n-3) & -(n-3) & \vdots \\ 2 & 2 & \cdots & \ddots & 2 & -(n-2) & -(n-2) \\ 1 & 1 & 1 & \cdots & 1 & 1 & -(n-1) \end{bmatrix} \in \mathbb{R}^{n-1\times n} \tag{255}$$

while

$$\mathcal{K}_{\mathcal{M}}^* = \{y \in \mathbb{R}^n \mid X^{*\dagger}y \succeq 0,\; X^{*\perp T}y = \mathbf{0}\} \tag{256}$$

is the dual monotone cone halfspace-description. □

2.9.2.3 More descriptions of pointed cone with equality constraint

Consider pointed polyhedral cone $\mathcal{K}$ whose subspace membership is explicit; *id est*, we are given the ordinary halfspace-description,

$$\mathcal{K} = \{x \mid Ax \succeq 0\,,\; Cx = \mathbf{0}\} \subseteq \mathbb{R}^n \qquad \text{(159a)}$$

where $A \in \mathbb{R}^{m\times n}$ and $C \in \mathbb{R}^{p\times n}$. This can be equivalently written in terms of nullspace of C and vector ξ:

$$\mathcal{K} = \{Z\xi \in \mathbb{R}^n \mid AZ\xi \succeq 0\} \tag{257}$$

where $\mathcal{R}(Z\in\mathbb{R}^{n\times n-\operatorname{rank}C})\triangleq\mathcal{N}(C)$. Assuming (224) is satisfied

$$\operatorname{rank}X \triangleq \operatorname{rank}\big((AZ)^\dagger\in\mathbb{R}^{n-\operatorname{rank}C\times m}\big) = m-\ell = \dim\operatorname{aff}\mathcal{K} \leq n-\operatorname{rank}C \tag{258}$$

where ℓ is the number of conically dependent rows in AZ (§2.6.7) that must be removed before the cone tables become applicable. Then the results collected in the cone tables imply the assignment $\hat{X}\triangleq(\hat{A}Z)^\dagger\in\mathbb{R}^{n-\operatorname{rank}C\times m-\ell}$, where $\hat{A}\in\mathbb{R}^{m-\ell\times n}$, can be followed with linear transformation by Z . So, we get the vertex-description

$$\mathcal{K}=\{Z(\hat{A}Z)^\dagger b \mid b\succeq 0\} \tag{259}$$

From this and (189) we get a halfspace-description of the dual cone,

$$\mathcal{K}^*=\{y\in\mathbb{R}^n \mid (Z^T\hat{A}^T)^\dagger Z^T y\succeq 0\} \tag{260}$$

From this and Cone Table **1** we get a vertex-description, (1175)

$$\mathcal{K}^*=\{[\,Z^{\dagger T}(\hat{A}Z)^T \quad C^T \quad -C^T\,]c \mid c\succeq 0\} \tag{261}$$

Yet because

$$\mathcal{K}=\{x \mid Ax\succeq 0\}\cap\{x \mid Cx=\mathbf{0}\} \tag{262}$$

then, by (179), we get an equivalent vertex-description for the dual cone

$$\begin{aligned}\mathcal{K}^*&=\overline{\{x \mid Ax\succeq 0\}^*+\{x \mid Cx=\mathbf{0}\}^*}\\&=\{[\,A^T \quad C^T \quad -C^T\,]b \mid b\succeq 0\}\end{aligned} \tag{263}$$

from which the conically dependent columns may, of course, be removed.

2.9.3 Dual of proper non-simplicial $\mathcal{K}$, X fat full-rank

Having found formula (239) to determine the dual of a simplicial cone, the easiest way to find the vertex-description for the dual of an arbitrary polyhedral proper cone $\mathcal{K}$ in $\mathbb{R}^n$ is to first decompose it into simplicial parts $\mathcal{K}_i$ so that $\mathcal{K}=\bigcup\mathcal{K}_i$.[2.49] The existence of multiple simplicial parts means the

[2.49] That proposition presupposes, of course, that we know how to perform the simplicial decomposition efficiently; also called *triangulation.* [74] [75, §3.1] [76, §3.1] biorthogonal expansion of $x \in \mathcal{K}$ like (223) can no longer be unique because the number of extreme directions in $\mathcal{K}$ exceeds n the dimension of the space.

Assume we are given a set of N conically independent generators[2.50] (§2.6.7) of proper $\mathcal{K}$ arranged columnar in $X \in \mathbb{R}^{n\times N}$ such that $n < N$ (*fat*) and $\operatorname{rank} X = n$. Each component simplicial cone in $\mathcal{K}$ corresponds to some subset of n linearly independent columns from X. The key idea, here, is how the extreme directions of the simplicial parts must remain extreme directions of $\mathcal{K}$. Finding the dual of $\mathcal{K}$ amounts to finding the dual of each simplicial part:

Theorem. *Dual cone intersection.* [31, §2.7] Suppose proper cone $\mathcal{K} \subset \mathbb{R}^n$ equals the union of M simplicial cones $\mathcal{K}_i$ whose extreme directions all coincide with those of $\mathcal{K}$. Then proper dual cone $\mathcal{K}^*$ is the intersection of M dual simplicial cones $\mathcal{K}_i^*$; *id est*,

$$\mathcal{K} = \bigcup_{i=1}^{M} \mathcal{K}_i \quad \Rightarrow \quad \mathcal{K}^* = \bigcap_{i=1}^{M} \mathcal{K}_i^* \tag{264}$$

◇

Proof. For $X_i \in \mathbb{R}^{n\times n}$, a matrix of extreme directions arranged columnar, corresponding simplicial $\mathcal{K}_i$ has vertex-description,

$$\mathcal{K}_i = \{X_i c \mid c \succeq 0\} \tag{265}$$

Now suppose,

$$\mathcal{K} \;=\; \bigcup_{i=1}^{M} \mathcal{K}_i \;=\; \bigcup_{i=1}^{M} \{X_i c \mid c \succeq 0\} \tag{266}$$

The union of all $\mathcal{K}_i$ can be equivalently expressed

$$\mathcal{K} \;=\; \left\{ [\, X_1 \; X_2 \; \cdots \; X_M \,] \begin{bmatrix} a \\ b \\ \vdots \\ c \end{bmatrix} \;\middle|\; a, b, \ldots, c \succeq 0 \right\} \tag{267}$$

Because extreme directions of the simplices $\mathcal{K}_i$ are extreme directions of $\mathcal{K}$ by assumption, then by the *extremes theorem*, (§2.6.4.0.1)

$$\mathcal{K} \;=\; \{ [\, X_1 \; X_2 \; \cdots \; X_M \,]\, d \mid d \succeq 0 \,\} \tag{268}$$

[2.50] We can always eliminate conically dependent columns from X to construct $\mathcal{K}$ or to determine $\mathcal{K}^*$. (§F.2)

Defining $X \triangleq [\,X_1\, X_2 \cdots X_M\,]$ (with any redundant columns optionally removed from X), then $\mathcal{K}^*$ can be expressed, (195) (Cone Table **S**)

$$\mathcal{K}^* \;=\; \{y \mid X^T y \succeq 0\} \;=\; \bigcap_{i=1}^{M} \{y \mid X_i^T y \succeq 0\} \;=\; \bigcap_{i=1}^{M} \mathcal{K}_i^* \tag{269}$$

♦

To find the extreme directions of the dual cone, first we observe that some facets of each simplicial part $\mathcal{K}_i$ are common to facets of $\mathcal{K}$ by assumption, and the union of all those common facets comprises the set of all facets of $\mathcal{K}$ by design. For any polyhedral proper cone $\mathcal{K}$, the extreme directions of the dual cone $\mathcal{K}^*$ are respectively orthogonal to the facets of $\mathcal{K}$. (§2.8.2.2) Then the extreme directions of the dual cone can be found among the inward-normals to facets of the component simplicial cones $\mathcal{K}_i$; those normals are extreme directions of the dual simplicial cones $\mathcal{K}_i^*$. From the theorem and Cone Table **S**,

$$\mathcal{K}^* \;=\; \bigcap_{i=1}^{M} \mathcal{K}_i^* \;=\; \bigcap_{i=1}^{M} \{X_i^{\dagger T} c \mid c \succeq 0\} \tag{270}$$

The set of extreme directions $\{\Gamma_i^*\}$ for the proper dual cone $\mathcal{K}^*$ is therefore constituted by the conically independent generators, from the columns of all the dual simplicial matrices $\{X_i^{\dagger T}\}$, that do not violate its discrete definition (195):

$$\left\{\Gamma_1^*,\, \Gamma_2^* \ldots \Gamma_N^*\right\} \;=\; \text{c.i.}\left\{X_i^{\dagger T}(:,j),\; i=1\ldots M,\; j=1\ldots n \mid X_i^{\dagger}(j,:)\Gamma_\ell \geq 0,\; \ell=1\ldots N\right\} \tag{271}$$

where c.i. denotes the selection of only the conically independent vectors from the argument set, argument $(:,j)$ denotes the j^{th} column while $(j,:)$ denotes the j^{th} row, and $\{\Gamma_\ell\}$ constitutes the extreme directions of $\mathcal{K}$. Figure **2.16**(b) (p.71) shows a cone and its dual found via this formulation.

Example. *Dual of* $\mathcal{K}$ *non-simplicial with respect to ambient space* $\operatorname{aff}\mathcal{K}$. Given conically independent generators for pointed closed convex $\mathcal{K}$ in $\mathbb{R}^4$, arranged columnar in

$$X \;=\; [\,\Gamma_1 \;\; \Gamma_2 \;\; \Gamma_3 \;\; \Gamma_4\,] \;=\; \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{bmatrix} \tag{272}$$

having $\dim\operatorname{aff}\mathcal{K} = \operatorname{rank} X = 3$, then performing the most inefficient simplicial decomposition in $\operatorname{aff}\mathcal{K}$ we find

$$X_1 = \begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},\quad X_2 = \begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix},\quad X_3 = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix},\quad X_4 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix} \tag{273}$$

The corresponding dual simplicial cones in $\operatorname{aff}\mathcal{K}$ have generators respectively columnar in

$$4X_1^{\dagger T} = \begin{bmatrix} 2 & 1 & 1 \\ -2 & 1 & 1 \\ 2 & -3 & 1 \\ -2 & 1 & -3 \end{bmatrix},\quad 4X_2^{\dagger T} = \begin{bmatrix} 1 & 2 & 1 \\ -3 & 2 & 1 \\ 1 & -2 & 1 \\ 1 & -2 & -3 \end{bmatrix},\quad 4X_3^{\dagger T} = \begin{bmatrix} 3 & 2 & -1 \\ -1 & 2 & -1 \\ -1 & -2 & 3 \\ -1 & -2 & -1 \end{bmatrix},\quad 4X_4^{\dagger T} = \begin{bmatrix} 3 & -1 & 2 \\ -1 & 3 & -2 \\ -1 & -1 & 2 \\ -1 & -1 & -2 \end{bmatrix} \tag{274}$$

Applying (271) we get

$$\begin{bmatrix} \Gamma_1^* & \Gamma_2^* & \Gamma_3^* & \Gamma_4^* \end{bmatrix} = \frac{1}{4}\begin{bmatrix} 1 & 2 & 3 & 2 \\ 1 & 2 & -1 & -2 \\ 1 & -2 & -1 & 2 \\ -3 & -2 & -1 & -2 \end{bmatrix} \tag{275}$$

whose rank is 3, and is the known result;[2.51] the conically independent generators for that pointed section of the dual cone $\mathcal{K}^*$ in $\operatorname{aff}\mathcal{K}$; *id est*, $\mathcal{K}^* \cap \operatorname{aff}\mathcal{K}$.

□

2.10 Polyhedral inscription in PSD cone

primal and dual inscribed cones

objective is bounded means number of faces not exponential as aspremont predicts.

inscription example in §2.8.3.1.1.

[2.51]These calculations proceed so as to be consistent with [77, §6]; as if the ambient vector space were the proper subspace $\operatorname{aff}\mathcal{K}$ whose dimension is 3. In that ambient space, $\mathcal{K}$ may be regarded as a proper cone. Yet that author (from the citation) erroneously states the dimension of the ordinary dual cone to be 3; it is, in fact, 4.

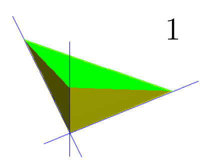


Figure 2.17: The unit simplex in $\mathbb{R}^{\mathbf{3}}$ is a unique solid tetrahedron, but is not regular.

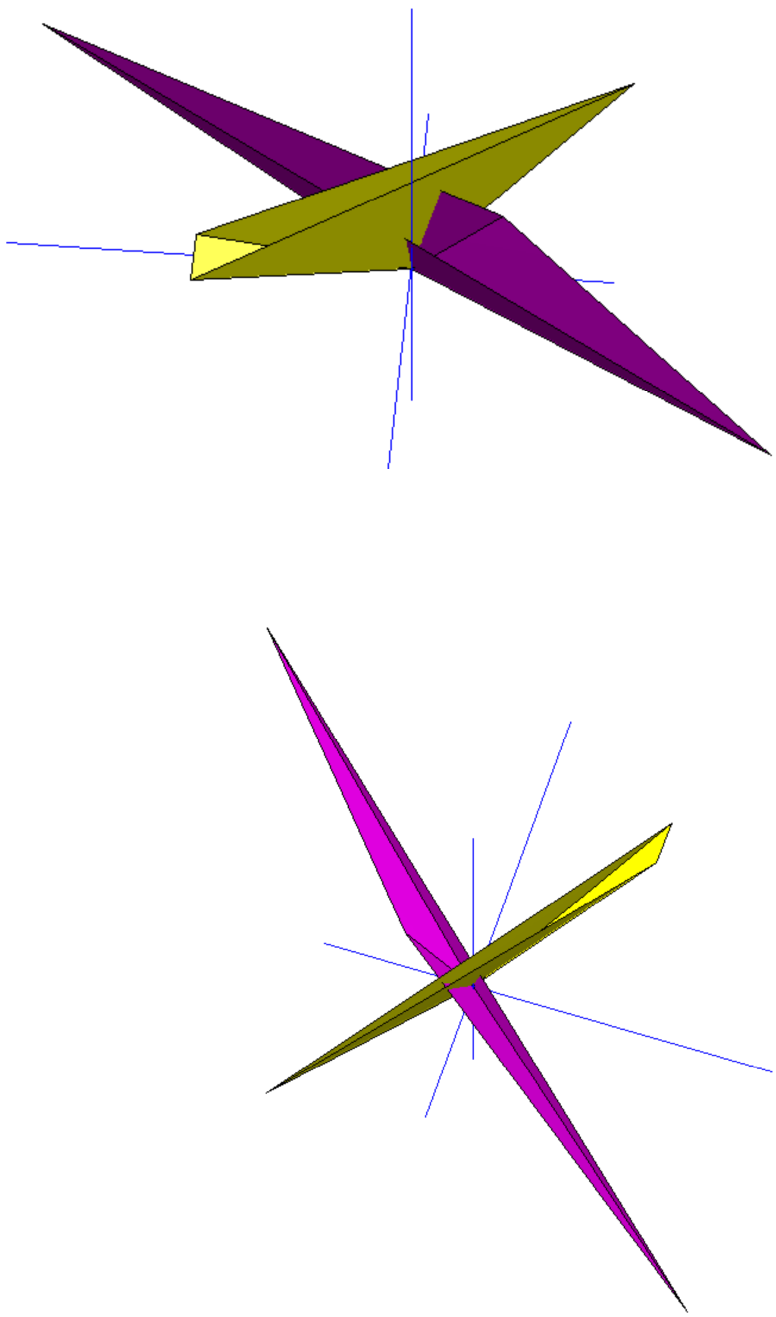


Figure 2.18: Two views of a simplicial cone and its dual in $\mathbb{R}^3$. The semi-infinite boundary of each cone is truncated for illustration. The Cartesian axes are drawn for reference.

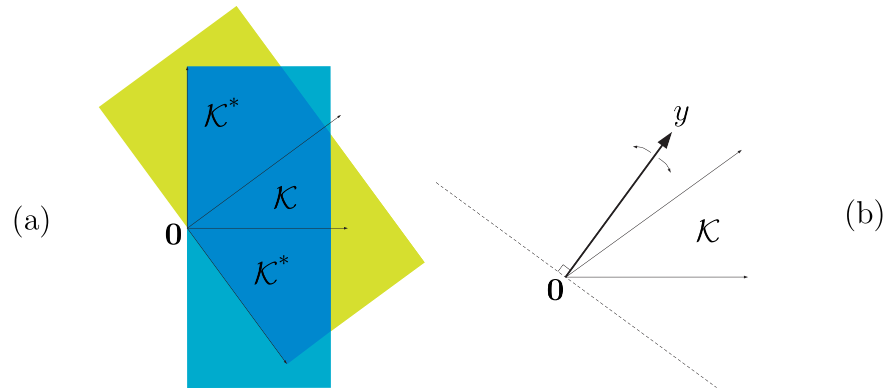


Figure 2.19: Two equivalent constructions of dual cone $\mathcal{K}^*$: **(a)** Showing construction by intersection of halfspaces. Only those two halfspaces whose bounding hyperplanes have inward-normal corresponding to an extreme direction of this pointed closed convex cone $\mathcal{K} \subset \mathbb{R}^2$ are drawn (truncated). **(b)** Suggesting construction by union of inward-normals y to each and every hyperplane supporting $\mathcal{K}$. This interpretation is valid when $\mathcal{K}$ is convex because existence of a supporting hyperplane is then guaranteed (§2.3.2.4).

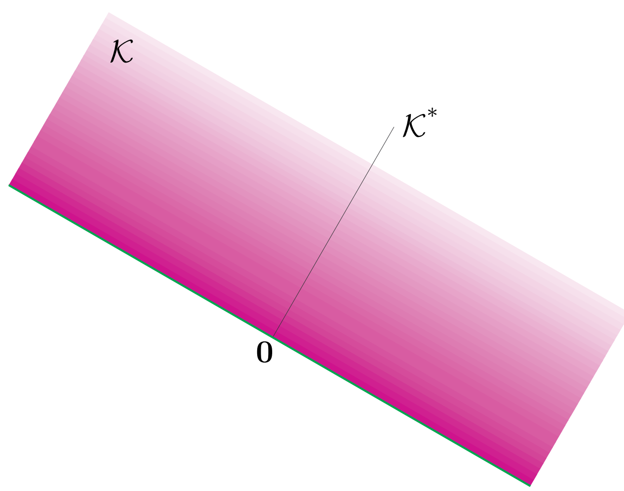


Figure 2.20: $\mathcal{K}$ is a halfspace about the origin in $\mathbb{R}^2$. $\mathcal{K}^*$ is a ray base $\mathbf{0}$, hence has empty interior in $\mathbb{R}^2$; so $\mathcal{K}$ cannot be pointed. (Both convex cones appear truncated.)

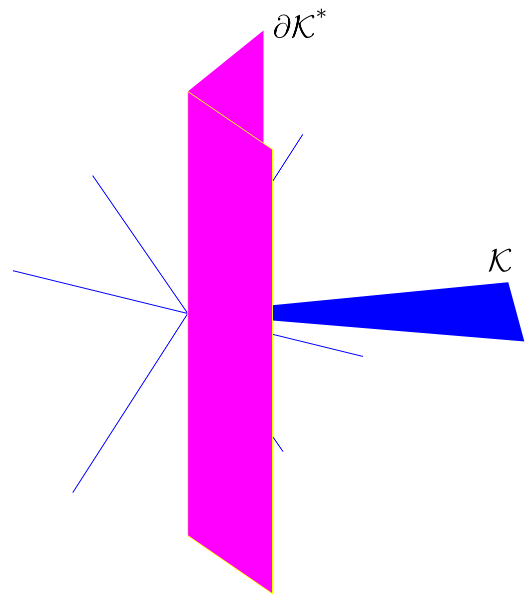


Figure 2.21: $\mathcal{K}$ is a pointed empty-interior polyhedral cone in $\mathbb{R}^3$ (drawn truncated and parallel to the floor on which you stand). $\mathcal{K}^*$ is a wedge whose truncated boundary is illustrated (drawn perpendicular to the floor). In this particular instance, $\mathcal{K} \subset \operatorname{int} \mathcal{K}^*$ (excepting the origin). Cartesian coordinate axes drawn for reference.

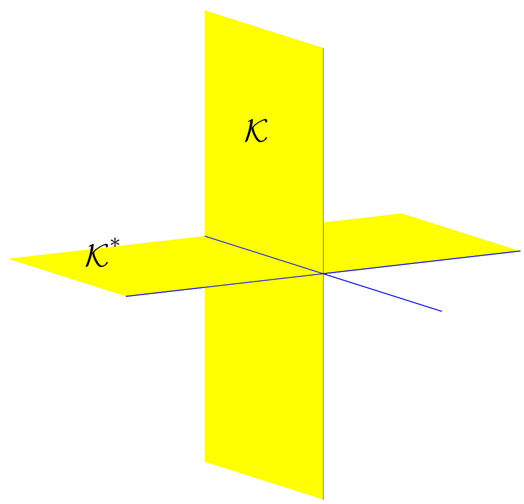


Figure 2.22: $\mathcal{K}$ and $\mathcal{K}^*$ are halfplanes in $\mathbb{R}^3$. Both semi-infinite convex cones appear truncated. Each cone is like $\mathcal{K}$ in Figure **2.20**, but embedded in a two-dimensional subspace of $\mathbb{R}^3$. Cartesian coordinate axes drawn for reference.

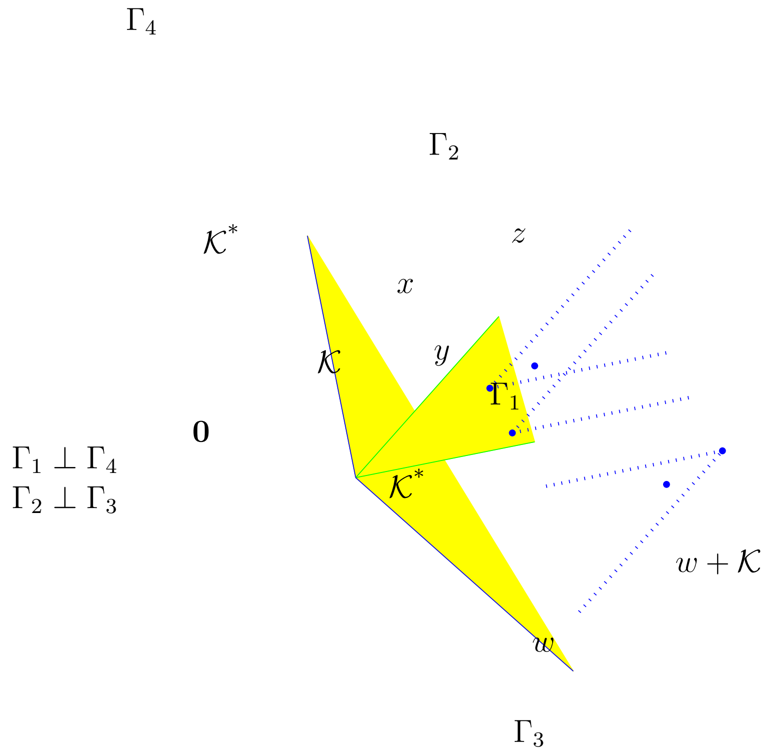
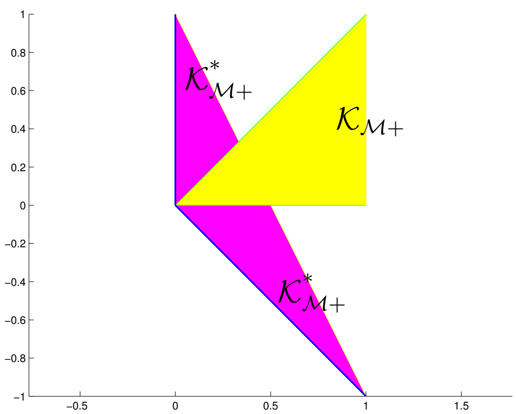


Figure 2.23: Polyhedral proper cone $\mathcal{K}$ in $\mathbb{R}^{\mathbf{2}}$ and its dual $\mathcal{K}^*$ in $\mathbb{R}^{\mathbf{2}}$ drawn truncated. Conically independent generators Γ_1 and Γ_2 constitute extreme directions of $\mathcal{K}$ while Γ_3 and Γ_4 constitute extreme directions of $\mathcal{K}^*$. Point x comparable to point z (and *vice versa*) but not to y; $z \succeq x \Leftrightarrow z - x \in \mathcal{K} \Leftrightarrow z - x \succeq_{\mathcal{K}} 0$ iff coordinates for biorthogonal expansion of $z - x$ are nonnegative. Point y not comparable to z because z does not belong to $y \pm \mathcal{K}$. Points need not belong to $\mathcal{K}$ to be comparable; *e.g.*, all points greater than w belong to $w + \mathcal{K}$. Were w lifted to three dimensions ($\mathcal{K}$ in $\mathbb{R}^{\mathbf{2}}$ and its ordinary dual $\mathcal{K}^*$ in $\mathbb{R}^{\mathbf{3}}$ for example), all members of the translated cone $w + \mathcal{K}$ would remain comparable to $w \in \mathbb{R}^{\mathbf{3}}$.

(a)



(b)

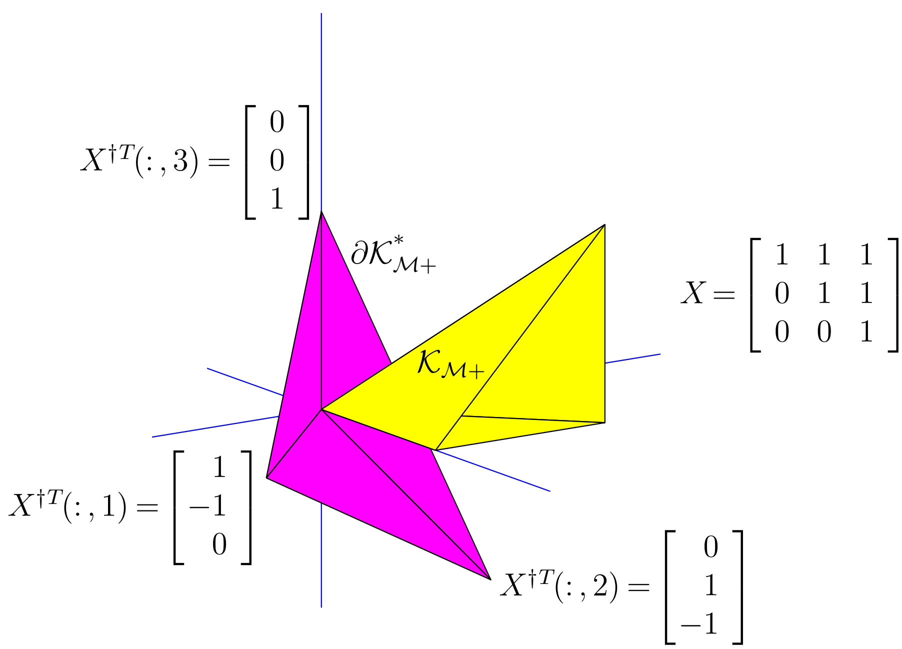


Figure 2.24: Simplicial cones. **(a)** Monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$ and its dual $\mathcal{K}^*_{\mathcal{M}+}$ (drawn truncated) in $\mathbb{R}^{\mathbf{2}}$. **(b)** Monotone nonnegative cone and boundary of its dual (both drawn truncated) in $\mathbb{R}^{\mathbf{3}}$. Extreme directions of $\mathcal{K}^*_{\mathcal{M}+}$ are indicated.

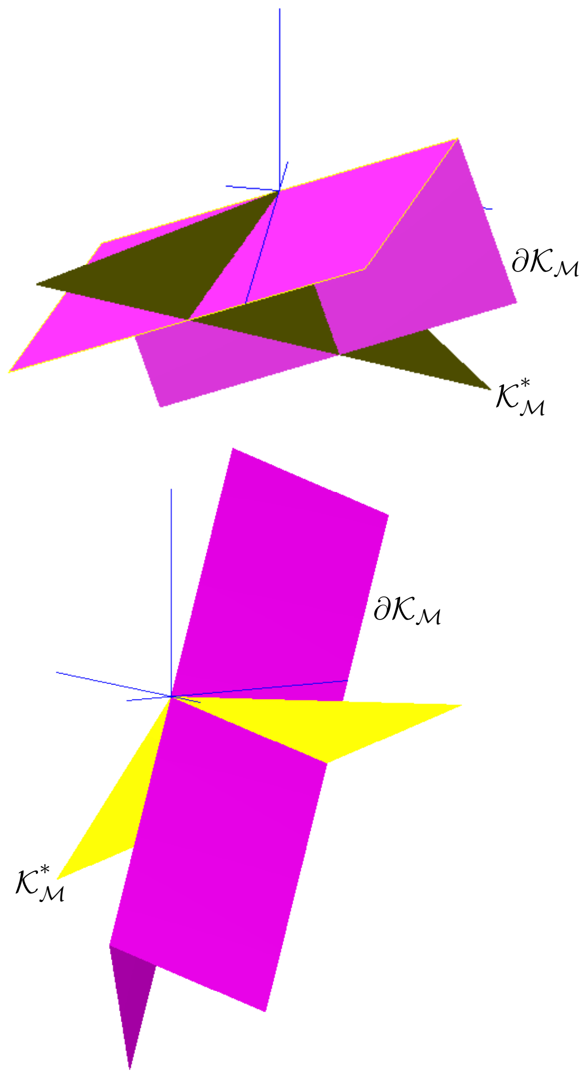


Figure 2.25: Two views of the monotone cone $\mathcal{K}_{\mathcal{M}}$ and its dual $\mathcal{K}_{\mathcal{M}}^*$ (drawn truncated) in $\mathbb{R}^{\mathbf{3}}$. The monotone cone is not pointed. The dual monotone cone has empty interior. The Cartesian coordinate axes are drawn for reference. In $\mathbb{R}^{\mathbf{2}}$, the monotone cone and its dual resembles Figure **2.20**.

Chapter 3

Geometry of convex functions

> *The link between convex sets and convex functions is via the epigraph: A* [real] *function is convex if and only if its epigraph is a convex set.*
>
> −Stephen Boyd & Lieven Vandenberghe [1, §3.1.7]

We limit our treatment of multidimensional functions to finite-dimensional Euclidean space. Then the icon for the one-dimensional *convex function* is bowl-shaped (Figure **3.2**), whereas the *concave* icon is the inverted bowl; respectively characterized by a unique global minimum and maximum whose existence is assumed. Because of this simple relationship, the usage of the term *convexity* is often implicitly inclusive of *concavity* in the literature. Despite the iconic imagery, the reader is reminded that the set of all convex, concave, *quasiconvex*, and *quasiconcave* functions contains the *monotone* [25] [24, §2.3.5] functions; *e.g.*, [1, §3.6, exer.3.46].

3.1 Convex function

3.1.1 Vector-valued function

The vector-valued continuous function $f(X):\mathbb{R}^{p\times k}\rightarrow\mathbb{R}^M$ is convex in X if and only if $\operatorname{dom} f$ is a convex set and, for each and every $Y,Z\in\operatorname{dom} f$ and all $0\leq\mu\leq 1$,

$$f(\mu Y + (1-\mu)Z) \underset{\mathbb{R}_+^M}{\preceq} \mu f(Y) + (1-\mu)f(Z) \tag{276}$$

Reversing the sense of the inequality flips this definition to concavity.

Since comparison of vectors here is with respect to $\mathbb{R}_+^M$ (196), the M-dimensional nonnegative orthant, the test prescribed by (276) is simply a comparison on $\mathbb{R}$ of each entry of the vector function. The vector-valued function case is therefore a straightforward generalization of conventional convexity theory for a real function. [1, §3, §4]

This same conclusion also follows from theory of generalized inequality (§2.8.2.0.1) that implies

$$f \text{ convex } \Leftrightarrow\; w^T f \text{ convex } \;\forall\, w\succeq 0 \tag{277}$$

shown by substituting the defining inequality (276). Discretization (§2.8.2.1.3) allows relaxation of the semi-infinite number of constraints $w\succeq 0$ to: for each and every $w\in\{e_i\,,\; i=1\ldots M\}$ (the standard basis for $\mathbb{R}^M$ and a minimal set of generators (§2.6.4.1) for $\mathbb{R}_+^M$) from which the stated conclusion follows.

Relation (277) further implies the space of all vector-valued convex functions is a closed convex cone. Indeed, any nonnegatively weighted sum of convex functions remains convex. Certainly any nonnegative sum of real convex functions remains convex.

When $f(X)$ instead satisfies, for each and every distinct Y and Z in $\operatorname{dom} f$ and all $0<\mu<1$,

$$f(\mu Y + (1-\mu)Z) \underset{\mathbb{R}_+^M}{\prec} \mu f(Y) + (1-\mu)f(Z) \tag{278}$$

then we shall say f is a *strictly convex function.* Like any convex function, a strictly convex function $f(X)$ has a unique minimum value. Yet it also has a unique minimizer $X^\star$ called the *optimal solution* of the *convex optimization* *problem* $\inf_{X\in\mathcal{C}} f(X)$ over some abstract convex set $\mathcal{C}$. The vector (Euclidean) 2-norm $\|x\|$ and Frobenius norm $\|X\|_{\mathrm{F}}$, for example, are strictly convex functions of their respective argument. [1, §8.1]

3.1.1.1 Affine function

A function $f(X)$ is *affine* when it is continuous and has the dimensionally extensible form (*confer* §2.6.6.3.4)

$$f(X) = AX + B \tag{279}$$

When $B = 0$ then $f(X)$ is a *linear function.* Variegated multidimensional affine functions are recognized by the existence of no multivariate terms in argument entries and no polynomial terms in argument entries of degree higher than 1; *id est*, entries of the function are characterized only by linear combinations of the argument entries plus constants.

All affine functions are simultaneously convex and concave.

For $X \in \mathbb{S}^M$ and matrices A, B, Q, R of any compatible dimensions, for example, the expression XAX is not affine in X, whereas

$$g(X) = \begin{bmatrix} R & B^T X \\ XB & Q + A^T X + XA \end{bmatrix} \tag{280}$$

is an affine multidimensional function. Such a function is typical in engineering control. [78, §2.2][3.1] [3] [5]

3.1.1.2 Epigraph

It is well established that a continuous real function $\hat{f}(X) : \mathbb{R}^{p\times k} \to \mathbb{R}$ is convex if and only if its *epigraph* makes a convex set;

$$\hat{f} \text{ convex } \Leftrightarrow \text{ epi}\, \hat{f} \text{ convex} \tag{281}$$

where the epigraph is defined, [29] [30] [35] [32] [37]

$$\text{epi}\, \hat{f} \triangleq \{(X, t) \mid X \in \text{dom}\, \hat{f}\,,\;\; \hat{f}(X) \le t\} \subseteq \mathbb{R}^{p\times k} \times \mathbb{R} \tag{282}$$

[3.1] The interpretation from this citation of $\{X \in \mathbb{S}^M \mid g(X) \succeq 0\}$ as "an intersection between a linear subspace and the cone of positive semidefinite matrices" is incorrect. (See §2.6.6.3.4 for a similar example.) The conditions they state under which strong duality holds for semidefinite programming are conservative. (*confer* §6.1.2.3.1)

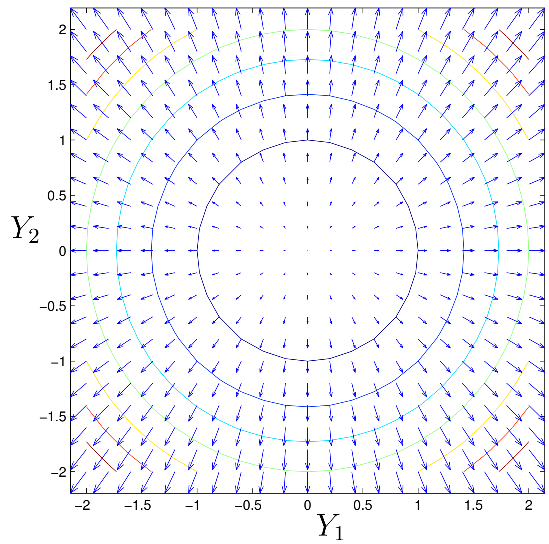


Figure 3.1: Gradient in $\mathbb{R}^{\mathbf{2}}$ evaluated on grid over some open disc in domain of convex quadratic bowl $\hat{f}(Y) = Y^T Y : \mathbb{R}^{\mathbf{2}} \to \mathbb{R}$ illustrated in Figure **3.2**. Circular contours are level sets.

Thus the epigraph is a classical connection between convex sets and real convex functions.

Generalization to a vector valued function $f(X) : \mathbb{R}^{p\times k} \to \mathbb{R}^M$ yields only a partial result; from (277):[3.2]

$$\begin{aligned} \operatorname{epi} f \;&=\; \{(X,t) \mid X \in \operatorname{dom} f\,,\;\; w^T f(X) \leq t\,,\;\; \forall\, w \succeq 0\} \;\subseteq\; \mathbb{R}^{p\times k} \times \mathbb{R} \\ &=\; \{(X,t) \mid X \in \operatorname{dom} f\,,\;\; f(X) \underset{\mathbb{R}^M_+}{\preceq} t\,\mathbf{1}\,\} \end{aligned} \tag{283}$$

id est,

$$f \text{ convex } \Rightarrow \operatorname{epi} f \text{ convex} \tag{284}$$

This partial result follows because a convex set can be formed from the intersection of non-convex sets, and (283) describes an intersection. Yet every real function constituting each entry of the convex vector-valued function must, of course, correspond to a convex epigraph.

[3.2] By generalized inequality (§2.8.2.0.1), $w^T(t\mathbf{1} - f) \geq 0 \;\; \forall\, w \succeq 0 \;\Leftrightarrow\; t\mathbf{1} - f \succeq 0$.

3.1.1.3 Gradient

The gradient ∇f (§D.1) of a multidimensional function f maps each entry f_i to a space having the same dimension as the ambient space of its domain; it can be considered a vector pointing in the direction of greatest change. [79, §15.6] For a one-dimensional function of real variable, for example, the gradient is just the slope of that function evaluated at any point in the domain. For the quadratic bowl in Figure **3.2**, the gradient maps to $\mathbb{R}^2$; illustrated in Figure **3.1**.

Example. *Hyperplane, line, described by affine function.* Consider the real affine function of vector variable,

$$\hat{f}(x) : \mathbb{R}^p \to \mathbb{R} \;=\; a^T x + b \tag{285}$$

whose domain is $\mathbb{R}^p$ and whose gradient $\nabla \hat{f}(x) = a$ is a constant vector (independent of x). This function describes the real line $\mathbb{R}$, its range, and it describes a *non-vertical* [29, §B.1.2] hyperplane $\partial\mathcal{H}$ in the space $\mathbb{R}^p \times \mathbb{R}$ for any vector a (*confer* §2.3.2);

$$\partial\mathcal{H} = \left\{ \begin{bmatrix} x \\ a^T x + b \end{bmatrix} \mid x \in \mathbb{R}^p \right\} \subset \mathbb{R}^p \times \mathbb{R} \tag{286}$$

having nonzero normal

$$\eta = \begin{bmatrix} a \\ -1 \end{bmatrix} \in \mathbb{R}^p \times \mathbb{R} \tag{287}$$

This equivalence to a hyperplane holds only for real functions.[3.3]

- The epigraph of the real affine function $\hat{f}(x)$ is therefore a halfspace, and so the real affine function is to convex functions as the halfspace is to convex sets.

[3.3] To prove that, consider a vector-valued affine function

$$f(x) : \mathbb{R}^p \to \mathbb{R}^M \;=\; Ax + b$$

having gradient $\nabla f(x) = A^T \in \mathbb{R}^{p \times M}$: The affine set

$$\left\{ \begin{bmatrix} x \\ Ax + b \end{bmatrix} \mid x \in \mathbb{R}^p \right\} \subset \mathbb{R}^p \times \mathbb{R}^M$$

Similarly, the matrix-valued affine function of real variable x, for any matrix $A\in\mathbb{R}^{M\times N}$,

$$h(x) : \mathbb{R}\to\mathbb{R}^{M\times N} = Ax + B \tag{288}$$

describes a line in $\mathbb{R}^{M\times N}$ in direction A

$$\{Ax + B \mid x\in\mathbb{R}\} \subseteq \mathbb{R}^{M\times N} \tag{289}$$

and describes a line in $\mathbb{R}\times\mathbb{R}^{M\times N}$

$$\left\{\begin{bmatrix} x \\ Ax+B \end{bmatrix} \mid x\in\mathbb{R}\right\} \subset \mathbb{R}\times\mathbb{R}^{M\times N} \tag{290}$$

whose slope with respect to x is A. □

3.1.1.3.1 First-order convexity condition, vector-valued function

When a real function $\hat{f}$ is differentiable at each point in its open domain, there is an intuitive geometric interpretation of function convexity in terms of its gradient $\nabla\hat{f}$ and its epigraph.

Consider the first-order necessary and sufficient condition for convexity: Differentiable vector-valued function $f(X) : \mathbb{R}^{p\times k}\to\mathbb{R}^M$ is convex if and only if $\operatorname{dom} f$ is open, convex, and for all $X, Y\in\operatorname{dom} f$,

$$f(Y) \underset{\mathbb{R}^M_+}{\succeq} f(X) + \overset{\to Y-X}{df(X)} \;=\; f(X) + \left.\frac{d}{dt}\right|_{t=0} f(X+t\,(Y-X)) \tag{291}$$

where $\overset{\to Y-X}{df(X)}$ is the *directional derivative*[3.4] [79] [80] of f at X in direction $Y-X$, and where the right-hand side of the inequality is the first-order Taylor series expansion of f about X.

---

is perpendicular to

$$\eta \triangleq \begin{bmatrix} \nabla f(x) \\ -I \end{bmatrix} \in \mathbb{R}^{p\times M}\times\mathbb{R}^{M\times M}$$

because

$$\eta^T\left(\begin{bmatrix} x \\ Ax+b \end{bmatrix} - \begin{bmatrix} 0 \\ b \end{bmatrix}\right) = 0\,, \quad \forall\, x\in\mathbb{R}^p$$

Yet η is a vector (in $\mathbb{R}^p\times\mathbb{R}^M$) only when $M=1$. ♦

[3.4] We extend the traditional definition of directional derivative in §D.1.4 so that direction may be indicated by a vector or a matrix, thereby broadening the scope of the Taylor series (§D.1.6).

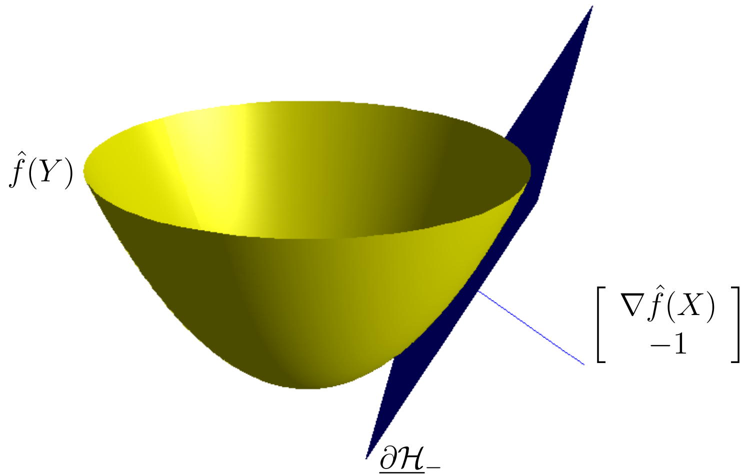


Figure 3.2: Drawn is a convex quadratic bowl in $\mathbb{R}^{\mathbf{3}}$ (*confer* Figure **D.1**, p.361); $\hat{f}(Y) = Y^TY : \mathbb{R}^{\mathbf{2}} \to \mathbb{R}$ *versus* Y on some open disc in $\mathbb{R}^{\mathbf{2}}$. The supporting hyperplane $\underline{\partial\mathcal{H}_-} \in \mathbb{R}^{\mathbf{2}}\times\mathbb{R}$ (which is tangent, only partially drawn) and its normal vector $[\,\nabla\hat{f}(X)^T \;\; -1\,]^T$ at the point of support $[\,X^T \;\; \hat{f}(X)\,]^T$ are also illustrated.

Necessary and sufficient discretization (§2.8.2.1.3) of $w \succeq 0$ in (277) invites refocus to the real-valued function: When $\hat{f}(X) : \mathbb{R}^{p\times k} \to \mathbb{R}$ is a real differentiable convex function with matrix argument on open convex domain, from (1138)

$$\hat{f}(Y) \geq \hat{f}(X) + \operatorname{tr}\Big(\nabla\hat{f}(X)^T(Y - X)\Big) \tag{292}$$

is the first-order necessary and sufficient condition for convexity.

When $\hat{f}(X) : \mathbb{R}^p \to \mathbb{R}$ is a real differentiable convex function with vector argument on open convex domain, there is further simplification of this first-order condition (291); [1, §3.1.3] [33, §1.2] [4, §1.2.3]

$$\hat{f}(Y) \geq \hat{f}(X) + \nabla\hat{f}(X)^T(Y - X) \tag{293}$$

From this we can find a unique [32, §5.5] non-vertical [29, §B.1.2] hyperplane $\underline{\partial\mathcal{H}_-}$ (§2.3), expressed in terms of the function gradient, supporting epi $\hat{f}$; *videlicet*, [1, §3.1.7] defining $\hat{f}(Y \notin \operatorname{dom}\hat{f}) = \infty$,

$$\begin{bmatrix} Y \\ t \end{bmatrix} \in \operatorname{epi}\hat{f} \;\Leftrightarrow\; t \geq \hat{f}(Y) \;\Rightarrow\; \begin{bmatrix} \nabla\hat{f}(X)^T & -1 \end{bmatrix}\left(\begin{bmatrix} Y \\ t \end{bmatrix} - \begin{bmatrix} X \\ \hat{f}(X) \end{bmatrix}\right) \leq 0 \tag{294}$$

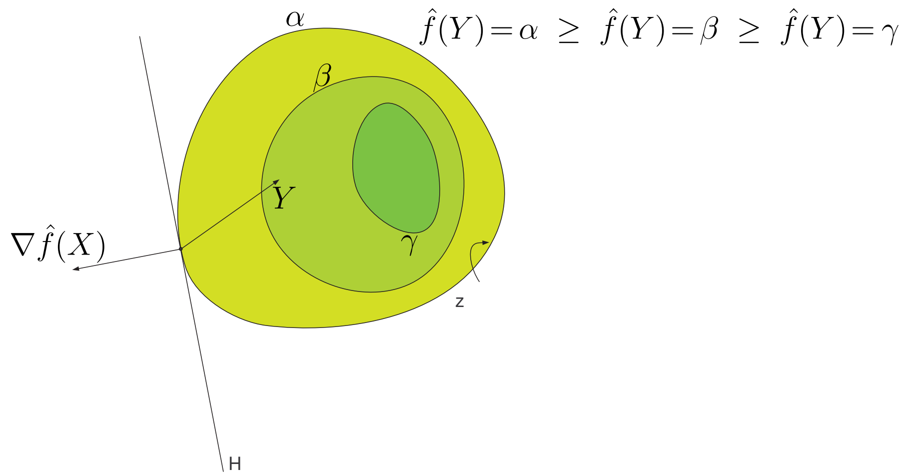


Figure 3.3: Shown is a plausible contour plot in $\mathbb{R}^{\mathbf{2}}$ of some arbitrary real convex function $\hat{f}(Y)$ at selected levels α , β , and γ ; contours in the function's domain of equal level $\hat{f}$ (level sets). A convex function has convex sublevel sets $\mathcal{L}_X\hat{f}(X)$ (296). [30, §4.6]

This means for each and every point X in the domain of a real convex function, there exists a hyperplane in $\mathbb{R}^p\times\mathbb{R}$ having normal $\begin{bmatrix}\nabla\hat{f}(X)\\ -1\end{bmatrix}$ supporting the function epigraph at $\begin{bmatrix}X\\ \hat{f}(X)\end{bmatrix}\in\underline{\partial\mathcal{H}}_-$. One such supporting hyperplane is illustrated in Figure **3.2** for a convex quadratic.

From (293) we deduce for all $X,Y\in\operatorname{dom}\hat{f}$:

$$\nabla\hat{f}(X)^T(Y-X)\geq 0 \ \Rightarrow \ \hat{f}(Y)\geq\hat{f}(X) \tag{295}$$

meaning, the gradient at X identifies a supporting hyperplane in $\mathbb{R}^p$ there to the *sublevel sets* of the function $\hat{f}$,

$$\mathcal{L}_X\hat{f}(X)=\{Y\in\operatorname{dom}\hat{f} \mid \hat{f}(Y)\leq\hat{f}(X)\}\subseteq\mathbb{R}^p \tag{296}$$

illustrated for an arbitrary real convex function in Figure **3.3**.

3.1.1.4 Second-order convexity condition, vector-valued function

Again, by discretization, we are obliged to consider only each separate entry of a vector function. For $f(X) : \mathbb{R}^p \rightarrow \mathbb{R}^M$, a twice differentiable vector function with vector argument on open convex domain,

$$\nabla^2 f_i(X) \underset{\mathbb{S}^p_+}{\succeq} 0 \quad \forall X \in \operatorname{dom} f\,, \quad i=1\ldots M \tag{297}$$

is a necessary and sufficient condition for convexity of f. Strict inequality is a sufficient condition for strict convexity.

For a twice-differentiable real function $\hat{f}(X) : \mathbb{R}^p \rightarrow \mathbb{R}$ having open domain, a consequence of the *mean value theorem* from calculus allows precise expression of its complete Taylor series expansion about $X \in \operatorname{dom} \hat{f}$ (§D.1.6) using only three terms: On some open interval of $\|Y\|$ so each and every line segment $[X, Y]$ belongs to $\operatorname{dom} \hat{f}$, there exists an $\alpha \in [0,1]$ such that [4, §1.2.3] [33, §1.1.4]

$$\hat{f}(Y) = \hat{f}(X) + \nabla \hat{f}(X)^T (Y - X) + \frac{1}{2}(Y - X)^T \nabla^2 \hat{f}\big(\alpha X + (1-\alpha)Y\big)(Y - X) \tag{298}$$

The first-order condition for convexity (293) follows directly from this and the second-order condition (297).

We need different tools for matrix argument:

3.1.2 Matrix-valued function

We are primarily interested in continuous matrix-valued functions $g(X)$. We choose symmetric $g(X) \in \mathbb{S}^M$ because matrix-valued functions are most often compared (299) with respect to the positive semidefinite cone $\mathbb{S}^M_+$ in the ambient space of symmetric matrices.[3.5]

[3.5] Function symmetry is not a necessary requirement for convexity; indeed, for $A \in \mathbb{R}^{m\times p}$ and $B \in \mathbb{R}^{m\times k}$, $g(X) = AX + B$ is a convex (affine) function in X on domain $\mathbb{R}^{p\times k}$ with respect to the nonnegative orthant $\mathbb{R}^{m\times k}_+$. Symmetric convex functions share the same benefits as symmetric matrices. Horn & Johnson [28, §7.7] liken symmetric matrices to real numbers, and (symmetric) positive definite matrices to positive real numbers.

Definition. *Convex matrix-valued function.*
1) *Matrix-definition.*
A function $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is convex in X iff $\operatorname{dom} g$ is a convex set and, for each and every $Y, Z \in \operatorname{dom} g$ and all $0 \leq \mu \leq 1$, [24, §2.3.7]

$$g(\mu Y + (1-\mu)Z) \underset{\mathbb{S}_+^M}{\preceq} \mu\, g(Y) + (1-\mu)g(Z) \tag{299}$$

Reversing the sense of the inequality flips this definition to concavity. Strict convexity is defined less a stroke of the pen in (299) similarly to (278).

2) *Scalar-definition.*
It follows that $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is convex in X iff $w^T g(X) w : \mathbb{R}^{p\times k} \to \mathbb{R}$ is convex in X for each and every $\|w\| = 1$; shown by substituting the defining inequality (299). By generalized inequality (§2.8.2.4) we have the equivalent but more general criterion,

$$g \text{ convex } \Leftrightarrow \langle W, g\rangle \text{ convex } \forall\, W \underset{\mathbb{S}_+^M}{\succeq} 0 \tag{300}$$

Because the set of all extreme directions for the positive semidefinite cone comprises a minimal set of generators for that cone, discretization (§2.8.2.1.3) allows replacement of matrix W with symmetric dyad ww^T as proposed. $\triangle$

The generalized inequality (300) from this *scalar-definition* implies the space of all matrix-valued convex functions is a closed convex cone.

3.1.2.1 First-order convexity condition, matrix-valued function

From the *scalar-definition* we have, for each and every real vector w of unit norm $\|w\| = 1$,

$$w^T g(Y) w \geq w^T g(X) w + w^T \overset{\to Y-X}{dg(X)}\, w \tag{301}$$

which follows immediately from the first-order condition for convexity of a real function (293). By generalized inequality (*confer* (291))

$$g(Y) \underset{\mathbb{S}_+^M}{\succeq} g(X) + \overset{\to Y-X}{dg(X)} \tag{302}$$

must therefore be necessary and sufficient for convexity of a matrix-valued function of matrix variable.

3.1.2.2 Epigraph of matrix-valued function

Observing for each and every $\|w\|=1$,

$$w^T g(X) w \leq t \;\Leftrightarrow\; g(X) \underset{\mathbb{S}_+^M}{\preceq} tI \tag{303}$$

[28, §7.7, prob.9] and by defining

$$\begin{aligned}\operatorname{epi} g &= \left\{(X,t) \mid X \in \operatorname{dom} g\,,\;\; w^T g(X) w \leq t\,,\;\; \|w\|=1\right\} \subseteq \mathbb{R}^{p\times k}\times\mathbb{R} \\ &= \{\,(X,t) \mid X \in \operatorname{dom} g\,,\;\; g(X) \underset{\mathbb{S}_+^M}{\preceq} tI\,\}\end{aligned} \tag{304}$$

it follows

$$g \text{ convex } \Rightarrow \operatorname{epi} g \text{ convex} \tag{305}$$

Given a continuous matrix-valued function $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ consequent to the *scalar-definition*, we defined the epigraph of $g(X)$ (304) in terms of the corresponding real function $w^T g(X) w$; *id est*,

$$\operatorname{epi} g \;=\; \bigcap_{\|w\|=1} \operatorname{epi}\left(w^T g\, w\right) \tag{306}$$

An epigraph made from an intersection of non-convex sets is possibly convex, hence the partial result (305).

3.1.2.3 Line Theorem

$g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is convex in X if and only if it remains convex on the intersection of any line with its domain. [1, §3.1.1] $\diamond$

3.1.2.4 Second-order convexity condition, matrix-valued function

Now we assume a twice differentiable function and drop the subscript $\mathbb{S}_+^M$ from the inequality when it is apparent.

Definition. *Differentiable convex matrix-valued function.*
$g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is convex in X iff $\operatorname{dom} g$ is an open convex set, and its second derivative $g''(X+t\,Y) : \mathbb{R} \to \mathbb{S}^M$ is positive semidefinite on each point along every line $X+t\,Y$ that intersects $\operatorname{dom} g$; *id est*, iff for each and every $X, Y \in \mathbb{R}^{p\times k}$ such that $X+t\,Y \in \operatorname{dom} g$ over some open interval of $t \in \mathbb{R}$,

$$\frac{d^2}{dt^2}\, g(X+t\,Y) \succeq 0 \tag{307}$$

Similarly, if

$$\frac{d^2}{dt^2}\, g(X+t\,Y) \succ 0 \tag{308}$$

then g is strictly convex; the converse is generally false. [1, §3.1.4][3.6]

△

Example. *Matrix inverse.* The matrix-valued function $g(X) = X^{-1}$ is convex on $\operatorname{int} \mathbb{S}^M_+$. For each and every $Y \in \mathbb{S}^M$, (§D.2.1.1, §A.3.1.0.5)

$$\frac{d^2}{dt^2}\, g(X+t\,Y) \;=\; 2(X+t\,Y)^{-1}Y(X+t\,Y)^{-1}Y(X+t\,Y)^{-1} \;\succeq\; 0 \tag{309}$$

on some open interval of $t \in \mathbb{R}$ such that $X+t\,Y \succ 0$. Hence, $g(X)$ is convex in X. This result is extensible;[3.7] $\operatorname{tr} X^{-1}$ is convex on that same domain. [28, §7.6, prob.2] □

Example. *Matrix squared.* The iconic real function $\hat{f}(x) = x^2$ is strictly convex on $\mathbb{R}$. Its matrix-valued counterpart $g(X) = X^2$ is convex on the domain of symmetric matrices; for $X, Y \in \mathbb{S}^M$ and any open interval of $t \in \mathbb{R}$, (§D.2.1.1)

$$\frac{d^2}{dt^2}\, g(X+t\,Y) \;=\; \frac{d^2}{dt^2}(X+t\,Y)^2 \;=\; 2Y^2 \tag{310}$$

which is positive semidefinite when Y is symmetric because then $Y^2 = Y^TY$ (848).[3.8] □

[3.6] Quadratic forms constitute a notable exception where the strict-case converse is reliably true.

[3.7] $d/dt \operatorname{tr} g(X+t\,Y) = \operatorname{tr} d/dt\, g(X+t\,Y)$.

[3.8] By (857) in §A.3.1, changing the domain instead to all symmetric and nonsymmetric positive semidefinite matrices, for example, will not produce a convex function.

Example. *Matrix exponential.* The matrix-valued function $g(X)=e^X:\mathbb{S}^M\to\mathbb{S}^M$ is convex on the subspace of circulant symmetric matrices [81]. Applying the *line theorem*, for all $t\in\mathbb{R}$ and for circulant $X,Y\in\mathbb{S}^M$ we have

$$\frac{d^2}{dt^2}e^{X+tY} = Ye^{X+tY}Y \succeq 0\,,\qquad (XY)^T = XY \tag{311}$$

because circulant matrices are commutative (§B.6) and, for symmetric matrices, $XY=YX \Leftrightarrow (XY)^T=XY$ (856). Given symmetric argument, the matrix exponential always resides interior to the cone of positive semidefinite matrices in the symmetric subspace; $e^A\succ 0\,,\ \forall A\in\mathbb{S}^M$ (1170). If matrix $e^A\in\mathbb{S}^M$ is positive (semi)definite then, for any matrix Y of compatible dimension, Y^Te^AY is positive semidefinite. (§A.3.1.0.5)

The second derivative, given in Table **D.2.7**, depends only upon commutativity; so, the domain of convex g may be broadened to all commutative symmetric matrices.

Changing the function domain to the subspace of all real diagonal matrices reduces the matrix exponential to a vector-valued function in an isometrically isomorphic subspace $\mathbb{R}^M$; [82, §5.3][3.9] known convex (276) from the real-valued function case [1, §3.1.5]. $\square$

There are, of course, multifarious methods to determine function convexity, [1] each of them efficient when appropriate.

3.2 Quasiconvex function

Quasiconvex functions [1, §3.4] [29] [31] [32] are useful in practical problem solving because they are *unimodal* (by definition when non-monotone); a global minimum is guaranteed to exist over any convex set in the function domain. The scalar definition of convexity carries over to quasiconvexity:

[3.9] The matrix exponential of a diagonal matrix exponentiates each individual diagonal entry.

Definition. *Quasiconvex matrix-valued function.*
$g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is a quasiconvex function of matrix X iff $\operatorname{dom} g$ is a convex set and for each and every: $Y, Z \in \operatorname{dom} g$, $0 \leq \mu \leq 1$, and real vector w of unit norm,

$$w^T g(\mu Y + (1-\mu)Z)w \;\leq\; \max\{w^T g(Y)w,\; w^T g(Z)w\} \tag{312}$$

A quasiconcave function is characterized

$$w^T g(\mu Y + (1-\mu)Z)w \;\geq\; \min\{w^T g(Y)w,\; w^T g(Z)w\} \tag{313}$$

In either case, vector w becomes superfluous for real functions.

△

When $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is a quasiconvex function of matrix X, then for each and every $\nu \in \mathbb{R}$ the corresponding sublevel set

$$\begin{aligned} \mathcal{L}_\nu g &= \left\{X \in \operatorname{dom} g \mid w^T g(X)w \leq \nu\,,\; \|w\| = 1\right\} \subseteq \mathbb{R}^{p\times k} & (314)\\ &= \{X \in \operatorname{dom} g \mid g(X) \preceq \nu I\} & (315) \end{aligned}$$

is convex. Convexity of all the sublevel sets is a necessary and sufficient condition for quasiconvexity of a real function $\hat{f}$, [83, §2] but it is not sufficient for a higher-dimensional function because the sublevel set $\mathcal{L}_\nu g$ of a matrix-valued function g is an intersection of sublevel sets of real functions $w^T g\, w$ (314).

Likewise, convexity of all superlevel sets[3.10] is a necessary and sufficient condition for quasiconcavity of a real function:

3.2.0.0.1 Example. *Rank function quasiconcavity.*
For $A, B \in \mathbb{R}^{m\times n}$ [28, §0.4]

$$\operatorname{rank} A + \operatorname{rank} B \;\geq\; \operatorname{rank}(A+B) \tag{316}$$

that follows from the fact [26, §3.6]

$$\dim \mathcal{R}(A) + \dim \mathcal{R}(B) \;=\; \dim \mathcal{R}(A+B) + \dim(\mathcal{R}(A) \cap \mathcal{R}(B)) \tag{317}$$

[3.10] The superlevel set is similarly defined:

$$\mathcal{L}_s g = \{X \in \operatorname{dom} g \mid g(X) \succeq sI\}$$

For $A, B \in \mathbb{S}_+^M$ [1, §3.4.2]

$$\operatorname{rank} A + \operatorname{rank} B \;\geq\; \operatorname{rank}(A+B) \;\geq\; \min\{\operatorname{rank} A\,,\ \operatorname{rank} B\} \tag{318}$$

that follows from the fact

$$\mathcal{N}(A+B) = \mathcal{N}(A) \cap \mathcal{N}(B)\,, \qquad A, B \in \mathbb{S}_+^M \tag{99}$$

Rank is a quasiconcave function on $\mathbb{S}_+^M$ because the right-hand side of (318) has the concave form of (312); *videlicet*,

$$\operatorname{rank}(A+B) = \operatorname{rank}(\mu A + (1-\mu)B) \tag{319}$$

over the open interval $(0,1)$ of μ, which follows from the *linearly independent dyads definition* in §B.1.1. □

From this example we see, unlike convex functions, quasiconvex functions are not necessarily continuous.

Definition. *Differentiable quasiconvex matrix-valued function.*
Assume that function $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ is twice differentiable, and $\operatorname{dom} g$ is an open convex set.

Then $g(X)$ is quasiconvex in X if wherever in its domain the directional derivative (§D.1.4) becomes $\mathbf{0}$, the second directional derivative (§D.1.5) is positive definite there [1, §3.4.3] in the same direction Y; *id est*, g is quasiconvex if for each and every point $X \in \operatorname{dom} g$, all nonzero directions $Y \in \mathbb{R}^{p\times k}$, and for $t \in \mathbb{R}$,

$$\left.\frac{d}{dt}\right|_{t=0} g(X + t\,Y) = \mathbf{0} \;\;\Rightarrow\;\; \left.\frac{d^2}{dt^2}\right|_{t=0} g(X + t\,Y) \succ 0 \tag{320}$$

If $g(X)$ is quasiconvex, conversely, then for each and every $X \in \operatorname{dom} g$ and all $Y \in \mathbb{R}^{p\times k}$,

$$\left.\frac{d}{dt}\right|_{t=0} g(X + t\,Y) = \mathbf{0} \;\;\Rightarrow\;\; \left.\frac{d^2}{dt^2}\right|_{t=0} g(X + t\,Y) \succeq 0 \tag{321}$$

△

3.3 Salient properties of convex and quasiconvex functions

1. • A convex (or concave) function is assumed continuous on the relative interior of its domain. [30, §10]
   • A quasiconvex (or quasiconcave) function is not necessarily a continuous function.

2. g convex $\Leftrightarrow$ $-g$ concave.
   g quasiconvex $\Leftrightarrow$ $-g$ quasiconcave.

3. convexity $\Rightarrow$ quasiconvexity $\Rightarrow$ convex sublevel sets.
   concavity $\Rightarrow$ quasiconcavity $\Rightarrow$ convex superlevel sets.[3.11]

4. The *scalar-definition* of matrix-valued function convexity and the *line theorem* (§3.1.2.3) [1, §3.4.2] translate identically to quasiconvexity (and quasiconcavity).

5. *Composition* $g\big(h(X)\big)$ of a convex (concave) function g with any affine mapping $h:\mathbb{R}^{m\times n}\to\mathbb{R}^{p\times k}$, such that $h(\mathbb{R}^{m\times n})\cap\operatorname{dom} g\neq\emptyset$, becomes convex (concave) in $X\in\mathbb{R}^{m\times n}$. [29, §B.2.1] Likewise for the quasiconvex (quasiconcave) functions g.

6. • A nonnegatively weighted sum of convex (concave) functions remains convex (concave).
   • A nonnegatively weighted maximum of quasiconvex functions remains quasiconvex. A nonnegatively weighted minimum of quasiconcave functions remains quasiconcave.

[3.11] For real functions, convex sublevel (superlevel) sets are necessary and sufficient for quasiconvexity (quasiconcavity).

Chapter 4

Euclidean Distance Matrix

These results were obtained by Schoenberg (1935), a surprisingly late date for such a fundamental property of Euclidean Geometry.

−John Clifford Gower [84, §3]

By itself, distance information between many points in Euclidean space is lacking. We might want to know more; such as, relative or absolute position or dimension of some hull. A question naturally arising in some fields (*e.g.*, geodesy, economics, genetics, psychology, biochemistry, engineering) [85] asks what facts can be deduced given only distance information. What can we know about the underlying points that the distance information purports to describe? We also ask what happens when the given distance information is incomplete; or suppose the distance information is not reliable, available, or specified only by certain tolerances. These questions motivate a study of inter-point distance, well represented in any spatial dimension by a simple matrix from linear algebra.[4.1] In what follows, we will answer some of these questions via Euclidean distance matrices.

[4.1] *e.g.*, $\sqrt{D} \in \mathbb{R}^{N\times N}$, a classical two-dimensional matrix representation of absolute inter-point distance because its entries (in ordered rows and columns) can be written neatly on a piece of paper. Matrix D will be reserved throughout to hold distance-square.

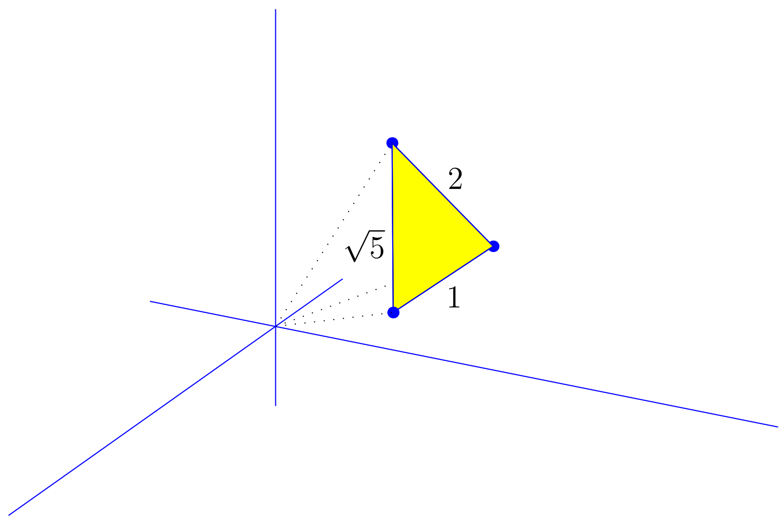


Figure 4.1: Convex hull of three points ($N = 3$) is shaded in $\mathbb{R}^3$ ($n = 3$). Dotted lines are imagined vectors to points.

4.1 EDM

Euclidean space $\mathbb{R}^n$ is a finite-dimensional real vector space having an inner product defined on it, hence a metric as well. [38, §3.1] A Euclidean distance matrix, an EDM in $\mathbb{R}_+^{N\times N}$, is an exhaustive table of distance-square d_{ij} between points taken by pair from a list of N points $\{x_\ell\,,\ \ell = 1 \ldots N\}$ in $\mathbb{R}^n$; the squared metric the measure of distance-square:

$$d_{ij} \;=\; \|x_i - x_j\|_2^2 \;\triangleq\; \langle x_i - x_j\,,\, x_i - x_j\rangle \tag{322}$$

Each point is labelled ordinally, hence the row or column index of an EDM, i or $j = 1 \ldots N$, individually addresses all the points in the list.

Consider the following example of an EDM for the case $N = 3$:

$$D \;=\; [d_{ij}] \;=\; \begin{bmatrix} d_{11} & d_{12} & d_{13} \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{bmatrix} = \begin{bmatrix} 0 & d_{12} & d_{13} \\ d_{12} & 0 & d_{23} \\ d_{13} & d_{23} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 5 \\ 1 & 0 & 4 \\ 5 & 4 & 0 \end{bmatrix} \tag{323}$$

Matrix D has N^2 entries but only $N(N-1)/2$ pieces of information. In Figure **4.1** we show three points in $\mathbb{R}^3$ that can be arranged in a list to correspond to D in (323). Such a list is not unique because any rotation, reflection, or translation (§4.5) of the points in Figure **4.1** would produce the same EDM D.

4.2 Metric requirements

For $i,j=1\ldots N$, the Euclidean distance between points x_i and x_j must satisfy the axiomatic requirements imposed by any metric space: [38, §1.1] [36, §1.7]

1. $\sqrt{d_{ij}} \geq 0,\ i \neq j$ — nonnegativity

2. $\sqrt{d_{ij}} = 0,\ i = j$ — self-distance

3. $\sqrt{d_{ij}} = \sqrt{d_{ji}}$ — symmetry

4. $\sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}\,,\ i\neq j\neq k$ — triangle inequality

where $\sqrt{d_{ij}}$ is the Euclidean metric in $\mathbb{R}^n$ (§4.4). Then all entries of an EDM must be in concord with these Euclidean axioms: specifically, each entry must be nonnegative,[4.2] the main diagonal must be $\mathbf{0}$,[4.3] an EDM must be symmetric. The fourth axiom provides upper and lower bounds for each entry. Axiom 4 is true more generally when there are no restrictions on indices i,j,k, but furnishes no new information.

4.3 $\exists$ fifth Euclidean axiom

The four axioms of the Euclidean metric provide information insufficient to certify that a bounded convex polyhedron more complicated than a triangle has a Euclidean realization. [84, §2] Yet any list of points or the vertices of any bounded convex polyhedron must conform to the axioms.

[4.2] Implicit from the terminology, $\sqrt{d_{ij}} \geq 0 \Leftrightarrow d_{ij} \geq 0$ is always assumed.

[4.3] What we call zero self-distance, Marsden calls *nondegeneracy*. [36, §1.6]

Example. *Triangle.* Consider the EDM in (323), but missing one of its entries:

$$D = \begin{bmatrix} 0 & 1 & d_{13} \\ 1 & 0 & 4 \\ d_{31} & 4 & 0 \end{bmatrix} \tag{324}$$

Can we determine the unknown entries of D by applying the axioms? Axiom 1 demands $\sqrt{d_{13}}\,, \sqrt{d_{31}} \geq 0$, axiom 2 requires the main diagonal be $\mathbf{0}$, while axiom 3 makes $\sqrt{d_{31}} = \sqrt{d_{13}}$. The fourth axiom tells us

$$1 \leq \sqrt{d_{13}} \leq 3 \tag{325}$$

Indeed, described over that closed interval $[1, 3]$ is a family of triangular polyhedra whose angle at vertex x_2 varies from 0 to π radians. So, yes we can determine the unknown entries of D, but they are not unique; nor should they be from the information given for this example. □

4.3.0.0.2 Example. *Small completion problem*, I. Now consider the polyhedron in Figure **4.2** formed from an unknown list $\{x_1, x_2, x_3, x_4\}$. The corresponding EDM less one critical piece of information, d_{14}, is given by

$$D = \begin{bmatrix} 0 & 1 & 5 & d_{14} \\ 1 & 0 & 4 & 1 \\ 5 & 4 & 0 & 1 \\ d_{14} & 1 & 1 & 0 \end{bmatrix} \tag{326}$$

From axiom 4 we may write a few inequalities for the two triangles common to d_{14}; we find

$$\sqrt{5}-1 \;\leq\; \sqrt{d_{14}} \;\leq\; 2 \tag{327}$$

We cannot further narrow those bounds on $\sqrt{d_{14}}$ using only the four axioms (§4.8.3.1.1). Yet there is only one possible choice for $\sqrt{d_{14}}$ because points x_2, x_3, x_4 must be collinear. All other values of $\sqrt{d_{14}}$ in the interval $[\sqrt{5}-1,\ 2]$ specify impossible distances in any dimension; *id est*, in this particular example the triangle inequality axiom does not yield an interval for $\sqrt{d_{14}}$ over which a family of convex polyhedra can be reconstructed.

□

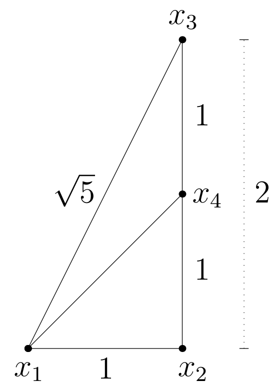


Figure 4.2: Four axioms of the Euclidean metric are not a recipe for reconstruction of this polyhedron.

We will return to this simple Example 4.3.0.0.2 to illustrate more elegant methods of solution in §4.9.3, §4.12.4.1, and §4.8.3.1.1. Until then, we can deduce some general principles from the foregoing examples:

- Unknown d_{ij} of an EDM are not necessarily uniquely determinable.
- The triangle inequality does not produce necessarily *tight* bounds.[4.4]
- The Euclidean axioms are insufficient for reconstruction.

4.3.1 Lookahead

There must exist at least one requirement more than the four axioms of the Euclidean metric that makes them altogether necessary and sufficient to certify realizability of bounded convex polyhedra. Indeed, there are infinitely many more; there are precisely $N+1$ necessary and sufficient Euclidean requirements for N points constituting a generating list (§2.2.2). Here is the fifth requirement:

[4.4]The term *tight* with reference to an inequality means equality is achievable.

Fifth Euclidean axiom. *Relative-angle inequality.* [86, §3.1] (*confer* §4.12.2.1) Augmenting the axioms of the Euclidean metric in $\mathbb{R}^n$, for all $i, j, \ell \neq k \in \{1 \ldots N\}$, $i<j<\ell$, and for $N \geq 4$ distinct points $\{x_k\}$, the inequalities

$$\begin{array}{c} \cos(\theta_{ik\ell} + \theta_{\ell kj}) \;\leq\; \cos\theta_{ikj} \;\leq\; \cos(\theta_{ik\ell} - \theta_{\ell kj}) \\ 0 \leq \theta_{ik\ell}\,, \theta_{\ell kj}\,, \theta_{ikj} \leq \pi \end{array} \tag{328}$$

where $\theta_{ikj} = \theta_{jki}$ is the angle between vectors at vertex x_k (371), must be satisfied at each point x_k regardless of affine dimension. $\diamond$

We will explore this in §4.12. One of our early objectives is to determine matrix criteria that subsume all the Euclidean axioms and any further requirements. Looking ahead, we will find (623) (352) (356)

$$\left.\begin{array}{r} -z^T D z \geq 0 \\ \mathbf{1}^T z = 0 \\ (\forall \, \|z\| = 1) \\ D \in \mathbb{S}^N_{\mathbf{0}} \end{array}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^N \tag{329}$$

where the convex cone of Euclidean distance matrices $\mathbb{EDM}^N \subseteq \mathbb{S}^N_{\mathbf{0}}$ belongs to the subspace of symmetric hollow[4.5] matrices (§2.1.2.2). Having found axiom-equivalent matrix criteria, we will see there is a bridge from bounded convex polyhedra to EDMs in §4.9 .[4.6]

In §4.15.1 we will show a new connection between the discrete Fourier transform and Euclidean distance matrices.

In §8.2 we explain how only $O(N)$ distances are required to uniquely reconstruct an N-vertex polyhedron existing in low affine dimension.

We now begin to develop some invaluable concepts and then link the axioms to matrix criteria.

[4.5] $\mathbf{0}$ main diagonal.

[4.6] From an EDM, a generating list (§2.2.2, §2.7.2) for a polyhedron can be found (§4.10) correct to within a rotation, reflection, and translation (§4.5).

4.4 EDM definition

Ascribe points in a list $\{x_\ell \in \mathbb{R}^n,\ \ell = 1 \ldots N\}$ to the columns of a matrix X ;

$$X = [\, x_1 \ \cdots \ x_N \,] \in \mathbb{R}^{n\times N} \qquad (54)$$

where N is regarded as the *cardinality* of list X . When matrix $D = [d_{ij}]$ is an EDM, its entries must be related to those points constituting the list by the Euclidean distance-square: for $i, j = 1 \ldots N$,

$$\begin{aligned} d_{ij} \;&=\; \|x_i - x_j\|^2 \;=\; (x_i - x_j)^T(x_i - x_j) \;=\; \|x_i\|^2 + \|x_j\|^2 - 2x_i^T x_j \\ &=\; \begin{bmatrix} x_i^T & x_j^T \end{bmatrix} \begin{bmatrix} I & -I \\ -I & I \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} \\ &=\; \operatorname{vec}(X)^T\, \Phi_{ij} \operatorname{vec} X \end{aligned} \qquad (330)$$

where Φ_{ij} has $I \in \mathbb{S}^n$ in its ii^{th} and jj^{th} block of entries while $-I \in \mathbb{S}^n$ fills its ij^{th} and ji^{th} block; *id est*,

$$\Phi_{ij} = (e_i e_i^T + e_j e_j^T - e_i e_j^T - e_j e_i^T) \otimes I \in \mathbb{S}_+^{nN} \qquad (331)$$

where $\{e_i \in \mathbb{R}^N,\ i = 1 \ldots N\}$ is the set of standard basis vectors, and $\otimes$ signifies the Kronecker product (§D.1.2.1). Thus each entry d_{ij} is a convex quadratic function [1, §3, §4] of $\operatorname{vec} X \in \mathbb{R}^{nN}$ (18). [30, §6]

The collection of all Euclidean distance matrices $\mathbb{EDM}^N$ is a convex subset of $\mathbb{R}_+^{N\times N}$ called the *EDM cone* (§5), hence not a subspace; (Figure **7.1**, p.246)

$$\mathbf{0} \;\in\; \mathbb{EDM}^N \;\subseteq\; \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N} \;\subset\; \mathbb{S}^N \qquad (332)$$

An EDM D must be expressible as a function of some list X ; *id est*, it must have the form

$$\mathbf{D}(X) \;\triangleq\; \delta(X^TX)\mathbf{1}^T + \mathbf{1}\delta(X^TX)^T - 2X^TX \;\in \mathbb{EDM}^N \qquad (333)$$

$$= \;(\mathbf{1} \otimes \operatorname{vec} X)^T \begin{bmatrix} \mathbf{0} & \Phi_{12} & \cdots & \Phi_{1N} \\ \Phi_{12} & \mathbf{0} & \ddots & \Phi_{2N} \\ \vdots & \ddots & \ddots & \vdots \\ \Phi_{1N} & \Phi_{2N} & \cdots & \mathbf{0} \end{bmatrix} (\mathbf{1} \otimes \operatorname{vec} X) \qquad (334)$$

Conversely, $\mathbf{D}(X)$ will make an EDM for any $X \in \mathbb{R}^{n\times N}$, but $\mathbf{D}(X)$ is not a convex function of X (§4.4.1). Now the EDM cone may be described:

$$\mathbb{EDM}^N = \left\{\mathbf{D}(X) \mid X \in \mathbb{R}^{n\times N}\right\} \tag{335}$$

Expression $\mathbf{D}(X)$ is a matrix definition of EDM and so conforms to the Euclidean axioms:

Nonnegativity of EDM entries (axiom 1, §4.2) is obvious from the distance-square definition (330), and so assumed to hold for any D expressible in the form $\mathbf{D}(X)$ in (333).

When we say D is an EDM, reading from (333), it implicitly means the main diagonal must be $\mathbf{0}$ (axiom 2, self-distance) and D must be symmetric (axiom 3); $\delta(D)=\mathbf{0}$ and $D^T=D$ or, equivalently, $D\in\mathbb{S}_{\mathbf{0}}^N$ are necessary matrix criteria.

The mapping $\mathbf{D}(X)$ is homogeneous in the sense, for $\zeta\in\mathbb{R}$,

$$\sqrt{\mathbf{D}(\zeta X)} = |\zeta|\sqrt{\mathbf{D}(X)} \tag{336}$$

where the square root is entry-wise.

4.4.1 $-V_{\mathcal{N}}^T\mathbf{D}(X)V_{\mathcal{N}}$ convexity

We saw that the EDM entries $d_{ij}\left(\begin{bmatrix} x_i \\ x_j \end{bmatrix}\right)$ are convex quadratic functions. Yet $-\mathbf{D}(X)$ (333) is not a quasiconvex function of matrix $X\in\mathbb{R}^{n\times N}$ because the second directional derivative (§3.2)

$$-\frac{d^2}{dt^2}\bigg|_{t=0}\mathbf{D}(X+t\,Y) = 2\left(-\delta(Y^TY)\mathbf{1}^T - \mathbf{1}\delta(Y^TY)^T + 2\,Y^TY\right) \tag{337}$$

is indefinite for any $Y\in\mathbb{R}^{n\times N}$ since its main diagonal is $\mathbf{0}$. [44, §4.2.8] [28, §7.1, prob.2] Hence $-\mathbf{D}(X)$ can neither be convex in X.

The outcome is different when instead we consider

$$-V_{\mathcal{N}}^T\mathbf{D}(X)V_{\mathcal{N}} = 2V_{\mathcal{N}}^TX^TXV_{\mathcal{N}} \tag{338}$$

where we introduce the full-rank skinny *auxiliary matrix* (§B.4.2)

$$V_{\mathcal{N}} \triangleq \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & -1 & \cdots & -1 \\ 1 & & & \mathbf{0} \\ & 1 & & \\ & & \ddots & \\ \mathbf{0} & & & 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} -\mathbf{1}^T \\ I \end{bmatrix} \in\mathbb{R}^{N\times N-1} \tag{339}$$

$(\mathcal{N}(V_{\mathcal{N}})=\mathbf{0})$ having range

$$\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)\,, \quad V_{\mathcal{N}}^T\mathbf{1} = \mathbf{0} \tag{340}$$

Matrix-valued function (338) meets the criterion for convexity in §3.1.2.4 over its domain that is all of $\mathbb{R}^{n\times N}$; *videlicet*, for any $Y\in\mathbb{R}^{n\times N}$,

$$-\frac{d^2}{dt^2}\,V_{\mathcal{N}}^T\mathbf{D}(X+t\,Y)V_{\mathcal{N}} \;=\; 4V_{\mathcal{N}}^T Y^T Y V_{\mathcal{N}} \succeq 0 \tag{341}$$

Quadratic matrix function $-V_{\mathcal{N}}^T\mathbf{D}(X)V_{\mathcal{N}}$ is therefore convex in X achieving its minimum, with respect to the positive semidefinite cone (§2.8.2.3), at $X=\mathbf{0}$. When the penultimate number of points exceeds the dimension of the space $n<N-1$, strict convexity of the quadratic (338) becomes impossible because (341) could not then be positive definite.

4.4.2 Gram-form EDM definition

Positive semidefinite matrix X^TX in (333), formed from an inner product of the list, is known as the *Gram matrix*; [37, §3.6]

$$\begin{aligned}
G \;\triangleq\; X^TX \;&=\; \begin{bmatrix} \|x_1\|^2 & x_1^Tx_2 & x_1^Tx_3 & \cdots & x_1^Tx_N \\ x_2^Tx_1 & \|x_2\|^2 & x_2^Tx_3 & \cdots & x_2^Tx_N \\ x_3^Tx_1 & x_3^Tx_2 & \|x_3\|^2 & \ddots & x_3^Tx_N \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ x_N^Tx_1 & x_N^Tx_2 & x_N^Tx_3 & \cdots & \|x_N\|^2 \end{bmatrix} \in \mathbb{S}_+^N \\
&= \delta\!\left(\begin{bmatrix} \|x_1\| \\ \|x_2\| \\ \vdots \\ \|x_N\| \end{bmatrix}\right) \begin{bmatrix} 1 & \cos\psi_{12} & \cos\psi_{13} & \cdots & \cos\psi_{1N} \\ \cos\psi_{12} & 1 & \cos\psi_{23} & \cdots & \cos\psi_{2N} \\ \cos\psi_{13} & \cos\psi_{23} & 1 & \ddots & \cos\psi_{3N} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \cos\psi_{1N} & \cos\psi_{2N} & \cos\psi_{3N} & \cdots & 1 \end{bmatrix} \delta\!\left(\begin{bmatrix} \|x_1\| \\ \|x_2\| \\ \vdots \\ \|x_N\| \end{bmatrix}\right) \\
&\triangleq\; \delta^2(G)^{1/2}\;\Psi\;\delta^2(G)^{1/2}
\end{aligned} \tag{342}$$

where ψ_{ij} is the angle between vectors x_i and x_j, and where δ^2 denotes a diagonal matrix in this case. Distance-square d_{ij} (330) is related to Gram matrix entries $G^T = G \triangleq [g_{ij}]$,

$$d_{ij} = g_{ii} + g_{jj} - 2g_{ij} \tag{343}$$

hence the linear EDM definition

$$\begin{array}{c}\mathbf{D}(G) \;\triangleq\; \delta(G)\mathbf{1}^T + \mathbf{1}\delta(G)^T - 2G \;\in \mathbb{EDM}^N \\ \Leftrightarrow \\ G \succeq 0\end{array} \tag{344}$$

We note from (342) that positive semidefiniteness of the *inter-point angle matrix* Ψ implies positive semidefiniteness of the Gram matrix G ; [1, §8.3]

$$\Psi \succeq 0 \;\Rightarrow\; G \succeq 0 \tag{345}$$

The EDM cone can be described,

$$\mathbb{EDM}^N = \left\{\mathbf{D}(G) \mid G \in \mathbb{S}_+^N\right\} \tag{346}$$

4.4.2.1 First point at the origin

Consider the calculation $(I - \mathbf{1}e_1^T)\mathbf{D}(G)(I - e_1\mathbf{1}^T)$; setting $\mathbf{D}(G) = D$ for convenience,

$$-\left(D - (De_1\mathbf{1}^T + \mathbf{1}e_1^T D)\right)\tfrac{1}{2} = G - (Ge_1\mathbf{1}^T + \mathbf{1}e_1^T G) + \mathbf{1}e_1^T Ge_1\mathbf{1}^T \tag{347}$$

where

$$e_1 \triangleq \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{348}$$

is the first vector from the standard basis. Under the assumption the first point x_1 in the unknown list X resides at the origin,

$$Xe_1 = \mathbf{0} \;\Leftrightarrow\; Ge_1 = \mathbf{0} \tag{349}$$

then it follows for D an EDM,

$$\begin{aligned} G &= -\left(D - (De_1\mathbf{1}^T + \mathbf{1}e_1^T D)\right)\tfrac{1}{2}\;, \qquad x_1 = \mathbf{0} \\ &= -\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix}^T D \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix}\tfrac{1}{2} \\ &= \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix} \end{aligned} \tag{350}$$

where

$$I - e_1\mathbf{1}^T = \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} \tag{351}$$

is a nonorthogonal projector (§E.1). From this we get the first matrix criterion for an EDM, first proved by Schoenberg in 1935; [87]

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \left\{ \begin{array}{c} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array} \right. \tag{352}$$

We provide a rigorous more geometric proof in §4.9.

By substituting $G = \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix}$ (350) into $\mathbf{D}(G)$ (344), assuming $x_1 = \mathbf{0}$,

$$D = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big) \end{bmatrix} \mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big)^T \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix} \tag{353}$$

4.4.2.2 0 geometric center

Now consider the calculation $(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T)\mathbf{D}(G)(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T)$ [88, §1] under the assumption that the *geometric center* (§4.5.1.0.1) of a corresponding list is the origin;

$$X\mathbf{1} = \mathbf{0} \;\Leftrightarrow\; G\mathbf{1} = \mathbf{0} \tag{354}$$

Setting $\mathbf{D}(G) = D$ for convenience,

$$\begin{aligned} G &= -\big(D - \tfrac{1}{N}(D\mathbf{1}\mathbf{1}^T + \mathbf{1}\mathbf{1}^T D) + \tfrac{1}{N^2}\mathbf{1}\mathbf{1}^T D \mathbf{1}\mathbf{1}^T\big)\tfrac{1}{2}\,, \qquad X\mathbf{1} = \mathbf{0} \\ &= -VDV\tfrac{1}{2} \end{aligned} \tag{355}$$

where properties of the auxiliary matrix

$$V \triangleq I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \tag{996}$$

are found in §B.4. From this, the more popular form of Schoenberg's criterion:

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \left\{ \begin{array}{c} -VDV \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array} \right. \tag{356}$$

Of particular utility when $D\in\mathbb{EDM}^N$ is the fact, (§B.4.2 no.11) (330)

$$\begin{aligned}\operatorname{tr}\!\left(-VDV\tfrac{1}{2}\right) &= \tfrac{1}{2N}\sum_{i,j} d_{ij} &&= \tfrac{1}{2N}\operatorname{vec}(X)^T\left(\sum_{i,j}\Phi_{ij}\right)\operatorname{vec}X \\ &= \operatorname{tr}G &&= \sum_{\ell=1}^{N}\|x_\ell\|^2\,, \qquad\qquad X\mathbf{1}=\mathbf{0}\end{aligned} \tag{357}$$

where $\sum\Phi_{ij}\in\mathbb{S}_+^{nN}$ (331), therefore convex in $\operatorname{vec}X$. We will find this trace useful as a heuristic to minimize affine dimension of an unknown list arranged columnar in X, (§7.2.2) but it tends to facilitate realization of a list configuration having least energy; *id est*, it compacts a reconstructed list by minimizing total norm-square of the vertices.

By substituting $G=-VDV\frac{1}{2}$ (355) into $\mathbf{D}(G)$ (344), assuming $X\mathbf{1}=\mathbf{0}$,

$$D=\delta\!\left(-VDV\frac{1}{2}\right)\mathbf{1}^T+\mathbf{1}\,\delta\!\left(-VDV\frac{1}{2}\right)^T-2\left(-VDV\frac{1}{2}\right) \tag{358}$$

These relationships will allow combination of distance and Gram constraints in any optimization problem we may pose:

- Constraining all diagonal entries of the Gram matrix to 1, for example, is equivalent to the constraint that all points lie on a hypersphere centered at the origin. Any further constraint on the Gram matrix then applies only to inter-point angle Ψ.

- More generally, constraint on inter-point angle Ψ can be accomplished by fixing all the individual point lengths $\delta(G)^{1/2}$; then

$$\Psi=-\frac{1}{2}\delta^2(G)^{-1/2}VDV\delta^2(G)^{-1/2} \tag{359}$$

  When $\delta^2(G)$ is nonsingular, then $\Psi\succeq 0 \Leftrightarrow G\succeq 0$. (§A.3.1.0.5)

4.4.2.2.1 Example. *Vector constraints via Gram matrix.*
Capitalizing again on identity (355) relating Gram and EDM matrices as in Example 4.4.2.2.3, a constraint set such as

$$\left.\begin{aligned}\operatorname{tr}\!\left(-\tfrac{1}{2}VDVe_ie_i^T\right) &= \|x_i\|^2 &&= \kappa_i \\ \operatorname{tr}\!\left(-\tfrac{1}{2}VDV(e_ie_j^T+e_je_i^T)\tfrac{1}{2}\right) &= x_i^Tx_j &&= \kappa_{ij} \\ \operatorname{tr}\!\left(-\tfrac{1}{2}VDVe_je_j^T\right) &= \|x_j\|^2 &&= \kappa_j\end{aligned}\right\} \tag{360}$$

(given constants κ_i , κ_{ij} , κ_j) unambiguously relates list member x_i to x_j to within an isometry through the inner product identity

$$\cos\psi_{ij} = \frac{x_i^T x_j}{\|x_i\|\,\|x_j\|} \tag{361}$$

$\square$

Consider the academic problem of finding a Gram matrix subject to some constraints on the entries of the corresponding EDM:

$$\begin{array}{rl} \text{find} & -VDV\frac{1}{2} \in \mathbb{S}^N \\ \text{subject to} & \left\langle (e_i e_j^T + e_j e_i^T)\frac{1}{2}\,,\, D\right\rangle = \hat{d}_{ij}\,, \quad i,j=1\ldots N\,, \quad i<j \\ & -VDV \succeq 0 \end{array} \tag{362}$$

where the $\hat{d}_{ij}$ are given nonnegative constants; EDM D can, of course, be replaced with the equivalent Gram form (358) in that constraint. Barvinok's proposition predicts[4.7] for $N>1$,[4.8]

$$\operatorname{rank} VDV \leq \left\lfloor \frac{\sqrt{8(N(N-1)/2)+1}-1}{2} \right\rfloor = N-1 \tag{363}$$

Of interest in this problem formulation (362) is the lack of explicit constraints on the main diagonal of EDM $D\in\mathbb{S}_{\mathbf{0}}^N$; finding the Gram matrix is logically disjoint from this EDM constraint.

Choice and number of constraints can affect uniqueness and affine dimension of solution as shown in this next example.

4.4.2.2.2 Example. *Trilateration in small wireless sensor network.* Given three known absolute point positions in $\mathbb{R}^{\mathbf{2}}$ (three *anchors* $\hat{x}_2\,, \hat{x}_3\,, \hat{x}_4$) and only one unknown point (one *sensor* $x_1 \in \mathbb{R}^{\mathbf{2}}$), it is easy to unambiguously determine the sensor's relative position when given its noiseless distance-square $\hat{d}_{i1}$ from only two of the three anchors under the assumption $x_1=\mathbf{0}$ (without loss of generality). The problem can be expressed as a feasibility problem in terms of the Gram matrix (350):

[4.7] Conditions required for tightening the upper bound as in (153) are not met here because the feasible set is not bounded.

[4.8] $-VDV|_{N\leftarrow 1} = 0$ (§B.4.1).

$$\begin{array}{rll}
\text{find} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{S}^{\mathbf{3}} & \\
\text{subject to} & \operatorname{tr}\big(D(e_i e_1^T + e_1 e_i^T)\tfrac{1}{2}\big) = \hat{d}_{i1}\,, & i=2,3 \\
& \operatorname{tr}\left(\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix}(e_i e_j^T + e_j e_i^T)\tfrac{1}{2}\right) = \hat{x}_i^T \hat{x}_j\,, & 2 \leq i < j = 3,4 \\
& \operatorname{tr}\left(\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix}\right) = \sum_{i=2}^{4} \|\hat{x}_i\|^2 & \\
& \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix} \succeq 0 &
\end{array} \tag{364}$$

having a total of six affine equality constraints, where the constraint on distance-square $\hat{d}_{i1}$ can be equivalently written as a constraint on the Gram matrix by substituting (353).

This Platonic feasibility problem explores the convex intersection of a face $\mathbb{S}_+^{\mathbf{3}}$ [23, §II.12] of the positive semidefinite cone in $\mathbb{S}^{\mathbf{4}}$ with an affine set in the proper subspace of symmetric matrices $\mathbb{S}^{\mathbf{3}}$, the intersection of six hyperplanes in isomorphic $\mathbb{R}^{\mathbf{6}}$. Because of the bounding Σ constraint (whose normal is I), there exists a feasible Gram matrix whose rank is bounded above by Barvinok's Proposition 2.6.6.4.1 (153); more precisely, if the feasible set is nonempty and nontrivial, then there exists a solution to (364) having affine dimension 1 or 2.[4.9] The sensor is thereby constrained to lie in the affine hull of the anchors. Having found the Gram matrix, we can locate the sensor relative to the anchors simply by using a *Cholesky factorization* (§4.10).

The sensor's relative location is unique when the six hyperplanes intersect at a point in isomorphic $\mathbb{R}^{\mathbf{6}}$ belonging to the positive semidefinite cone. The hyperplane intersection is a point whenever their normals are linearly independent in $\mathbb{R}^{\mathbf{6}}$. To find each normal for the two $\hat{d}_{i1}$ hyperplanes, we substitute the Gram-form definition (344) for D and then utilize the self-adjointness property (813) of the linear diagonal operator δ; for $i=2,3$,

$$\left\langle \delta(G)\mathbf{1}^T + \mathbf{1}\delta(G)^T - 2G\,,\, (e_i e_1^T + e_1 e_i^T)\tfrac{1}{2}\right\rangle = \left\langle G\,,\, \delta\big((e_i e_1^T + e_1 e_i^T)\mathbf{1}\big) - (e_i e_1^T + e_1 e_i^T)\right\rangle \tag{365}$$

The first row and column for these and the remaining four constraint normals in $\mathbb{S}^{\mathbf{4}}$ are truncated because, for $n>m$,

$$\{x \in \mathbb{R}^n \mid a^T x = b\} \cap \mathbb{R}^m = \{x \in \mathbb{R}^m \mid a(1:m)^T x = b\} \tag{366}$$

[4.9] Intuitively, the bounding constraint might, for example, be met by rotating a planar configuration of four points in $\mathbb{R}^{\mathbf{3}}$.

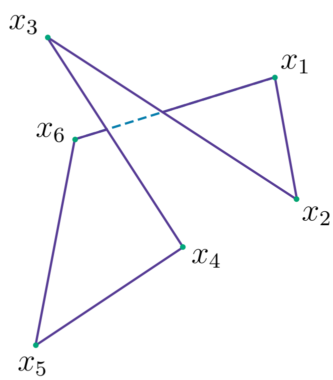


Figure 4.3: Arbitrary hexagon in $\mathbb{R}^3$ whose vertices are labelled clockwise.

These six truncated normals in isometrically isomorphic $\mathbb{R}^6$ are arranged columnar in a matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{367}$$

whose rank is obviously 6 independent of the problem data. This means the isometric realization is always unique when it exists, and if the nonempty feasible set consisting of one positive semidefinite point is nonzero, then the affine dimension (§4.7.2) of this solution must be 1 or 2 by Barvinok's proposition. □

4.4.2.2.3 Example. *Hexagon.* Barvinok [89, §2.6] poses a problem in *geometric realizability* of an arbitrary hexagon (Figure **4.3**) having:

1. prescribed (one-dimensional) face-lengths,
2. prescribed angles between the three pairs of opposing faces, and
3. a constraint on the sum of norm-square of each and every vertex;

ten affine equality constraints in all on the Gram matrix $G \in \mathbb{S}^{\mathbf{6}}$. Let's realize this as a convex *feasibility problem* (with constraints written in the same order) under the assumption of $\mathbf{0}$ geometric center:

$$\begin{array}{rll}\text{find} & -VDV\frac{1}{2} \in \mathbb{S}^{\mathbf{6}} & \\ \text{subject to} & \operatorname{tr}\big(D(e_i e_j^T + e_j e_i^T)\frac{1}{2}\big) \,=\, l_{ij}^2\;, & j-1 = (i=1\ldots 6) \bmod 6 \\ & \operatorname{tr}\big(-\frac{1}{2}VDV(A_i + A_i^T)\frac{1}{2}\big) \,=\, \cos\varphi_i\;, & i=1\ldots 3 \\ & \operatorname{tr}(-\frac{1}{2}VDV) = 1 & \\ & -VDV \succeq 0 & \end{array} \tag{368}$$

where, for $A_i \in \mathbb{R}^{\mathbf{6}\times\mathbf{6}}$,

$$\begin{array}{l} A_1 = (e_1 - e_6)(e_3 - e_4)^T/(l_{61}l_{34}) \\ A_2 = (e_2 - e_1)(e_4 - e_5)^T/(l_{12}l_{45}) \\ A_3 = (e_3 - e_2)(e_5 - e_6)^T/(l_{23}l_{56}) \end{array} \tag{369}$$

and where the first constraint on length-square l_{ij}^2 can be equivalently written as a constraint on the Gram matrix by substituting (358). We show how to numerically solve such a problem by alternating projection in §E.9.2.1.1. Barvinok's Proposition 2.6.6.4.1 asserts the existence of a list corresponding to Gram matrix G solving this feasibility problem whose corresponding affine dimension (§4.7.2) does not exceed 3 because the convex feasible set[4.10] is bounded by the third constraint. □

4.4.3 Inner-product form EDM definition

Equivalent to (330) is [90, §1-7] [26, §3.2]

$$\begin{aligned} d_{ij} \;&=\; d_{ik} + d_{kj} - 2\sqrt{d_{ik}d_{kj}}\cos\theta_{ikj} \\ &=\; \begin{bmatrix}\sqrt{d_{ik}} & \sqrt{d_{kj}}\end{bmatrix} \begin{bmatrix} 1 & -e^{\imath\theta_{ikj}} \\ -e^{-\imath\theta_{ikj}} & 1 \end{bmatrix} \begin{bmatrix}\sqrt{d_{ik}} \\ \sqrt{d_{kj}}\end{bmatrix} \end{aligned} \tag{370}$$

called the *law of cosines*, where $\imath \overset{\Delta}{=} \sqrt{-1}\,,\;\; i,k,j$ are positive integers, and θ_{ikj} is the angle at vertex x_k formed by vectors $x_i - x_k$ and $x_j - x_k$;

$$\cos\theta_{ikj} \;=\; \frac{\frac{1}{2}(d_{ik} + d_{kj} - d_{ij})}{\sqrt{d_{ik}d_{kj}}} \;=\; \frac{(x_i - x_k)^T(x_j - x_k)}{\|x_i - x_k\|\,\|x_j - x_k\|} \tag{371}$$

[4.10] the presumably nonempty set of all points D solving this feasibility problem.

where the numerator forms an inner product of vectors. Distance-square $d_{ij}\left(\begin{bmatrix}\sqrt{d_{ik}}\\ \sqrt{d_{kj}}\end{bmatrix}\right)$ is a convex quadratic function[4.11] on $\mathbb{R}^{\mathbf{2}}_+$ whereas $d_{ij}(\theta_{ikj})$ is quasiconvex (§3.2) minimized over domain $-\pi\leq\theta_{ikj}\leq\pi$ by $\theta^\star_{ikj}=0$, we get the *Pythagorean theorem* when $\theta_{ikj}=\pm\pi/2$, and $d_{ij}(\theta_{ikj})$ is maximized when $\theta^\star_{ikj}=\pm\pi$;

$$\begin{array}{rll} d_{ij} =& \left(\sqrt{d_{ik}}\,+\sqrt{d_{kj}}\,\right)^2, & \theta_{ikj} = \pm\pi\\ d_{ij} =& d_{ik}+d_{kj}\,, & \theta_{ikj} = \pm\frac{\pi}{2}\\ d_{ij} =& \left(\sqrt{d_{ik}}\,-\sqrt{d_{kj}}\,\right)^2, & \theta_{ikj} = \quad 0 \end{array} \tag{372}$$

so

$$|\sqrt{d_{ik}}\,-\sqrt{d_{kj}}\,| \;\leq\; \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}}\,+\sqrt{d_{kj}} \tag{373}$$

Hence the triangle inequality, axiom 4 of the Euclidean metric, holds for any EDM D.

We may construct the inner-product form of the EDM definition for matrices by evaluating (370) for $k=1$: By defining

$$\Theta^T\Theta \triangleq \begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214} & \cdots & \sqrt{d_{12}d_{1N}}\cos\theta_{21N}\\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & \cdots & \sqrt{d_{13}d_{1N}}\cos\theta_{31N}\\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14} & \ddots & \sqrt{d_{14}d_{1N}}\cos\theta_{41N}\\ \vdots & \vdots & \ddots & \ddots & \vdots\\ \sqrt{d_{12}d_{1N}}\cos\theta_{21N} & \sqrt{d_{13}d_{1N}}\cos\theta_{31N} & \sqrt{d_{14}d_{1N}}\cos\theta_{41N} & \cdots & d_{1N} \end{bmatrix} \in \mathbb{S}^{N-1} \tag{374}$$

then any EDM may be expressed

$$\mathbf{D}(\Theta) \triangleq \begin{bmatrix} 0\\ \delta(\Theta^T\Theta) \end{bmatrix}\mathbf{1}^T + \mathbf{1}\begin{bmatrix}0 & \delta(\Theta^T\Theta)^T\end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T\\ \mathbf{0} & \Theta^T\Theta \end{bmatrix} \;\in \mathbb{EDM}^N \tag{375}$$

$$\mathbb{EDM}^N = \left\{\mathbf{D}(\Theta) \mid \Theta\in\mathbb{R}^{n\times N-1}\right\} \tag{376}$$

for which all Euclidean axioms hold. The entries of $\Theta^T\Theta$ result from inner products as in (371); *id est*,

$$\Theta = [\,x_2-x_1 \quad x_3-x_1 \quad \cdots \quad x_N-x_1\,] \in \mathbb{R}^{n\times N-1} \tag{377}$$

4.11 $\begin{bmatrix} 1 & -e^{\imath\theta_{ikj}}\\ -e^{-\imath\theta_{ikj}} & 1 \end{bmatrix} \succeq 0$, having eigenvalues $\{0,2\}$. Minimum is achieved for $\begin{bmatrix}\sqrt{d_{ik}}\\ \sqrt{d_{kj}}\end{bmatrix} = \begin{cases} \mu\mathbf{1}\,, & \mu\geq 0\,,\ \theta_{ikj}=0\\ \mathbf{0}\,, & -\pi\leq\theta_{ikj}\leq\pi\,,\ \theta_{ikj}\neq 0 \end{cases}$. (§D.2.1, [1, exmp.4.5])

The inner product $\Theta^T\Theta$ is obviously related to the Gram matrix (342),

$$G = \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Theta^T\Theta \end{bmatrix}, \qquad x_1 = \mathbf{0} \tag{378}$$

For $\mathbf{D}(\Theta) = D$ and no constraint on the list X, (*confer* (350) (355))

$$\Theta^T\Theta = -V_{\mathcal{N}}^T D V_{\mathcal{N}} \ \in \mathbb{R}^{N-1\times N-1} \tag{379}$$

4.4.3.1 Relative-angle form

Like $\mathbf{D}(X)$ (333), $\mathbf{D}(\Theta)$ will make an EDM for any $\Theta \in \mathbb{R}^{n\times N-1}$, it is neither a convex function of Θ (§4.4.3.2), and it is homogeneous in the sense (336). Scrutinizing $\Theta^T\Theta$ we find that because of the arbitrary choice $k=1$, distances therein are all with respect to point x_1. Similarly, relative angles in $\Theta^T\Theta$ are between all vector pairs having vertex x_1. Yet picking arbitrary θ_{i1j} to fill $\Theta^T\Theta$ will not necessarily make an EDM; $\Theta^T\Theta$ must be positive semidefinite.

$$\Theta^T\Theta \;=\; \delta(\sqrt{d}\,)\,\Omega\,\delta(\sqrt{d}\,) \;\triangleq$$

$$\begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \begin{bmatrix} 1 & \cos\theta_{213} & \cdots & \cos\theta_{21N} \\ \cos\theta_{213} & 1 & \ddots & \cos\theta_{31N} \\ \vdots & \ddots & \ddots & \vdots \\ \cos\theta_{21N} & \cos\theta_{31N} & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \tag{380}$$

Expression $\mathbf{D}(\Theta)$ defines an EDM for any positive semidefinite *relative-angle matrix*

$$\Omega \;=\; [\cos\theta_{i1j}\,,\ i,j = 2\ldots N] \in \mathbb{S}^{N-1} \tag{381}$$

and any nonnegative distance vector

$$\sqrt{d} \;=\; [\sqrt{d_{1j}}\,,\ j = 2\ldots N] \;=\; \sqrt{\delta(\Theta^T\Theta)} \in \mathbb{R}^{N-1} \tag{382}$$

because (§A.3.1.0.5)

$$\Omega \succeq 0 \;\Rightarrow\; \Theta^T\Theta \succeq 0 \tag{383}$$

The decomposition (380) and the *relative-angle matrix inequality* $\Omega \succeq 0$ lead to a different expression of the inner-product form EDM definition (375):

$$\mathbf{D}(\Omega\,,d) \;\triangleq\; \begin{bmatrix} 0 \\ d \end{bmatrix} \mathbf{1}^T + \mathbf{1}\,[0 \quad d^T] - 2\,\delta\!\left(\begin{bmatrix} 0 \\ \sqrt{d} \end{bmatrix}\right) \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Omega \end{bmatrix} \delta\!\left(\begin{bmatrix} 0 \\ \sqrt{d} \end{bmatrix}\right) \;\in\; \mathbb{EDM}^N \tag{384}$$

$$\mathbb{EDM}^N = \left\{\mathbf{D}(\Omega\,,d) \mid \Omega \succeq 0,\ \sqrt{d} \succeq 0\right\} \tag{385}$$

In the particular circumstance $x_1 = \mathbf{0}$, we can relate inter-point angle matrix Ψ from the Gram-form in (342) to relative-angle matrix Ω in (380). Thus,

$$\Psi \equiv \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Omega \end{bmatrix}, \qquad x_1 = \mathbf{0} \tag{386}$$

4.4.3.2 Inner-product form $-V_{\mathcal{N}}^T\mathbf{D}(\Theta)V_{\mathcal{N}}$ convexity

We saw that d_{ij} is a convex quadratic function of $\begin{bmatrix}\sqrt{d_{ik}} \\ \sqrt{d_{kj}}\end{bmatrix}$ and a quasiconvex function of θ_{ikj}. Here the situation for the inner-product form $\mathbf{D}(\Theta)$ (375) of the EDM definition is identical to that in §4.4.1: $-\mathbf{D}(\Theta)$ is not a quasiconvex function of Θ by the same reasoning, and from (379)

$$-V_{\mathcal{N}}^T\mathbf{D}(\Theta)V_{\mathcal{N}} = \Theta^T\Theta \tag{387}$$

is a convex quadratic function of Θ on the domain $\mathbb{R}^{n\times N-1}$ achieving its minimum at $\Theta = 0$.

4.4.3.3 Inner-product form conclusion

We deduce that knowledge of inter-point distance is equivalent to knowledge of distance and angle from the perspective of one point, x_1 in our chosen case. The total amount of information in $\Theta^T\Theta$, $N(N-1)/2$, is unchanged[4.12] with respect to EDM D.

4.5 Invariance

When D is an EDM, there exist an infinite number of corresponding N-point lists X (54) in Euclidean space. All those lists are related by isometric transformation: rotation, reflection, and translation (*offset* or *shift*).

[4.12] The reason for the amount $O(N^2)$ information is because of the relative measurements. The use of a fixed reference in the measurement of angles and distances would reduce the required information but is antithetical. In the particular case $n = 2$, for example, ordering all points x_ℓ in a length-N list by increasing angle of vector $x_\ell - x_1$ with respect to $x_2 - x_1$, θ_{i1j} becomes equivalent to $\sum\limits_{k=i}^{j-1}\theta_{k,1,k+1} \leq 2\pi$ and the amount of information is reduced to $2N-3$; rather, $O(N)$.

4.5.1 Translation

Any translation common among all the points x_ℓ in a list will be cancelled in the formation of each d_{ij} . Proof follows directly from (330). Knowing that translation α in advance, we may remove it from the list constituting the columns of X by subtracting $\alpha\mathbf{1}^T$. Then it stands to reason by definition (333) of an EDM, for any translation $\alpha\in\mathbb{R}^n$,

$$\mathbf{D}(X-\alpha\mathbf{1}^T)=\mathbf{D}(X) \tag{388}$$

In words, inter-point distances are unaffected by offset; EDM D is *translation invariant.* When $\alpha=x_1$ in particular,

$$\mathbf{D}(X-x_1\mathbf{1}^T) \;=\; \mathbf{D}(X-Xe_1\mathbf{1}^T) \;=\; \mathbf{D}\big(X\begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix}\big) \;=\; \mathbf{D}(X) \tag{389}$$

4.5.1.0.1 Example. *Translating geometric center to origin.*
We might choose to shift the geometric center α_g of an N-point list $\{x_\ell\}$ arranged columnar in X to the origin; [47] [91]

$$\alpha \;=\; \alpha_g \;\triangleq\; Xb_g \;\triangleq\; \frac{1}{N}X\mathbf{1}\in\mathcal{P}\subseteq\mathcal{A} \tag{390}$$

If we were to associate a point-mass m_ℓ with each of the points x_ℓ in the list, then their *center of mass* (or *gravity*) would be $(\sum x_\ell\, m_\ell)\,/\sum m_\ell$. The geometric center is the same as the center of mass under the assumption of uniform mass density across points. [79] The geometric center always lies in the convex hull $\mathcal{P}$ of the list; *id est*, $\alpha_g\in\mathcal{P}$ because $b_g^T\mathbf{1}=1$ and $b_g\succeq 0$. Subtracting the geometric center from every list member,

$$X-\alpha_g\mathbf{1}^T \;=\; X-\frac{1}{N}X\mathbf{1}\mathbf{1}^T \;=\; X(I-\frac{1}{N}\mathbf{1}\mathbf{1}^T) \;=\; XV\in\mathbb{R}^{n\times N} \tag{391}$$

So we have (*confer* (333))

$$\mathbf{D}(X) \;=\; \mathbf{D}(XV) \;=\; \delta(V^TX^TXV)\mathbf{1}^T+\mathbf{1}\delta(V^TX^TXV)^T-2V^TX^TXV \;\in\; \mathbb{EDM}^N \tag{392}$$

$\square$

More generally, any b from $\alpha=Xb$ chosen such that $b^T\mathbf{1}=1$, makes an auxiliary V-matrix. (§B.4.5)

For the inner-product form EDM definition $\mathbf{D}(\Theta)$ (375) and $\alpha \in \mathbb{R}^n$, it generally holds

$$\mathbf{D}(\Theta - \alpha\mathbf{1}^T) \neq \mathbf{D}(\Theta) \tag{393}$$

But because (377)

$$\Theta = X\sqrt{2}V_{\mathcal{N}} \tag{394}$$

and for the list form EDM definition (333)

$$\mathbf{D}(X - x_1\mathbf{1}^T) \;=\; \mathbf{D}\big(X[\,\mathbf{0}\quad \sqrt{2}V_{\mathcal{N}}\,]\big) \;=\; \mathbf{D}([\mathbf{0}\;\;\Theta]) \;=\; \mathbf{D}(X) \tag{395}$$

then we have translation invariance in the following sense:

$$\mathbf{D}\big([\,-\alpha\quad \Theta - \alpha\mathbf{1}^T\,]\big) \;=\; \mathbf{D}([\mathbf{0}\;\;\Theta]) \tag{396}$$

4.5.1.1 Gram form invariance

The Gram form EDM definition (344) exhibits invariance to translation by a *doublet* (§B.2) $u\mathbf{1}^T + \mathbf{1}u^T$;

$$\mathbf{D}(G) = \mathbf{D}\big(G - (u\mathbf{1}^T + \mathbf{1}u^T)\big) \tag{397}$$

because, for any $u \in \mathbb{R}^N$, $\mathbf{D}(u\mathbf{1}^T + \mathbf{1}u^T) = \mathbf{0}$.

4.5.2 Rotation/Reflection

Rotation of the list $X \in \mathbb{R}^{n\times N}$ about some arbitrary point $\alpha \in \mathbb{R}^n$, or reflection through some affine subset containing α is accomplished via $QX - \alpha\mathbf{1}^T$, where Q is an orthogonal matrix (§B.5).

We rightfully expect

$$\mathbf{D}(QX - \alpha\mathbf{1}^T) = \mathbf{D}\big(Q(X - \alpha\mathbf{1}^T)\big) = \mathbf{D}(QX) = \mathbf{D}(X) \tag{398}$$

Because $\mathbf{D}(X)$ is translation invariant, we may safely ignore offset and consider only the impact of matrices that pre-multiply X. Inter-point distances are unaffected by rotation or reflection; we say, EDM D is *rotation/reflection invariant.* Proof follows from the fact, $Q^T = Q^{-1} \Rightarrow X^TQ^TQX = X^TX$. So (398) follows directly from (333).

The class of pre-multiplying matrices for which inter-point distances are unaffected is a little more broad than orthogonal matrices. Looking at EDM definition (333), it appears that any matrix Q_p such that

$$X^T Q_p^T Q_p X = X^T X \tag{399}$$

will have the property

$$\mathbf{D}(Q_p X) = \mathbf{D}(X) \tag{400}$$

An example is skinny $Q_p \in \mathbb{R}^{m\times n}$ $(m>n)$ having orthonormal columns.

4.5.2.1 Inner-product form invariance

Likewise, $\mathbf{D}(\Theta)$ (375) is rotation/reflection invariant;

$$\mathbf{D}(Q\Theta) = \mathbf{D}(\Theta) \tag{401}$$

so (399) and (400) would similarly apply.

4.5.3 Invariance conclusion

In the construction of an EDM, absolute rotation, reflection, and translation information is lost. Given an EDM, reconstruction of point position (§4.10, the list X) can be guaranteed correct only in affine dimension r; *id est*, in relative position. Given a noiseless complete EDM, this *isometric reconstruction* is unique in so far as every realization of a corresponding list X is *congruent*: (§4.6)

4.6 Injectivity of D. Unique reconstruction

Injectivity implies uniqueness of an isometric reconstruction; hence we endeavor to demonstrate it.

EDM definitions $\mathbf{D}(X)$ (333), $\mathbf{D}(G)$ (344), and $\mathbf{D}(\Theta)$ (375) are many-to-one surjections (§4.5) onto the same range; the EDM cone (§5): Independent of Euclidean dimension n,

$$\begin{aligned}\mathbb{EDM}^N &= \left\{\mathbf{D}(X) : \mathbb{R}^{n\times N} \rightarrow \mathbb{S}_{\mathbf{0}}^N \mid X \in \mathbb{R}^{n\times N}\right\}\\ &= \left\{\mathbf{D}(G) : \mathbb{S}^N \rightarrow \mathbb{S}_{\mathbf{0}}^N \mid G \in \mathbb{S}_+^N\right\}\\ &= \left\{\mathbf{D}(\Theta) : \mathbb{R}^{n\times N-1} \rightarrow \mathbb{S}_{\mathbf{0}}^N \mid \Theta \in \mathbb{R}^{n\times N-1}\right\}\end{aligned} \tag{402}$$

4.6.0.1 Inner-product form injectivity and surjectivity

Substituting $\Theta^T\Theta \leftarrow -V_{\mathcal{N}}^T D V_{\mathcal{N}}$ (387) into the inner-product form EDM definition (375), $\mathbf{D}(\Theta)$ may be further decomposed: (*confer* (353))

$$\mathbf{D}(D) = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big) \end{bmatrix} \mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big)^T \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix} \tag{403}$$

This linear operator $\mathbf{D}$ is an *injective* (one-to-one) map of the EDM cone onto itself. Yet when its domain is instead the entire symmetric hollow subspace $\mathbb{S}_{\mathbf{0}}^N = \operatorname{aff}\mathbb{EDM}^N$ (633), $\mathbf{D}(D)$ becomes an injective map onto that same subspace. Proof follows directly from the fact: linear $\mathbf{D}$ has no nullspace on $\mathbb{S}_{\mathbf{0}}^N$. [92, §A.1]

4.6.0.2 Gram-form bijectivity

The Gram-form

$$\mathbf{D}(G) \;=\; \delta(G)\mathbf{1}^T + \mathbf{1}\delta(G)^T - 2G \tag{344}$$

is an injective map, for example, on the subspace of symmetric matrices having all zeros in the first row and column

$$\begin{aligned} \mathbb{S}_{\mathbf{1}}^N &\triangleq \{G\in\mathbb{S}^N \mid Ge_1 = \mathbf{0}\} \\ &= \left\{\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} Y \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} \mid Y\in\mathbb{S}^N\right\} \end{aligned} \tag{1296}$$

because it obviously has no nullspace there. Since $Ge_1 = \mathbf{0}$ (349) means the first point in the list X resides at the origin (342), then $\mathbf{D}(G)$ on $\mathbb{S}_{\mathbf{1}}^N \cap \mathbb{S}_+^N$ must be surjective onto $\mathbb{EDM}^N$.

Because it has no nullspace on the geometric center subspace (§E.7.1.0.2), $\mathbf{D}(G)$ is also injective on that subspace

$$\begin{aligned} \mathbb{S}_g^N &\triangleq \{G\in\mathbb{S}^N \mid G\mathbf{1} = \mathbf{0}\} \\ &= \{G\in\mathbb{S}^N \mid \mathcal{N}(G) \supseteq \mathbf{1}\} \;=\; \{G\in\mathbb{S}^N \mid \mathcal{R}(G) \subseteq \mathcal{N}(\mathbf{1}^T)\} &&(1292) \\ &= \{VYV \mid Y\in\mathbb{S}^N\} \subset \mathbb{S}^N &&(1293) \end{aligned}$$

where $V\in\mathbb{S}^N$ is the auxiliary orthogonal projector having $\mathcal{R}(V)=\mathcal{N}(\mathbf{1}^T)$ (B.4.1).

To prove injectivity of $\mathbf{D}(G)$ on $\mathbb{S}_g^N$ (1292) (1293): Any matrix $Y\in\mathbb{S}^N$ can be decomposed into orthogonal components in $\mathbb{S}^N$

$$Y = VYV + (Y - VYV) \tag{404}$$

where $VYV\in\mathbb{S}_g^N$ and $Y-VYV\in\mathbb{S}_g^{N\perp}=\{u\mathbf{1}^T+\mathbf{1}u^T \mid u\in\mathbb{R}^N\}$ (1294). Because of translation invariance (§4.5) and linearity, $\mathbf{D}(Y-VYV)=\mathbf{0}$ hence $\mathcal{N}(\mathbf{D}(Y))\supseteq\mathbb{S}_g^{N\perp}$. It remains only to show $\mathbf{D}(VYV)=\mathbf{0}\Leftrightarrow VYV=\mathbf{0}$ $\big(\Leftrightarrow Y=u\mathbf{1}^T+\mathbf{1}u^T$ for some particular $u\in\mathbb{R}^N\big)$. $\mathbf{D}(VYV)$ will vanish whenever $2VYV=\delta(VYV)\mathbf{1}^T+\mathbf{1}\delta(VYV)^T$. But this implies $\mathcal{R}(\mathbf{1})$ were a subset of $\mathcal{R}(VYV)$ (§B), which is contradictory. We thus have

$$\mathcal{N}(\mathbf{D}(Y)) = \mathbb{S}_g^{N\perp} \tag{405}$$

♦

Since $G\mathbf{1}=\mathbf{0}\Leftrightarrow X\mathbf{1}=\mathbf{0}$ means the list X is geometrically centered at the origin, and because $\mathcal{N}(\mathbf{D}(G))$ is the orthogonal complement $\mathbb{S}_g^{N\perp}$, then $\mathbf{D}(G)$ on $\mathbb{S}_g^N\cap\mathbb{S}_+^N$ must be surjective onto $\mathbb{EDM}^N$.

4.6.1 Inversion of D

Injectivity of linear operator $\mathbf{D}(D)$ (403) suggests inversion of the linear operator

$$\mathbf{V}_{\mathcal{N}}(D) \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}} \tag{406}$$

whose nullspace is $\{u\mathbf{1}^T+\mathbf{1}u^T \mid u\in\mathbb{R}^N\}=\mathbb{S}_g^{N\perp}$ (1294). Thus $\mathbf{V}_{\mathcal{N}}(D)$ is injective on $\mathbb{S}_{\mathbf{0}}^N$ because $\mathbb{S}_g^{N\perp}\cap\mathbb{S}_{\mathbf{0}}^N=\mathbf{0}$. Indeed, revising the argument of that linear operator $\mathbf{D}$,

$$\mathbf{D}\big(-V_{\mathcal{N}}^TDV_{\mathcal{N}}\big) = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^TDV_{\mathcal{N}}\big) \end{bmatrix}\mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^TDV_{\mathcal{N}}\big)^T \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^TDV_{\mathcal{N}} \end{bmatrix} \tag{407}$$

we have, for $D\in\mathbb{S}_{\mathbf{0}}^N$,

$$D = \mathbf{D}\big(\mathbf{V}_{\mathcal{N}}(D)\big) \tag{408}$$

$$-V_{\mathcal{N}}^TDV_{\mathcal{N}} = \mathbf{V}_{\mathcal{N}}\big(\mathbf{D}(-V_{\mathcal{N}}^TDV_{\mathcal{N}})\big) \tag{409}$$

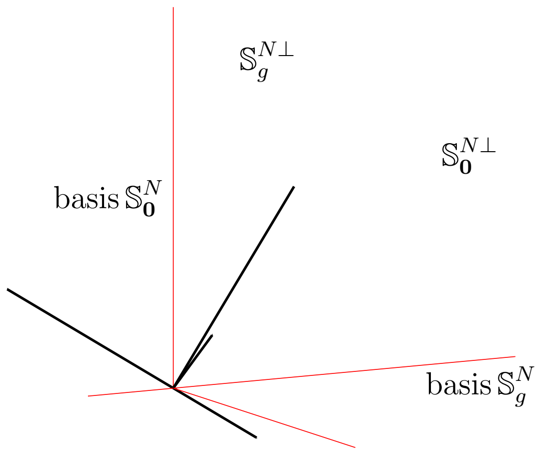


Figure 4.4: Two pairs of orthogonal complements in $\mathbb{S}^N$. $\dim \mathbb{S}_g^N = \dim \mathbb{S}_{\mathbf{0}}^N = N(N-1)/2$ in isomorphic $\mathbb{R}^{N^2}$. Orthogonal projection of the basis for $\mathbb{S}_{\mathbf{0}}^N$ on $\mathbb{S}_g^N$ yields another basis for $\mathbb{S}_g^N$.

or

$$\mathbb{S}_{\mathbf{0}}^N = \mathbf{D}\big(\mathbf{V}_{\mathcal{N}}(\mathbb{S}_{\mathbf{0}}^N)\big) \tag{410}$$

$$-V_{\mathcal{N}}^T \mathbb{S}_{\mathbf{0}}^N V_{\mathcal{N}} = \mathbf{V}_{\mathcal{N}}\big(\mathbf{D}(-V_{\mathcal{N}}^T \mathbb{S}_{\mathbf{0}}^N V_{\mathcal{N}})\big) \tag{411}$$

These operators $\mathbf{V}_{\mathcal{N}}$ and $\mathbf{D}$ are therefore mutual inverses.

Now instead we apply the injective Gram-form operator (344) $\mathbf{D}(G)$. Define the linear *geometric centering operator* (§E.7.1.0.2)

$$\mathbf{V}(D) \triangleq -VDV\frac{1}{2} \tag{412}$$

This orthogonal projector $\mathbf{V}(D)$ has no nullspace on $\mathbb{S}_{\mathbf{0}}^N$ because the projection of $-D/2$ on $\mathbb{S}_g^N$ (1292) can be $\mathbf{0}$ if and only if $D \in \mathbb{S}_g^{N\perp}$; but $\mathbb{S}_g^{N\perp} \cap \mathbb{S}_{\mathbf{0}}^N = \mathbf{0}$. Projector $\mathbf{V}(D)$ is therefore injective hence invertible on $\mathbb{S}_{\mathbf{0}}^N$. We find, for $D \in \mathbb{S}_{\mathbf{0}}^N$, (*confer* (358))

$$\mathbf{D}(-VDV\tfrac{1}{2}) = \delta(-VDV\tfrac{1}{2})\mathbf{1}^T + \mathbf{1}\delta(-VDV\tfrac{1}{2})^T - 2(-VDV\tfrac{1}{2}) \tag{413}$$

id est,

$$D = \mathbf{D}\big(\mathbf{V}(D)\big) \tag{414}$$

$$-VDV = \mathbf{V}\big(\mathbf{D}(-VDV)\big) \tag{415}$$

or

$$\mathbb{S}_{\mathbf{0}}^N = \mathbf{D}\big(\mathbf{V}(\mathbb{S}_{\mathbf{0}}^N)\big) \tag{416}$$

$$-V\mathbb{S}_{\mathbf{0}}^N V = \mathbf{V}\big(\mathbf{D}(-V\mathbb{S}_{\mathbf{0}}^N V)\big) \tag{417}$$

reestablished in §4.10.2.1. These operators $\mathbf{V}$ and $\mathbf{D}$ are mutual inverses.

Further, $-V\mathbb{S}_{\mathbf{0}}^N V/2$ is equivalent to the geometric center subspace $\mathbb{S}_g^N$ in the ambient space of symmetric matrices;

$$\mathbb{S}_g^N \;=\; -V\mathbb{S}^N V/2 \;=\; -V\big(\mathbb{S}_{\mathbf{0}}^N \oplus \mathbb{S}_{\mathbf{0}}^{N\perp}\big)V/2 \;=\; -V\mathbb{S}_{\mathbf{0}}^N V/2 \tag{418}$$

because (51)

$$-V\mathbb{S}_{\mathbf{0}}^N V/2 \;\supseteq\; -V\mathbb{S}_{\mathbf{0}}^{N\perp} V/2 \;=\; -V\delta^2(\mathbb{S}^N)V/2 \tag{419}$$

which holds if and only if $\mathbb{S}_{\mathbf{0}}^{N\perp} \cap \mathbb{S}_g^N = \mathbf{0}$. The geometry is abstracted in Figure **4.4**. Gram-form $\mathbf{D}\big(\mathbb{S}_g^N\big)$ (344) is equivalent to $\mathbb{S}_{\mathbf{0}}^N$; by (416)

$$\mathbf{D}\big(\mathbb{S}_g^N\big) \;=\; \mathbf{D}\big(-V(\mathbb{S}_{\mathbf{0}}^N \oplus \mathbb{S}_{\mathbf{0}}^{N\perp})V/2\big) \;=\; \mathbb{S}_{\mathbf{0}}^N + \mathbf{D}\big(-V\mathbb{S}_{\mathbf{0}}^{N\perp}V/2\big) \;=\; \mathbb{S}_{\mathbf{0}}^N \tag{420}$$

because $\mathbb{S}_{\mathbf{0}}^N \;\supseteq\; \mathbf{D}\big(-V\delta^2(\mathbb{S}^N)V/2\big)$. We have, finally, [93, §2.1] [94, §2] [95, §18.2.1] [96, §2.1]

$$\mathbb{S}_{\mathbf{0}}^N = \mathbf{D}(\mathbb{S}_g^N) \tag{421}$$

$$\mathbb{S}_g^N = \mathbf{V}(\mathbb{S}_{\mathbf{0}}^N) \tag{422}$$

and from the bijectivity results in §4.6.0.2,

$$\mathbb{EDM}^N = \mathbf{D}(\mathbb{S}_g^N \cap \mathbb{S}_+^N) \tag{423}$$

$$\mathbb{S}_g^N \cap \mathbb{S}_+^N = \mathbf{V}(\mathbb{EDM}^N) \tag{424}$$

4.7 Embedding in the affine hull

The affine hull $\mathcal{A}$ (56) of a point list $\{x_\ell\}$, arranged columnar in $X \in \mathbb{R}^{n\times N}$ (54), is identical to the affine hull of that polyhedron $\mathcal{P}$ (60) formed from all convex combinations of the x_ℓ ; [1, §2] [30, §17]

$$\mathcal{A} \;=\; \operatorname{aff} X \;=\; \operatorname{aff} \mathcal{P} \tag{425}$$

Comparing definitions (56) and (60), it becomes obvious that the x_ℓ and their convex hull $\mathcal{P}$ are embedded in their unique affine hull $\mathcal{A}$;

$$\mathcal{A} \supseteq \mathcal{P} \supseteq \{x_\ell\} \tag{426}$$

Recall that affine dimension r is a lower bound on embedding, equal to the dimension of the subspace parallel to that nonempty affine set $\mathcal{A}$ in which the points are embedded. (§2.2.1) We define the dimension of the convex hull $\mathcal{P}$ to be the same as the dimension r of the affine hull $\mathcal{A}$ [30, §2], but r is not necessarily equal to the rank of X (444).

For the particular example illustrated in Figure **4.1**, $\mathcal{P}$ is the triangle plus its relative interior while its three vertices constitute the entire list X. The affine hull $\mathcal{A}$ is the unique plane that contains the triangle, so $r=2$ in that example while the rank of X is 3. Were there only two points in Figure **4.1**, then the affine hull would instead be the unique line passing through them; r would become 1 while the rank would then be 2.

4.7.1 Determining affine dimension

Knowledge of affine dimension r is important because we lose any absolute offset component common to all the generating x_ℓ in $\mathbb{R}^n$ when reconstructing convex polyhedra given only distance information. (§4.5.1) To calculate r, we first eliminate any offset that serves to increase dimensionality of the subspace required to contain $\mathcal{P}$; subtracting $\alpha \in \mathcal{A}$ from every list member will work,

$$X - \alpha\mathbf{1}^T \tag{427}$$

translating $\mathcal{A}$ to the origin:

$$\mathcal{A} - \alpha \;=\; \operatorname{aff}(X - \alpha\mathbf{1}^T) \;=\; \operatorname{aff}(X) - \alpha \tag{428}$$

$$\mathcal{P} - \alpha \;=\; \operatorname{conv}(X - \alpha\mathbf{1}^T) \;=\; \operatorname{conv}(X) - \alpha \tag{429}$$

which follow from their definitions. Because (425) and (426) translate,

$$\mathbb{R}^n \;\supseteq\; \mathcal{A}-\alpha \;=\; \operatorname{aff}(X-\alpha\mathbf{1}^T) \;=\; \operatorname{aff}(\mathcal{P}-\alpha) \;\supseteq\; \mathcal{P}-\alpha \;\supseteq\; \{x_\ell-\alpha\} \tag{430}$$

where from the previous relations it is easily shown

$$\operatorname{aff}(\mathcal{P} - \alpha) = \operatorname{aff}(\mathcal{P}) - \alpha \tag{431}$$

Translating $\mathcal{A}$ neither changes its dimension or the dimension of the embedded polyhedron $\mathcal{P}$; (55)

$$r \stackrel{\Delta}{=} \dim \mathcal{A} = \dim(\mathcal{A} - \alpha) \stackrel{\Delta}{=} \dim(\mathcal{P} - \alpha) = \dim \mathcal{P} \tag{432}$$

For any $\alpha \in \mathbb{R}^n$, (428)-(432) remain true. [30, p.4, p.12] Yet when $\alpha \in \mathcal{A}$, the affine set $\mathcal{A} - \alpha$ becomes a unique subspace of $\mathbb{R}^n$ in which the $\{x_\ell - \alpha\}$ and their convex hull $\mathcal{P} - \alpha$ are embedded (430), and whose dimension is more easily calculated.

4.7.1.0.1 Example. *Translating first list-member to origin.*
Subtracting the first member $\alpha \stackrel{\Delta}{=} x_1$ from every list member will translate their affine hull $\mathcal{A}$ and their convex hull $\mathcal{P}$ and, in particular, $x_1 \in \mathcal{P} \subseteq \mathcal{A}$ to the origin in $\mathbb{R}^n$; *videlicet*,

$$X - x_1\mathbf{1}^T = X - Xe_1\mathbf{1}^T = X(I - e_1\mathbf{1}^T) = X\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} \in \mathbb{R}^{n\times N} \tag{433}$$

where $V_{\mathcal{N}}$ is defined in (339), and e_1 in (348). Applying (430) to (433),

$$\mathbb{R}^n \supseteq \mathcal{R}(XV_{\mathcal{N}}) = \mathcal{A} - x_1 = \operatorname{aff}(X - x_1\mathbf{1}^T) = \operatorname{aff}(\mathcal{P} - x_1) \supseteq \mathcal{P} - x_1 \ni \mathbf{0} \tag{434}$$

where $XV_{\mathcal{N}} \in \mathbb{R}^{n\times N-1}$. Hence

$$r = \dim \mathcal{R}(XV_{\mathcal{N}}) \tag{435}$$

□

Since shifting the geometric center to the origin (§4.5.1.0.1) translates the affine hull to the origin as well, then it must also be true

$$r = \dim \mathcal{R}(XV) \tag{436}$$

For any matrix whose range is $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$ we get the same result; *e.g.*,

$$r = \dim \mathcal{R}(XV_{\mathcal{N}}^{\dagger T}) \tag{437}$$

because $\mathcal{R}(XV) = \{Xz \mid z \in \mathcal{N}(\mathbf{1}^T)\}$ and $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{R}(V_{\mathcal{N}}^{\dagger T})$ (§E). These auxiliary matrices (§B.4.2) are more closely related;

$$V = V_{\mathcal{N}} V_{\mathcal{N}}^{\dagger} \tag{438}$$

4.7.2 Affine dimension r *versus* rank

Now, suppose D is an EDM as in (333) and we pre-multiply by $-V_{\mathcal{N}}^T$ and post-multiply by $V_{\mathcal{N}}$. Then because $V_{\mathcal{N}}^T\mathbf{1}=\mathbf{0}$ (340),

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^T G V_{\mathcal{N}} \in \mathbb{S}^{N-1} \tag{439}$$

where G is the Gram matrix. Similarly pre- and post-multiplying by V,

$$-VDV \;=\; 2VX^TXV \;=\; 2VGV \in \mathbb{S}^N \tag{440}$$

because $V\mathbf{1}=\mathbf{0}$ (997). Likewise, multiplying the inner-product form EDM definition (375),

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \Theta^T\Theta \in \mathbb{S}^{N-1} \tag{379}$$

For any matrix A, $\operatorname{rank} A^TA = \operatorname{rank} A = \operatorname{rank} A^T$. [28, §0.4][4.13] Hence

$$\begin{aligned}\operatorname{rank} VDV \;&=\; \operatorname{rank} VGV \;=\; \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \operatorname{rank} V_{\mathcal{N}}^T G V_{\mathcal{N}}\\ &=\; \operatorname{rank} XV \;=\; \operatorname{rank} XV_{\mathcal{N}} \;=\; \operatorname{rank}\Theta \;=\; r\end{aligned} \tag{441}$$

By *conservation of dimension*, (§A.7.2.0.1)

$$r + \dim \mathcal{N}(V_{\mathcal{N}}^T D V_{\mathcal{N}}) \;=\; N-1 \tag{442}$$

$$r + \dim \mathcal{N}(VDV) \;=\; N \tag{443}$$

The general fact[4.14] (*confer* (363))

$$r \le \min\{n\,,\, N-1\} \tag{444}$$

is evident from (433) but can be visualized in the example illustrated in Figure **4.1**. There we imagine a vector from the origin to each point in the list. Those three vectors are linearly independent in $\mathbb{R}^3$, but the affine dimension r is 2 because the three points lie in a plane. When that plane is translated to the origin, it becomes the only subspace of dimension $r=2$ that can contain the translated triangular polyhedron.

[4.13] For $A\in\mathbb{R}^{m\times n}$, $\mathcal{N}(A^TA)=\mathcal{N}(A)$. [26, §3.3]

[4.14] $\operatorname{rank} X \le \min\{n\,,\, N\}$

4.7.3 Précis

We collect expressions for the affine dimension: for $X\in\mathbb{R}^{n\times N}$,

$$\begin{array}{rl}
r \;\stackrel{\Delta}{=} & \dim(\mathcal{P}-\alpha) \;=\; \dim\mathcal{P} \;=\; \dim\operatorname{conv}X \\
= & \dim(\mathcal{A}-\alpha) \;=\; \dim\mathcal{A} \;=\; \dim\operatorname{aff}X \\
= & \operatorname{rank}(X - x_1\mathbf{1}^T) \;=\; \operatorname{rank}(X-\alpha_g\mathbf{1}^T) \\
= & \operatorname{rank}\Theta \quad (377) \\
= & \operatorname{rank}XV_{\mathcal{N}} \;=\; \operatorname{rank}XV \;=\; \operatorname{rank}XV_{\mathcal{N}}^{\dagger T} \\
= & \operatorname{rank}V_{\mathcal{N}}^TGV_{\mathcal{N}} \;=\; \operatorname{rank}VGV \;=\; \operatorname{rank}V_{\mathcal{N}}^{\dagger}GV_{\mathcal{N}} \\
\left.\begin{array}{rl}
= & \operatorname{rank}V_{\mathcal{N}}^TDV_{\mathcal{N}} \;=\; \operatorname{rank}VDV \;=\; \operatorname{rank}V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}} \quad (\S 4.14.3) \\
= & \operatorname{rank}\Lambda \quad (486) \\
= & N-1-\dim\mathcal{N}\!\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0\end{bmatrix}\right) \;=\; \operatorname{rank}\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0\end{bmatrix} - 2 \quad (447)
\end{array}\right\} & D\in\mathbb{EDM}^N
\end{array} \tag{445}$$

4.7.3.0.1 Theorem. *EDM rank versus affine dimension r.*
[91, §3] [97, §3] For $D\in\mathbb{EDM}^N$, (*confer* (604))

1. $r = \operatorname{rank}(D) - 1 \;\Leftrightarrow\; \mathbf{1}^TD^{\dagger}\mathbf{1} \neq 0$
   Points constituting a generating list for the corresponding polyhedron lie on the relative boundary of an r-dimensional *circumhypersphere* having
   $$\text{diameter} \;=\; \sqrt{2}\,\big(\mathbf{1}^TD^{\dagger}\mathbf{1}\big)^{-1/2} \tag{446}$$

2. $r = \operatorname{rank}(D) - 2 \;\Leftrightarrow\; \mathbf{1}^TD^{\dagger}\mathbf{1} = 0$
   There can be no circumhypersphere whose relative boundary contains a generating list for the corresponding polyhedron.

3. In *Cayley-Menger form* [22, §3.3] [98, §40] (§4.12.3.1),
   $$r \;=\; N-1-\dim\mathcal{N}\!\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0\end{bmatrix}\right) \;=\; \operatorname{rank}\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0\end{bmatrix} - 2 \tag{447}$$

$\diamond$

For all practical purposes,

$$\max\{0\,,\ \operatorname{rank}(D)-2\} \;\leq\; r \;\leq\; \min\{n\,,\ N-1\} \tag{448}$$

4.8 Euclidean metric *versus* matrix criteria

4.8.1 Nonnegativity axiom 1

When D is an EDM (333), then it is apparent from (439) that

$$2V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \;=\; -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \tag{449}$$

because for any A, $A^T A \succeq 0$.[4.15] We claim that nonnegativity of the d_{ij} is enforced primarily by the matrix inequality (449); *id est*,

$$\left.\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array}\right\} \Rightarrow\; d_{ij} \geq 0,\; i \neq j \tag{450}$$

(The matrix criterion to enforce strict positivity differs by a stroke of the pen. (453))

We now support our claim: If any matrix $A \in \mathbb{R}^{m\times m}$ is positive semidefinite, then its main diagonal $\delta(A) \in \mathbb{R}^m$ must have all nonnegative entries. [44, §4.2] Given $D \in \mathbb{S}_{\mathbf{0}}^N$,

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} =$$

$$\begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) & \frac{1}{2}(d_{1,i+1}+d_{1,j+1}-d_{i+1,j+1}) & \cdots & \frac{1}{2}(d_{12}+d_{1N}-d_{2N}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} & \frac{1}{2}(d_{1,i+1}+d_{1,j+1}-d_{i+1,j+1}) & \cdots & \frac{1}{2}(d_{13}+d_{1N}-d_{3N}) \\ \frac{1}{2}(d_{1,j+1}+d_{1,i+1}-d_{j+1,i+1}) & \frac{1}{2}(d_{1,j+1}+d_{1,i+1}-d_{j+1,i+1}) & d_{1,i+1} & \ddots & \frac{1}{2}(d_{14}+d_{1N}-d_{4N}) \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{1}{2}(d_{12}+d_{1N}-d_{2N}) & \frac{1}{2}(d_{13}+d_{1N}-d_{3N}) & \frac{1}{2}(d_{14}+d_{1N}-d_{4N}) & \cdots & d_{1N} \end{bmatrix}$$

$$\in \mathbb{S}^{N-1} \tag{451}$$

where row,column indices $i,j \in \{1 \ldots N-1\}$. [87] It follows:

$$\left.\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array}\right\} \Rightarrow\; \delta(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \begin{bmatrix} d_{12} \\ d_{13} \\ \vdots \\ d_{1N} \end{bmatrix} \succeq 0 \tag{452}$$

[4.15] For $A \in \mathbb{R}^{m\times n}$, $A^T A \succeq 0 \;\Leftrightarrow\; y^T A^T A y \;=\; \|Ay\|^2 \;\geq\; 0$ for all $\|y\| = 1$. When A is full-rank skinny-or-square, $A^T A \succ 0$.

Multiplication of $V_{\mathcal{N}}$ by any permutation matrix Ξ has null effect on its range and nullspace. In other words, any permutation of the rows or columns of $V_{\mathcal{N}}$ produces a basis for $\mathcal{N}(\mathbf{1}^T)$; *id est*, $\mathcal{R}(\Xi_r V_{\mathcal{N}}) = \mathcal{R}(V_{\mathcal{N}}\,\Xi_c) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$. Hence, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \Leftrightarrow -V_{\mathcal{N}}^T \Xi_r^T D \Xi_r V_{\mathcal{N}} \succeq 0$ $(\Leftrightarrow -\Xi_c^T V_{\mathcal{N}}^T D V_{\mathcal{N}}\,\Xi_c \succeq 0)$. Various permutation matrices[4.16] will sift the remaining d_{ij} similarly to (452) thereby proving their nonnegativity. Hence $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ is a sufficient test of the first axiom (§4.2) of the Euclidean metric, nonnegativity. ♦

4.8.1.1 Strict positivity

Should we require the points in $\mathbb{R}^n$ to be distinct, then entries of D off the main diagonal must be strictly positive $\{d_{ij} > 0,\ i \neq j\}$, and only those entries along the main diagonal of D are 0. By similar argument, the strict matrix inequality is a sufficient test for strict positivity of Euclidean distance-square;

$$\left.\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array}\right\} \Rightarrow\ d_{ij} > 0,\ i \neq j \tag{453}$$

4.8.2 Triangle inequality axiom 4

In light of Kreyszig's observation [38, §1.1, prob.15] that axioms 2 through 4 of the Euclidean metric (§4.2) together imply axiom 1, the nonnegativity criterion (450) suggests that the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ might somehow take on the role of triangle inequality; *id est*,

$$\left.\begin{array}{r} \delta(D) = \mathbf{0} \\ D^T = D \\ -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \end{array}\right\} \Rightarrow \sqrt{d_{ij}}\ \leq\ \sqrt{d_{ik}} + \sqrt{d_{kj}}\,,\ i \neq j \neq k \tag{454}$$

We now show that is indeed the case: Let T be the *leading principal submatrix* in $\mathbb{S}^{\mathbf{2}}$ of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ (upper left 2×2 submatrix from (451));

$$T \triangleq \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} \end{bmatrix} \tag{455}$$

[4.16] The rule of thumb is: If $\Xi_r(i,1) = 1$, then $\delta(-V_{\mathcal{N}}^T \Xi_r^T D \Xi_r V_{\mathcal{N}}) \in \mathbb{R}^{N-1}$ is some permutation of the i^{th} row or column of D excepting the 0 entry from the main diagonal.

Submatrix T must be positive (semi)definite whenever $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ is. (§A.3.1.0.4, §4.8.3) Now we have,

$$\begin{array}{l} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \;\Rightarrow\; T \succeq 0 \;\Leftrightarrow\; \sigma_1 \geq \sigma_2 \geq 0 \\ -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \;\Rightarrow\; T \succ 0 \;\Leftrightarrow\; \sigma_1 > \sigma_2 > 0 \end{array} \tag{456}$$

where σ_1 and σ_2 are the eigenvalues of T, real due only to symmetry of T:

$$\begin{array}{l} \sigma_1 = \frac{1}{2}\left(d_{12} + d_{13} + \sqrt{d_{23}^2 - 2(d_{12}+d_{13})d_{23} + 2(d_{12}^2 + d_{13}^2)}\right) \in \mathbb{R} \\ \sigma_2 = \frac{1}{2}\left(d_{12} + d_{13} - \sqrt{d_{23}^2 - 2(d_{12}+d_{13})d_{23} + 2(d_{12}^2 + d_{13}^2)}\right) \in \mathbb{R} \end{array} \tag{457}$$

Nonnegativity of eigenvalue σ_1 is guaranteed by only the nonnegativity of the d_{ij} which in turn is guaranteed by the matrix inequality (450). The inequality between the eigenvalues in (456) follows from only the realness of the d_{ij}. Since σ_1 always exceeds or equals σ_2, conditions for the positive (semi)definiteness of submatrix T can be completely determined by examining σ_2, the smaller of its two eigenvalues. A triangle inequality is made apparent when we express T eigenvalue nonnegativity in terms of D matrix entries; *videlicet*,

$$\begin{array}{c} T \succeq 0 \quad\Leftrightarrow\quad \det T = \sigma_1\sigma_2 \geq 0\,, \quad d_{12}, d_{13} \geq 0 \\ \Leftrightarrow \\ \sigma_2 \geq 0 \\ \Leftrightarrow \\ |\sqrt{d_{12}} - \sqrt{d_{23}}\,| \;\leq\; \sqrt{d_{13}} \;\leq\; \sqrt{d_{12}} + \sqrt{d_{23}} \qquad \text{(a)} \end{array} \tag{458}$$

Triangle inequality (458a) (*confer* (373) (470)), in terms of three entries from D, is equivalent to axiom 4

$$\begin{array}{l} \sqrt{d_{13}} \leq \sqrt{d_{12}} + \sqrt{d_{23}} \\ \sqrt{d_{23}} \leq \sqrt{d_{12}} + \sqrt{d_{13}} \\ \sqrt{d_{12}} \leq \sqrt{d_{13}} + \sqrt{d_{23}} \end{array} \tag{459}$$

for the corresponding points x_1, x_2, x_3 from some length-N list.[4.17]

[4.17] Accounting for symmetry axiom 3, the fourth axiom demands three inequalities be satisfied per one of type (458a). The first of those inequalities in (459) is self evident from (458a), while the two remaining follow from the left-hand side of (458a) and the fact for scalars, $|a| \leq b \Leftrightarrow a \leq b$ and $-a \leq b$.

4.8.2.1 Comment

Given D whose dimension N equals or exceeds 3, there are $N!/(3!(N-3)!)$ distinct triangle inequalities in total like (373) that must be satisfied, of which each d_{ij} is involved in $N-2$, and each point x_i is in $(N-1)!/(2!(N-1-2)!)$. We have so far revealed only one of those triangle inequalities; namely, (458a) that came from T (455). Yet we claim if $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ then all triangle inequalities will be satisfied simultaneously;

$$|\sqrt{d_{ik}} - \sqrt{d_{kj}}\,| \;\leq\; \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}} + \sqrt{d_{kj}}\,, \quad i<k<j \tag{460}$$

(There are no more.) To verify our claim, we must prove the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ to be a sufficient test of all the triangle inequalities; more efficient, we add, for larger N :

4.8.2.1.1 Shore

The columns of $\Xi_r V_{\mathcal{N}} \Xi_c$ hold a basis for $\mathcal{N}(\mathbf{1}^T)$ when Ξ_r and Ξ_c are permutation matrices. In other words, any permutation of the rows or columns of $V_{\mathcal{N}}$ leaves its range and nullspace unchanged; *id est*, $\mathcal{R}(\Xi_r V_{\mathcal{N}} \Xi_c) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$ (340). Hence, two distinct matrix inequalities can be equivalent tests of the positive semidefiniteness of D on $\mathcal{R}(V_{\mathcal{N}})$; *id est*, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \Leftrightarrow -(\Xi_r V_{\mathcal{N}} \Xi_c)^T D (\Xi_r V_{\mathcal{N}} \Xi_c) \succeq 0$. By properly choosing the permutation matrices,[4.18] the leading principal submatrix $T_{\Xi} \in \mathbb{S}^{\mathbf{2}}$ of $-(\Xi_r V_{\mathcal{N}} \Xi_c)^T D (\Xi_r V_{\mathcal{N}} \Xi_c)$ may be loaded with the entries of D needed to test any particular triangle inequality (similarly to (451)-(458)). Because all the triangle inequalities can be individually tested using a test equivalent to the lone matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$, it logically follows that the lone matrix inequality tests all those triangle inequalities simultaneously. We conclude that $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ is a sufficient test of the fourth axiom of the Euclidean metric, triangle inequality. ⧫

4.8.2.2 Strict triangle inequality

Without exception, all the inequalities in (458) and (459) can be made strict while their corresponding implications remain true. The then strict inequality (458a) or (459) may be interpreted as a *strict triangle inequality* under

[4.18] To individually test triangle inequality $|\sqrt{d_{ik}} - \sqrt{d_{kj}}\,| \leq \sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}$ for particular i, k, j, set $\Xi_r(i,1) = \Xi_r(k,2) = \Xi_r(j,3) = 1$, and $\Xi_c = I$.

which collinear arrangement of points is not allowed. [57, §24/6, p.322] Hence by similar reasoning, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$ is a sufficient test of all the strict triangle inequalities; *id est*,

$$\left.\begin{array}{r}\delta(D)=\mathbf{0}\\ D^T=D\\ -V_{\mathcal{N}}^T D V_{\mathcal{N}}\succ 0\end{array}\right\}\Rightarrow \sqrt{d_{ij}}\;<\;\sqrt{d_{ik}}+\sqrt{d_{kj}}\;,\quad i\neq j\neq k \tag{461}$$

4.8.3 $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ nesting

From (455) observe that $T = -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 3}$. In fact, for $D\in\mathbb{EDM}^N$, the leading principal submatrices of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ form a nested sequence (by inclusion) whose members are individually positive semidefinite [44] [28] [26] and have the same form as T; *videlicet*,

$$\begin{array}{lll}
[\,-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 1} & = & [\,\emptyset\,]\;, \qquad\qquad \text{(o)}\\[6pt]
-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 2} & = & [d_{12}]\in\mathbb{S}_+\;, \qquad\qquad \text{(a)}\\[6pt]
-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 3} & = & \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23})\\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13}\end{bmatrix} \;=\; T\in\mathbb{S}_+^{\mathbf{2}}\;, \qquad \text{(b)}\\[6pt]
-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 4} & = & \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) & \frac{1}{2}(d_{12}+d_{14}-d_{24})\\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} & \frac{1}{2}(d_{13}+d_{14}-d_{34})\\ \frac{1}{2}(d_{12}+d_{14}-d_{24}) & \frac{1}{2}(d_{13}+d_{14}-d_{34}) & d_{14}\end{bmatrix}, \qquad \text{(c)}\\[6pt]
 & \vdots & \\[6pt]
-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow i} & = & \begin{bmatrix} -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow i-1} & \nu(i)\\ \\ \nu^T(i) & d_{1i}\end{bmatrix}\in\mathbb{S}_+^{i-1}, \qquad \text{(d)}\\
 & \vdots & \\[6pt]
-V_{\mathcal{N}}^T D V_{\mathcal{N}} & = & \begin{bmatrix} -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow N-1} & \nu(N)\\ \\ \nu^T(N) & d_{1N}\end{bmatrix}\in\mathbb{S}_+^{N-1} \qquad \text{(e)}\\
]
\end{array} \tag{462}$$

where[4.19]

$$\nu(i) \triangleq \frac{1}{2}\begin{bmatrix} d_{12}+d_{1i}-d_{2i} \\ d_{13}+d_{1i}-d_{3i} \\ \vdots \\ d_{1,i-1}+d_{1i}-d_{i-1,i} \end{bmatrix} \in \mathbb{R}^{i-2}, \quad i>2 \tag{463}$$

Hence, the leading principal submatrices of EDM D must also be EDMs.[4.20]

Bordered symmetric matrices in the form (462d) are known to have *intertwined* [26, §6.4] (or *interlaced* [28, §4.3] [99, §IV.4.1]) eigenvalues; (*confer* §4.14.1) that means, for the particular submatrices (462a) and (462b),

$$\sigma_2 \leq d_{12} \leq \sigma_1 \tag{464}$$

where d_{12} is the eigenvalue of the submatrix (462a), and σ_1, σ_2 are the eigenvalues of T (462b) (455). Intertwining in (464) predicts that should d_{12} become 0, then σ_2 must go to 0.[4.21] The eigenvalues are similarly intertwined for submatrices (462b) and (462c);

$$\gamma_3 \leq \sigma_2 \leq \gamma_2 \leq \sigma_1 \leq \gamma_1 \tag{465}$$

where $\gamma_1, \gamma_2, \gamma_3$ are the eigenvalues of submatrix (462c). Intertwining likewise predicts that should σ_2 become 0 (a possibility revealed in §4.8.3.1), then γ_3 must go to 0. Combining results so far for $N=2,3,4$: (464) (465)

$$\gamma_3 \leq \sigma_2 \leq d_{12} \leq \sigma_1 \leq \gamma_1 \tag{466}$$

The preceding logic extends by induction through the remaining members of the sequence (462).

4.8.3.1 Tightening the triangle inequality

Now we apply the Schur complement from §A.4 to tighten the triangle inequality. We find that the gains by doing so are modest. From (462) we identify

$$G \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 4} \tag{467}$$

$$A \triangleq T = -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 3} \tag{468}$$

4.19 $-VDV|_{N\leftarrow 1} = 0 \in \mathbb{S}_+^{\mathbf{0}}$ (§B.4.1)

4.20 In fact, each and every principal submatrix of an EDM D is another EDM. [86, §4.1]

4.21 If d_{12} were 0, eigenvalue σ_2 becomes 0 (457) because d_{13} must then be equal to d_{23}; *id est*, $d_{12}=0 \Leftrightarrow x_1 = x_2$. (54)

both positive semidefinite by assumption, $B=\nu(4)$ defined in (463), and $C=d_{14}$. Using the latter non-strict form of (886), $C\geq 0$ by assumption (§4.8.1) and $CC^\dagger=I$. So by the *positive semidefinite ordering of eigenvalues theorem* (§A.3.1.0.1),

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 4}\succeq 0 \;\Leftrightarrow\; T\succeq d_{14}^{-1}\nu(4)\nu^T(4) \;\Rightarrow \left\{\begin{array}{l}\sigma_1\geq d_{14}^{-1}\|\nu(4)\|^2\\ \sigma_2\geq 0\end{array}\right. \tag{469}$$

where $\{d_{14}^{-1}\|\nu(4)\|^2,\,0\}$ are the eigenvalues of $d_{14}^{-1}\nu(4)\nu^T(4)$ and $\sigma_1\,,\sigma_2$ are the eigenvalues of T.

4.8.3.1.1 Example. *Small completion problem*, IV.
Applying the inequality for σ_1 in (469) to the *small completion problem* on page 132, Figure **4.2** (*confer* §4.9.3, §4.12.4.1), the lower bound on $\sqrt{d_{14}}$, 1.236 in (327), is tightened to 1.289. The correct value of $\sqrt{d_{14}}$ to three significant figures is 1.414. □

4.8.4 Affine dimension reduction in two dimensions

(*confer* §4.12.4) The leading principal 2×2 submatrix T of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has largest eigenvalue σ_1 (457) which is a convex function of D.[4.22] σ_1 can never be 0 unless $d_{12}=d_{13}=d_{23}=0$. σ_1 can never be negative while the d_{ij} are nonnegative. The remaining eigenvalue σ_2 is a concave function of D that becomes 0 only at the upper and lower bounds of inequality (458a) and its equivalent forms: (*confer* (460))

$$\begin{array}{rclcll}
|\sqrt{d_{12}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{13}} & \leq & \sqrt{d_{12}}+\sqrt{d_{23}} & \text{(a)}\\
 & & \Leftrightarrow & & & \\
|\sqrt{d_{12}}-\sqrt{d_{13}}\,| & \leq & \sqrt{d_{23}} & \leq & \sqrt{d_{12}}+\sqrt{d_{13}} & \text{(b)}\\
 & & \Leftrightarrow & & & \\
|\sqrt{d_{13}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{12}} & \leq & \sqrt{d_{13}}+\sqrt{d_{23}} & \text{(c)}
\end{array} \tag{470}$$

[4.22] The maximum eigenvalue of any symmetric matrix is always a convex function of its entries, while the minimum eigenvalue is always concave. [1, exmp.3.10] In our particular case, say $\underline{d}\triangleq\begin{bmatrix}d_{12}\\ d_{13}\\ d_{23}\end{bmatrix}\in\mathbb{R}^3$. Then the Hessian (1072) $\nabla^2\sigma_1(\underline{d})\succeq 0$ certifies convexity whereas $\nabla^2\sigma_2(\underline{d})\preceq 0$ certifies concavity. Each Hessian has rank equal to 1. The respective gradients $\nabla\sigma_1(\underline{d})$ and $\nabla\sigma_2(\underline{d})$ are nowhere $\mathbf{0}$.

In between those bounds, σ_2 is strictly positive; otherwise, it would be negative but prevented by the condition $T \succeq 0$.

When σ_2 becomes 0, it means that triangle $\triangle_{123}$ has collapsed to a line segment; a potential reduction in affine dimension r. The same logic is valid for any principal 2×2 submatrix of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$, hence applicable to other triangles.

4.9 Bridge: Convex polyhedra to EDMs

The criteria for the existence of an EDM include, by definition (333) (375), the axioms imposed upon its entries d_{ij} by the Euclidean metric. From §4.8.1 and §4.8.2, we know there is a relationship of matrix criteria to those axioms. Here is a snapshot of what we are sure thus far: for $i,j,k \in \{1 \ldots N\}$, (*confer* §4.2)

$$\begin{array}{l} \sqrt{d_{ij}} \geq 0, \;\; i \neq j \\ \sqrt{d_{ij}} = 0, \;\; i = j \\ \sqrt{d_{ij}} = \sqrt{d_{ji}} \\ \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}} + \sqrt{d_{kj}}\,, \;\; i \neq j \neq k \end{array} \quad \Leftarrow \quad \begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ \delta(D) = \mathbf{0} \\ D^T = D \end{array} \quad \Leftarrow \quad D \in \mathbb{EDM}^N \tag{471}$$

In words, these Euclidean axioms are necessary conditions for D to be a distance matrix. At this moment, we have no converse for (471). As of concern in §4.3, we have yet to establish metric requirements beyond the four Euclidean axioms that would allow D to be certified an EDM or might facilitate polyhedron or list reconstruction from an incomplete EDM. Our present goal is to establish *ab initio* the necessary and sufficient matrix criteria that will subsume all the Euclidean axioms and any further requirements[4.23] for all $N > 0$ (§4.8.3); *id est*,

$$\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array} \quad \Leftrightarrow \quad D \in \mathbb{EDM}^N \tag{352}$$

[4.23] In 1935, Schoenberg [87, (1)] first extolled expansion (451) (predicated on symmetry and zero self-distance) specifically incorporating $V_{\mathcal{N}}$, albeit algebraically. He showed that nonnegativity $-y^T V_{\mathcal{N}}^T D V_{\mathcal{N}}\, y \geq 0$, for all (normalized) $y \in \mathbb{R}^{N-1}$, is necessary and sufficient for D to be an EDM. Gower [84, §3] remarks how surprising it is that such a fundamental property of Euclidean geometry was obtained so late.

or since $-V_{\mathcal{N}}^T D V_{\mathcal{N}} = \Theta^T\Theta$ (379), then for relative-angle matrix Ω and distance vector $\sqrt{d}$ as in (380) and EDM definition (384),

$$\begin{array}{r}\Omega \succeq 0\\ \sqrt{d} \succeq 0\end{array} \quad\Leftrightarrow\quad D = \mathbf{D}(\Omega\,, d) \in \mathbb{EDM}^N \tag{472}$$

From (340) we know $\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$, so (352) is the same as (329). In fact, any matrix V in place of $V_{\mathcal{N}}$ will satisfy (352) whenever $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$.

4.9.1 Geometric criterion

We derive matrix criteria for D to be an EDM, validating (352) using simple geometry: distance to the polyhedron formed by the convex hull of a list of points (54) in Euclidean space $\mathbb{R}^n$.

EDM assertion. D is a Euclidean distance matrix if and only if $D \in \mathbb{S}_{\mathbf{0}}^N$ and distances-square from the origin

$$\{\|p(y)\|^2 = -y^T V_{\mathcal{N}}^T D V_{\mathcal{N}}\, y \mid y \in \mathcal{S} - \beta\} \tag{473}$$

correspond to points p in some bounded convex polyhedron

$$\mathcal{P} - \alpha \;=\; \{p(y) \mid y \in \mathcal{S} - \beta\} \tag{474}$$

having N or fewer vertices embedded in an r-dimensional subspace $\mathcal{A} - \alpha$ of $\mathbb{R}^n$, where $\alpha \in \mathcal{A} = \operatorname{aff} \mathcal{P}$, and where the domain of linear surjection $p(y)$ is the unit simplex $\mathcal{S} \subset \mathbb{R}_+^{N-1}$ shifted such that its vertex at the origin is translated to $-\beta$ in $\mathbb{R}^{N-1}$. When $\beta = 0$, $\alpha = x_1$. $\diamond$

In terms of $V_{\mathcal{N}}$, the unit simplex (166) in $\mathbb{R}^{N-1}$ has an equivalent representation:

$$\mathcal{S} \;=\; \{s \in \mathbb{R}^{N-1} \mid \sqrt{2}V_{\mathcal{N}}\, s \succeq -e_1\} \tag{475}$$

where e_1 is as in (348). Incidental to the *EDM assertion*, shifting the unit-simplex domain in $\mathbb{R}^{N-1}$ translates the polyhedron $\mathcal{P}$ in $\mathbb{R}^n$. Indeed, there is a one-to-one correspondence between vertices of the unit simplex and members of the list generating $\mathcal{P}$;

$$
\begin{array}{rcccc}
p & : & \mathbb{R}^{N-1} & \to & \mathbb{R}^n \\
& & p\left(\left\{\begin{array}{c} -\beta \\ e_1-\beta \\ e_2-\beta \\ \vdots \\ e_{N-1}-\beta \end{array}\right\}\right) & = & \left\{\begin{array}{c} x_1-\alpha \\ x_2-\alpha \\ x_3-\alpha \\ \vdots \\ x_N-\alpha \end{array}\right\}
\end{array}
\tag{476}
$$

4.9.1.0.2 Proof. *EDM assertion.*
($\Longrightarrow$) We demonstrate that if D is an EDM, then each distance-square $\|p(y)\|^2$ described by (473) corresponds to a point p in some embedded polyhedron $\mathcal{P}-\alpha$. Assume D is indeed an EDM; *id est*, D can be made from some list X of N unknown points in Euclidean space $\mathbb{R}^n$; $D=\mathbf{D}(X)$ for $X\in\mathbb{R}^{n\times N}$ as in (333). Since D is translation invariant (§4.5.1), we may shift the affine hull $\mathcal{A}$ of those unknown points to the origin as in (427). Then take any point p in their convex hull (60);

$$
\mathcal{P}-\alpha \;=\; \{p=(X-Xb\,\mathbf{1}^T)a \mid a^T\mathbf{1}=1,\ a\succeq 0\} \tag{477}
$$

where $\alpha=Xb\in\mathcal{A}\;\Leftrightarrow\; b^T\mathbf{1}=1$. Solutions to $a^T\mathbf{1}=1$ are:[4.24]

$$
a=e_1+\sqrt{2}V_{\mathcal{N}}\,s \tag{478}
$$

where $s\in\mathbb{R}^{N-1}$ and e_1 is as in (348). Similarly, $b=e_1+\sqrt{2}V_{\mathcal{N}}\beta$.

$$
\begin{aligned}
\mathcal{P}-\alpha \;&=\; \{p=X(I-(e_1+\sqrt{2}V_{\mathcal{N}}\beta)\mathbf{1}^T)(e_1+\sqrt{2}V_{\mathcal{N}}\,s) \mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\} \\
&=\; \{p=X\sqrt{2}V_{\mathcal{N}}(s-\beta) \mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\}
\end{aligned}
\tag{479}
$$

that describes the domain of $p(s)$ as the unit simplex $\mathcal{S}$;

$$
\mathcal{S}=\{s \mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\}\subset\mathbb{R}_+^{N-1} \tag{480}
$$

Making the substitution $y\leftarrow s-\beta$,

$$
\mathcal{P}-\alpha \;=\; \{p=X\sqrt{2}V_{\mathcal{N}}\,y \mid y\in\mathcal{S}-\beta\} \tag{481}
$$

[4.24] Since $\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^T)$ and $\mathcal{N}(\mathbf{1}^T)\perp\mathcal{R}(\mathbf{1})$, then over all $s\in\mathbb{R}^{N-1}$, $V_{\mathcal{N}}\,s$ is a hyperplane through the origin orthogonal to $\mathbf{1}$. Thus the solutions a constitute a hyperplane orthogonal to the vector $\mathbf{1}$, and offset from the origin in $\mathbb{R}^N$ by any particular solution; in this case, $a=e_1$.

Point p belongs to a convex polyhedron $\mathcal{P}-\alpha$ embedded in an r-dimensional subspace of $\mathbb{R}^n$ because the convex hull of any list forms a polyhedron, and because the translated affine hull $\mathcal{A}-\alpha$ contains the translated polyhedron $\mathcal{P}-\alpha$ (430) and the origin (when $\alpha\in\mathcal{A}$), and because $\mathcal{A}$ has dimension r by definition (432). Now, any distance-square from the origin to the polyhedron $\mathcal{P}-\alpha$ can be formulated

$$\{p^Tp \;=\; \|p\|^2 \;=\; 2y^TV_{\mathcal{N}}^TX^TXV_{\mathcal{N}}\,y \mid y\in\mathcal{S}-\beta\} \tag{482}$$

Applying (439) to (482) we get (473).

($\Longleftarrow$) To validate the *EDM assertion* in the reverse direction, we prove: If each distance-square $\|p(y)\|^2$ (473) on the shifted unit-simplex $\mathcal{S}-\beta\subset\mathbb{R}^{N-1}$ corresponds to a point $p(y)$ in some embedded polyhedron $\mathcal{P}-\alpha$, then D is an EDM. The r-dimensional subspace $\mathcal{A}-\alpha\subseteq\mathbb{R}^n$ is spanned by

$$p(\mathcal{S}-\beta)=\mathcal{P}-\alpha \tag{483}$$

because $\mathcal{A}-\alpha=\operatorname{aff}(\mathcal{P}-\alpha)\supseteq\mathcal{P}-\alpha$ (430). So, outside the domain $\mathcal{S}-\beta$ of linear surjection $p(y)$, the simplex complement $\backslash\mathcal{S}-\beta\subset\mathbb{R}^{N-1}$ must contain the domain of the distance-square $\|p(y)\|^2=p(y)^Tp(y)$ to remaining points in the subspace $\mathcal{A}-\alpha$; *id est*, to the polyhedron's relative exterior $\backslash\mathcal{P}-\alpha$. For $\|p(y)\|^2$ to be nonnegative on the entire subspace $\mathcal{A}-\alpha$, $-V_{\mathcal{N}}^TDV_{\mathcal{N}}$ must be positive semidefinite and is assumed symmetric;[4.25]

$$-V_{\mathcal{N}}^TDV_{\mathcal{N}} \;\stackrel{\Delta}{=}\; \Phi^T\Phi \tag{484}$$

where[4.26] $\Phi\in\mathbb{R}^{m\times N-1}$ for some $m\geq r$. Because $p(\mathcal{S}-\beta)$ is a convex polyhedron, it is necessarily a set of linear combinations of points from some length-N list because every convex polyhedron having N or fewer vertices can be generated that way (§2.7.2). Equivalent to (473) are

$$\{p^Tp \mid p\in\mathcal{P}-\alpha\} \;=\; \{p^Tp=y^T\Phi^T\Phi\,y \mid y\in\mathcal{S}-\beta\} \tag{485}$$

Because $p\in\mathcal{P}-\alpha$ may be found by factoring (485), the list Φ is found by factoring (484). A unique EDM can be constructed from that list using the inner-product form definition $\mathbf{D}(\Theta)|_{\Theta=\Phi}$ (375). That EDM will be identical to D if $\delta(D)=\mathbf{0}$, by injectivity of $\mathbf{D}$ (403). ♦

[4.25] The antisymmetric part $\big(-V_{\mathcal{N}}^TDV_{\mathcal{N}}-(-V_{\mathcal{N}}^TDV_{\mathcal{N}})^T\big)/2$ is annihilated by $\|p(y)\|^2$. By the same reasoning, any positive (semi)definite matrix A is generally assumed symmetric because only the symmetric part $(A+A^T)/2$ survives the test $y^TAy\geq 0$. [28, §7.1]

[4.26] $A^T=A\succeq 0 \;\Leftrightarrow\; A=R^TR$ for some real matrix R. [26, §6.3]

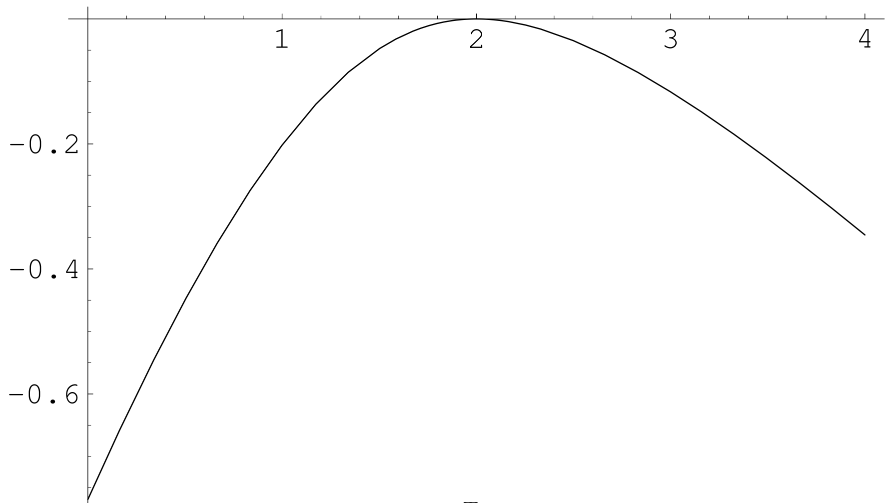


Figure 4.5: Minimum eigenvalue of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$, positive semidefinite for only one value of d_{14} ; 2.

4.9.2 Necessity and sufficiency

From (449) we learned that the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ is a necessary test for D to be an EDM. In §4.9.1, the connection between convex polyhedra and EDMs was pronounced by the *EDM assertion*; the matrix inequality together with $D \in \mathbb{S}_{\mathbf{0}}^N$ became a sufficient test when the *EDM assertion* demanded that every bounded convex polyhedron have a corresponding EDM. For all $N > 0$ (§4.8.3), the matrix criteria for the existence of an EDM in (352), (472), and (329) are therefore necessary and sufficient and subsume all the Euclidean axioms and further requirements.

4.9.3 Example revisited

Now we apply the necessary and sufficient EDM criteria (352) to an earlier problem.

Example. *Small completion problem*, II. Continuing the Example on page 132 that pertains to Figure **4.2** where $N = 4$, d_{14} is ascertainable from the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$. Because all distances in (326) are known except $\sqrt{d_{14}}$, we may simply calculate the minimum eigenvalue of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ over a range of d_{14} as in Figure **4.5**. We observe a unique value of d_{14} satisfying (352) where the abscissa is tangent to the hypograph of the minimum eigenvalue. Since the minimum eigenvalue of a symmetric matrix is known to be a concave function (§4.8.4), we calculate its second partial derivative with respect to d_{14} evaluated at 2 and find $-1/3$. We conclude there are no other satisfying values of d_{14}. Further, that value of d_{14} does not meet an upper or lower bound of a triangle inequality like (460), so neither does it cause the collapse of any triangle. Because the minimum eigenvalue is 0, the affine dimension r of any point list corresponding to D cannot exceed $N-2$. (§4.7.2) $\square$

4.10 List reconstruction

Isometric reconstruction (§4.5.3) of point list X is generally performed by factorization of some quantity involving inter-point distance-square data.

4.10.1 via Gram

For quick reconstruction of a generating list, we may simply perform a Cholesky factorization[4.27] of the Gram matrix (350) or (355) from given $D \in \mathbb{EDM}^N$; *id est*, $G = X^T X$ where reconstruction X provided by the factorization is upper triangular. Alternatively, we may factorize $-V_{\mathcal{N}}^T D V_{\mathcal{N}} = \Theta^T \Theta$ (379) to find upper triangular reconstruction Θ (377).

We now consider how rotation/reflection and translation invariance factor into a reconstruction. Alternatively, the reader may skip ahead to the examples.

4.10.2 x_1 at the origin. $V_{\mathcal{N}}$

At the stage of reconstruction, we have $D \in \mathbb{EDM}^N$ and we wish to find a generating list (§2.2.2) for $\mathcal{P} - \alpha$ by factoring positive semidefinite $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ (484) as suggested in §4.9.1.0.2. One way to factor $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ is via *diagonalization* of symmetric matrices; [26, §5.6] [28] (§A.5, §A.3)

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \triangleq Q \Lambda Q^T \tag{486}$$

$$Q \Lambda Q^T \succeq 0 \;\Leftrightarrow\; \Lambda \succeq 0 \tag{487}$$

[4.27] A very stable numerical algorithm (not requiring definiteness) is given in §F.1.1.5.

where $Q \in \mathbb{R}^{N-1\times N-1}$ is an orthogonal matrix containing eigenvectors while $\Lambda \in \mathbb{R}^{N-1\times N-1}$ is a diagonal matrix containing corresponding nonnegative eigenvalues ordered by nonincreasing value. From the diagonalization, identify the list using (439);

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \;\stackrel{\Delta}{=}\; Q\sqrt{\Lambda}\,Q_p^T Q_p \sqrt{\Lambda}\,Q^T \tag{488}$$

where $\sqrt{\Lambda}\,Q_p^T Q_p \sqrt{\Lambda} \stackrel{\Delta}{=} \Lambda = \sqrt{\Lambda}\sqrt{\Lambda}$, and where $Q_p \in \mathbb{R}^{n\times N-1}$ is unknown as is its dimension n. Rotation/reflection is accounted for by Q_p yet only its first r columns are necessarily orthonormal.[4.28] Assuming membership to the unit simplex $y \in \mathcal{S}$ (481), then point $p = X\sqrt{2}V_{\mathcal{N}}\, y = Q_p \sqrt{\Lambda}\,Q^T y$ in $\mathbb{R}^n$ belongs to the polyhedron

$$\mathcal{P} - x_1 \tag{489}$$

whose generating list constitutes the columns of (433)

$$\begin{bmatrix} \mathbf{0} & X\sqrt{2}V_{\mathcal{N}} \end{bmatrix} \;=\; \begin{bmatrix} \mathbf{0} & Q_p\sqrt{\Lambda}\,Q^T \end{bmatrix} \in \mathbb{R}^{n\times N} \tag{490}$$

The simplest choice of Q_p has n set to $N-1$; *id est*, $Q_p = I$. Each member of the generating list then has $N-1-r$ zeros in its higher-dimensional coordinates because $r \leq N-1$. (444) To truncate those zeros, choose n to be

$$\operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \operatorname{rank} Q_p \sqrt{\Lambda}\,Q^T \;=\; \operatorname{rank}\Lambda \;=\; r \tag{491}$$

which is the smallest n possible because $XV_{\mathcal{N}}$ has rank $r \leq n$ (441).[4.29] In that case, the simplest choice for Q_p is $[\,I \;\; \mathbf{0}\,]$ having dimensions $r \times N-1$.

[4.28] Q_p is not necessarily an orthogonal matrix. Q_p is constrained such that only its first r columns are necessarily orthonormal because there are only r nonzero eigenvalues in Λ when $V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has rank r (§4.7.2). The remaining columns of Q_p are arbitrary.

[4.29] If we write $Q^T = \begin{bmatrix} q_1^T \\ \vdots \\ q_{N-1}^T \end{bmatrix}$ as row-wise eigenvectors, $\Lambda = \begin{bmatrix} \lambda_1 & & & & \mathbf{0} \\ & \ddots & & & \\ & & \lambda_r & & \\ & & & 0 & \\ & & & & \ddots \\ \mathbf{0} & & & & 0 \end{bmatrix}$ in terms of eigenvalues, and $Q_p = \begin{bmatrix} q_{p_1} \cdots q_{p_{N-1}} \end{bmatrix}$ as column vectors, then $Q_p \sqrt{\Lambda}\,Q^T = \sum\limits_{i=1}^{r} \sqrt{\lambda_i}\, q_{p_i} q_i^T$ is a sum of r linearly independent rank-one matrices (§B.1.1). Hence the summation has rank r.

We may wish to verify the list (490) found from the diagonalization of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$. Because of rotation/reflection and translation invariance (§4.5), EDM D can be uniquely constructed from that list by calculating: (333)

$$\mathbf{D}(X) \;=\; \mathbf{D}(X[\,\mathbf{0}\quad \sqrt{2}V_{\mathcal{N}}\,]) \;=\; \mathbf{D}(Q_p[\,\mathbf{0}\quad \sqrt{\Lambda}\,Q^T\,]) \;=\; \mathbf{D}([\,\mathbf{0}\quad \sqrt{\Lambda}\,Q^T\,]) \tag{492}$$

This suggests a way to find EDM D given $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$; (*confer* (408))

$$D = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big) \end{bmatrix} \mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^T D V_{\mathcal{N}}\big)^T \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T D V_{\mathcal{N}} \end{bmatrix} \tag{353}$$

4.10.2.1 0 geometric center. V

Alternatively, we may perform reconstruction using instead the auxiliary matrix V (§B.4.1), corresponding to the polyhedron

$$\mathcal{P} - \alpha_g \tag{493}$$

whose geometric center has been translated to the origin. Redimensioning $Q\,,\Lambda\in\mathbb{R}^{N\times N}$ and $Q_p\in\mathbb{R}^{n\times N}$, (440)

$$-\,VDV \;=\; 2VX^TXV \;\triangleq\; Q\sqrt{\Lambda}\,Q_p^TQ_p\sqrt{\Lambda}\,Q^T \tag{494}$$

where the generating list now constitutes (*confer* (490))

$$XV = \frac{1}{\sqrt{2}}\,Q_p\sqrt{\Lambda}\,Q^T \in \mathbb{R}^{n\times N} \tag{495}$$

Now, EDM D can be uniquely constructed from the list found by calculating: (333)

$$\mathbf{D}(X) \;=\; \mathbf{D}(XV) \;=\; \mathbf{D}(\frac{1}{\sqrt{2}}\,Q_p\sqrt{\Lambda}\,Q^T) \;=\; \mathbf{D}(\sqrt{\Lambda}\,Q^T)\frac{1}{2} \tag{496}$$

This EDM is, of course, identical to (492). Similarly to (353), from $-VDV$ we can find EDM D; (*confer* (414))

$$D = \delta(-VDV\tfrac{1}{2})\mathbf{1}^T + \mathbf{1}\delta(-VDV\tfrac{1}{2})^T - 2(-VDV\tfrac{1}{2}) \tag{358}$$

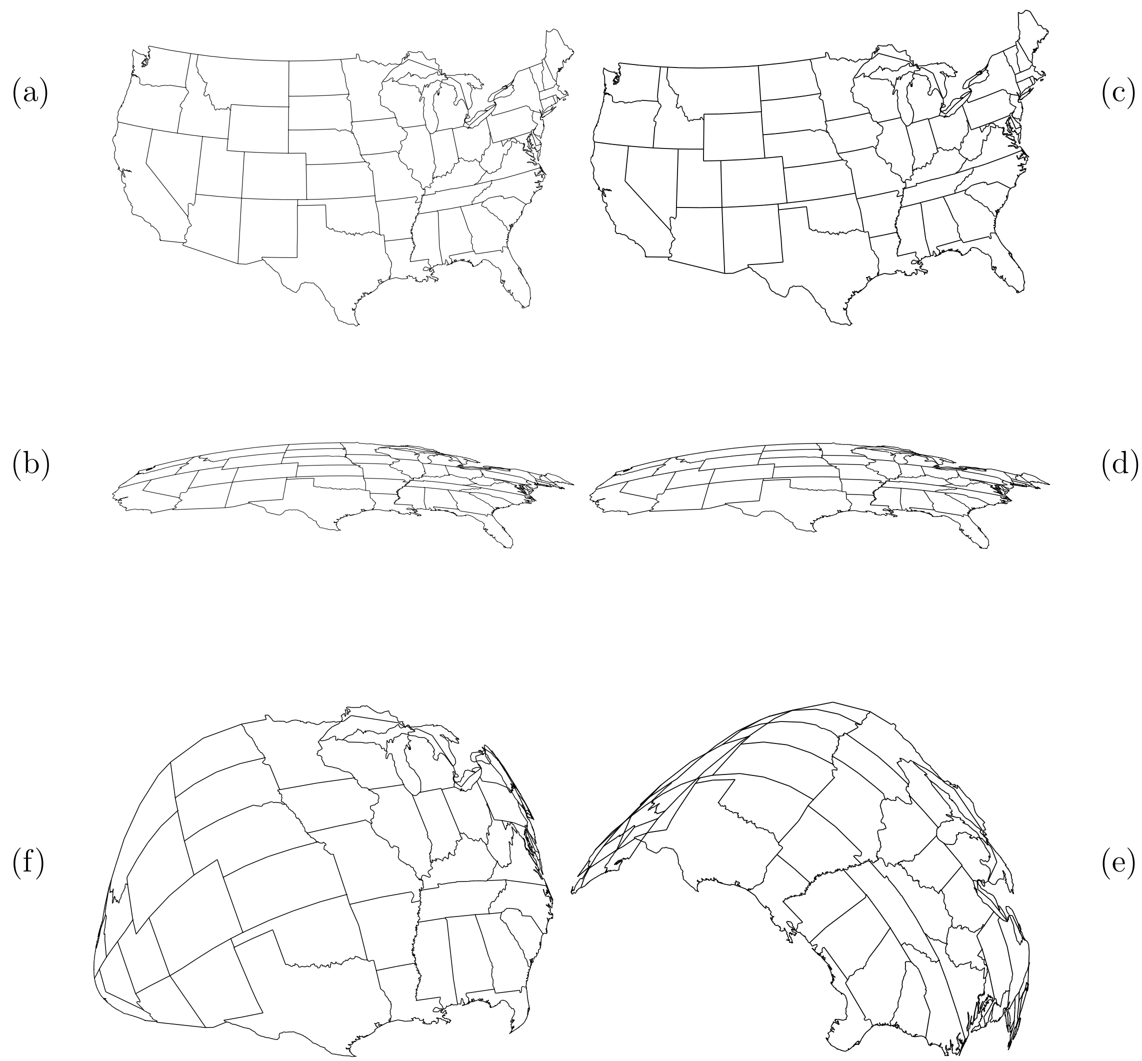


Figure 4.6: Map of United States of America showing some state boundaries and the Great Lakes. All plots made using 5020 connected points. Any difference in scale in (a) through (d) is an artifact of plotting routine.
(a) shows original map made from decimated (latitude, longitude) data.
(b) shows original map data rotated to highlight curvature of Earth.
(c) Map isometrically reconstructed from the EDM.
(d) Same reconstructed map illustrating curvature.
(e)(f) Two views of one isotonic reconstruction; problem (506) with no sort constraint $\Xi\,\underline{d}$ (and no removal of hidden lines).

4.11 Reconstruction examples

4.11.1 Isometric reconstruction

4.11.1.0.1 Example. *Map of the USA.*
The most fundamental application of EDMs is to reconstruct relative point position given only inter-point distance information. Drawing a map of the United States is a good illustration of isometric reconstruction from complete distance data. We obtained latitude and longitude information for the coast, border, states, and Great Lakes from the *usalo atlas data file* within the MATLAB Mapping Toolbox; the conversion to Cartesian coordinates $(x\,,y\,,z)$ via:

$$\begin{aligned}
\phi &\triangleq \pi/2 - \text{latitude}\\
\theta &\triangleq \text{longitude}\\
x &= \sin(\phi)\cos(\theta)\\
y &= \sin(\phi)\sin(\theta)\\
z &= \cos(\phi)
\end{aligned} \tag{497}$$

We used 64% of the available map data to calculate EDM D from $N=5020$ points. The original (decimated) data and its isometric reconstruction are shown in Figure **4.6**(a)-(d). The MATLAB code is in §F.3.1. The eigenvalues computed for (486) are

$$\lambda(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \{199.8\,,\ 152.3\,,\ 2.465\,,\ 0\,,\ 0\,,\ 0\,,\ \ldots\} \tag{498}$$

The 0 eigenvalues have numerical error on the order of `2E-13`; meaning, the EDM data indicates three dimensions ($r=3$) are required for reconstruction to nearly machine precision. □

4.11.2 Isotonic reconstruction

Sometimes only comparative information about distance is known (*e.g.*, the Earth is closer to the Moon than it is to the Sun). Suppose, for example, the EDM D for three points is unknown:

$$D = [d_{ij}] = \begin{bmatrix} 0 & d_{12} & d_{13}\\ d_{12} & 0 & d_{23}\\ d_{13} & d_{23} & 0 \end{bmatrix} \in \mathbb{S}_{\mathbf{0}}^{\mathbf{3}} \tag{323}$$

but the comparative data is available:

$$d_{12} \leq d_{23} \leq d_{13} \tag{499}$$

With the vectorization $\underline{d} = [d_{12}\ d_{13}\ d_{23}]^T \in \mathbb{R}^{\mathbf{3}}$, we express the comparative distance relationship as the nondecreasing sorting

$$\Xi\,\underline{d} \;=\; \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} d_{12} \\ d_{13} \\ d_{23} \end{bmatrix} \;=\; \begin{bmatrix} d_{12} \\ d_{23} \\ d_{13} \end{bmatrix} \in \mathcal{K}_{+\mathcal{M}} \tag{500}$$

where Ξ is a given permutation matrix expressing the known sorting action on the entries of unknown EDM D, and $\mathcal{K}_{+\mathcal{M}}$ is the monotone nonnegative cone (§2.9.2.2.1) with reversed indices,

$$\mathcal{K}_{+\mathcal{M}} \triangleq \{z \mid 0 \leq z_1 \leq z_2 \leq \cdots \leq z_{N(N-1)/2}\} \subseteq \mathbb{R}_+^{N(N-1)/2} \tag{501}$$

where $N(N-1)/2 = 3$ for the present example. From the sorted vectorization (500) we create the *sort-index matrix*

$$O = \begin{bmatrix} 0 & 1^2 & 3^2 \\ 1^2 & 0 & 2^2 \\ 3^2 & 2^2 & 0 \end{bmatrix} \in \mathbb{S}_{\mathbf{0}}^{\mathbf{3}} \cap \mathbb{R}_+^{\mathbf{3}\times\mathbf{3}} \tag{502}$$

where, for $j \neq i$,

$$O_{ij} = k^2 \mid d_{ij} = \big(\Xi\,\underline{d}\big)_k \tag{503}$$

Replacing EDM data with indices-square of a nondecreasing sorting like this is, of course, a heuristic we invented. Any process of reconstruction that leaves comparative distance information intact is called *ordinal multidimensional scaling* or *isotonic reconstruction.* Beyond rotation, reflection, and translation error, (§4.5) list reconstruction by isotonic reconstruction is subject to error in absolute scale (*dilation*) and distance ratio. Yet Borg and Groenen argue: [100, §2.2] reconstruction from complete comparative distance information for a large number of points is as highly constrained as reconstruction from an EDM; the larger the number, the better.

4.11.2.0.1 Example. *Isotonic map of the USA.*

To test that conjecture, suppose we make a complete sort-index matrix $O \in \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N}$ for the map of the USA and then substitute O in place of

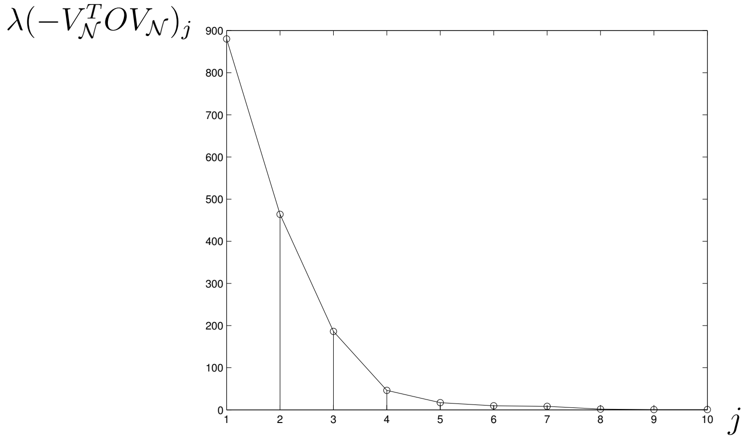


Figure 4.7: Largest ten eigenvalues of $-V_{\mathcal{N}}^T O V_{\mathcal{N}}$ for map of USA, sorted by nonincreasing value. In the code (§F.3.2), we normalize O by $(N(N-1)/2)^2$.

EDM D in the reconstruction process of §4.10. Whereas EDM D returned only three significant eigenvalues (498), the sort-index matrix O is generally not an EDM, certainly not an EDM with corresponding affine dimension 3, so returns many more. The eigenvalues, calculated with numerical error `5E-7`, are plotted in Figure **4.7**:

$$\lambda(-V_{\mathcal{N}}^T O V_{\mathcal{N}}) = \{880.1\,,\ 463.9\,,\ 186.1\,,\ 46.20\,,\ 17.12\,,\ 9.625\,,\ 8.257\,,\ 1.701\,,\ 0.7128\,,\ 0.6460\,,\ \ldots\} \tag{504}$$

The extra eigenvalues indicate that affine dimension corresponding to an EDM near O is likely to exceed 3. To realize the map, we must simultaneously reduce that dimensionality and find an EDM D closest to O in some sense (a problem explored more in §7) while maintaining the known comparative distance relationship; *e.g.*, given permutation matrix Ξ that expresses the known sorting action on the entries $\underline{d}$ of unknown $D \in \mathbb{S}_{\mathbf{0}}^N$, (52)

$$\underline{d} \triangleq \frac{1}{\sqrt{2}} \operatorname{dvec} D = \begin{bmatrix} d_{12} \\ d_{13} \\ d_{23} \\ d_{14} \\ d_{24} \\ d_{34} \\ \vdots \\ d_{N-1,N} \end{bmatrix} \in \mathbb{R}^{N(N-1)/2} \tag{505}$$

we can make the sort-index matrix O input to the optimization problem

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-O)V_{\mathcal{N}}\|_{\mathrm{F}}\\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq 3\\ & \Xi\,\underline{d} \in \mathcal{K}_{+\mathcal{M}}\\ & D \in \mathbb{EDM}^N\end{array} \tag{506}$$

that finds the EDM D corresponding to affine dimension not exceeding 3 in $\frac{1}{\sqrt{2}}\operatorname{dvec}\mathbb{EDM}^N \cap \Xi^T\mathcal{K}_{+\mathcal{M}}$ closest to O in the sense of Schoenberg (352).

The analytical solution to this problem, ignoring the sort constraint ($\Xi\,\underline{d}\in\mathcal{K}_{+\mathcal{M}}$), is known [73] (§7.1): Only the three largest nonnegative eigenvalues in (504) need be retained to make (490); the rest are discarded. The reconstruction from the EDM D found in this manner is plotted in Figure **4.6**(e)(f) from which it becomes clear that inclusion of the sort constraint is necessary for isotonic reconstruction. Ignoring the sort constraint, apparently, violates it. Yet it is remarkable, in light of the many violations, how much the map reconstructed using only ordinal data so resembles the original map. □

4.11.2.1 Isotonic solution with sort constraint

Because problems involving rank are generally difficult, we will partition (506) into two problems we know how to solve and alternate their solution until convergence:

$$\begin{array}{cll}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-O)V_{\mathcal{N}}\|_{\mathrm{F}} & \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq 3 & \text{(a)}\\ & D \in \mathbb{EDM}^N & \\ & & \\ \underset{\underline{o}}{\text{minimize}} & \underline{o}^T(\underline{o}-\Xi\,\underline{d}) & \\ \text{subject to} & \underline{o} \in \mathcal{K}_{+\mathcal{M}} & \text{(b)}\\ & \underline{o}-\Xi\,\underline{d} \in \mathcal{K}_{+\mathcal{M}}^* & \end{array} \tag{507}$$

where $\mathcal{K}_{+\mathcal{M}}^*$ is the dual of the reversed monotone nonnegative cone (501), and where the sort-index matrix O (a given constant in (a)) becomes a vectorized variable $\underline{o}$ in (b) related by

$$\underline{o} \triangleq \frac{1}{\sqrt{2}}\operatorname{dvec} O \in \mathbb{R}^{N(N-1)/2} \tag{508}$$

A closed-form solution to problem (507a) exists. (§7.1) Only the first iteration of (507a) sees the original sort-index matrix O whose entries are nonnegative whole numbers; *id est*, $O_0 = O$ (503). Subsequent iterations i take

$$O_i = \operatorname{dvec}^{-1}(\sqrt{2}\,\underline{o}_i) \in \mathbb{R}^{N\times N} \tag{509}$$

as input, where O_i is a real successor to the sort-index matrix O at the i^{th} iteration, and where $\underline{o}_i \in \mathbb{R}^{N(N-1)/2}$ is a new vector variable that solves the i^{th} instance of (507b).

The new problem (507b) we devised from the necessary and sufficient conditions in §E.8.1.0.1 for unique projection of $\Xi\,\underline{d}$ on convex cone $\mathcal{K}_{+\mathcal{M}}$. Its objective function $\underline{o}^T(\underline{o} - \Xi\,\underline{d})$ cannot fall below the optimal value 0 by (183) because simplicial $\mathcal{K}_{+\mathcal{M}}$ is closed and convex. By defining (§2.9.2.2.1)

$$\begin{aligned} Y &\triangleq [\,e_m \quad e_m + e_{m-1} \quad e_m + e_{m-1} + e_{m-2} \quad \cdots \quad \mathbf{1}\,] \in \mathbb{R}^{m\times m} \\ Y^{\dagger T} &\triangleq [\,e_m - e_{m-1} \quad e_{m-1} - e_{m-2} \quad e_{m-2} - e_{m-3} \quad \cdots \quad e_1\,] \in \mathbb{R}^{m\times m} \end{aligned} \tag{510}$$

where $m \triangleq N(N-1)/2$, we may rewrite (507b) as an equivalent *quadratic program*; a convex optimization problem [1, §4] in terms of halfspace-descriptions of the cone and its dual:

$$\begin{array}{ll} \underset{\underline{o}}{\text{minimize}} & \underline{o}^T(\underline{o} - \Xi\,\underline{d}) \\ \text{subject to} & Y^{\dagger}\underline{o} \succeq 0 \\ & Y^T(\underline{o} - \Xi\,\underline{d}) \succeq 0 \end{array} \tag{511}$$

4.11.2.2 Convergence

In §E.9 we discuss convergence of *alternating projection* on intersecting convex sets; convergence to a point in their intersection. Here the situation is a little different because sets of positive semidefinite matrices having an upper bound on rank are generally not convex. Yet in §7.1.3.0.1 we prove (507a) is equivalent to a projection of eigenvalues on a polyhedral cone $\mathcal{K}_{\mathcal{M}+}^{\mathbf{3}}$ (720):

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D - O)V_{\mathcal{N}}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq 3 \\ & D \in \mathbb{EDM}^N \end{array} \quad\equiv\quad \begin{array}{ll} \underset{\Upsilon}{\text{minimize}} & \|\Upsilon - \Lambda\|_{\mathrm{F}} \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}+}^{\mathbf{3}} \end{array} \tag{512}$$

where $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \stackrel{\Delta}{=} U\Upsilon U^T \in \mathbb{S}^{N-1}$ and $-V_{\mathcal{N}}^T O V_{\mathcal{N}} \stackrel{\Delta}{=} Q\Lambda Q^T \in \mathbb{S}^{N-1}$ are ordered diagonalizations (§A.5). It so happens: optimal orthogonal U always equals Q given. An operator T acting on matrix A, as in $T(A) = U^T A U$, is linear and bijective, hence an isomorphism; an isometry because the Frobenius norm is orthogonally invariant. (28) This isometric isomorphism T thus maps a non-convex problem to a convex one that preserves distance. The alternation (507) therefore converges to a point, in the set of all EDMs corresponding to affine dimension not in excess of 3, belonging to $\frac{1}{\sqrt{2}}\operatorname{dvec}\mathbb{EDM}^N \cap \Xi^T \mathcal{K}_{+\mathcal{M}}$.

We have not implemented the second half of the alternation (511) because memory-demands exceed the capability of our laptop computer.

4.11.3 Isotonic reconstruction, alternating projection

Perhaps a computationally simpler approach is to find a feasible point; (Boyd)

$$\begin{array}{ll} \text{find} & D \in \mathbb{EDM}^N \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq 3 \\ & \langle A_j \,,\, D\rangle \leq 0\,, \quad j = 1 \ldots N(N-1)/2 - 1 \end{array} \tag{513}$$

Pick an arbitrary starting point somewhere in the EDM cone corresponding to affine dimension 3, then alternately project (§E.9) on all the halfspaces specified by the inequalities and on the subset of the EDM cone corresponding to affine dimension not in excess of 3. The inequalities denote the known ordinal information; *e.g.*, for $D \in \mathbb{EDM}^{\mathbf{3}}$, ordinal data

$$d_{12} \leq d_{23} \leq d_{13} \tag{499}$$

would be represented by two inequalities where...

$$\begin{aligned} A_1 &= \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \frac{1}{2} \\ A_2 &= \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix} \frac{1}{2} \end{aligned} \tag{514}$$

4.11.3.0.1 Example... *Global positioning system (GPS).*
Twenty four satellites orbit the earth constantly transmitting...

```
http://www.trimble.com/gps/what.html

http://205.236.5.89/~eric/tril.html

here's one, related to GPS: suppose each of n nodes transmits a
pseudo-random code, and hears all others.   the clocks are not
synchronized, but each one is off by a fixed bias from a common clock.
then each node gets the distances to all other nodes, plus the
difference in clock offsets.  can you solve the problem of figuring out
the clock offsets?
```

□

4.12 Fifth Euclidean requirement

We continue now with the question raised in §4.3 regarding the necessity for at least one requirement more than the four axioms of the Euclidean metric (§4.2) to certify realizability of a bounded convex polyhedron or to reconstruct a generating list for it from incomplete distance information. There we saw the Euclidean axioms are necessary for $D\in\mathbb{EDM}^N$ in the case $N=3$, but become insufficient when the cardinality N exceeds 3 (regardless of affine dimension).

4.12.1 Recapitulate

In the particular case $N = 3$, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ (456) and $D\in\mathbb{S}_{\mathbf{0}}^{\mathbf{3}}$ are the necessary and sufficient conditions for D to be an EDM. From (458), the triangle inequality is then the only Euclidean constraint on the bounds of the necessarily nonnegative d_{ij}, and those bounds are tight. That means the four axioms of the Euclidean metric are necessary and sufficient requirements for D to be an EDM in the case $N=3$; for $i,j\in\{1,2,3\}$,

$$\begin{array}{l}\sqrt{d_{ij}} \geq 0,\ i \neq j\\ \sqrt{d_{ij}} = 0,\ i = j\\ \sqrt{d_{ij}} = \sqrt{d_{ji}}\\ \sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}\,,\ i\neq j\neq k\end{array} \quad\Leftrightarrow\quad \begin{array}{r}-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0\\ D\in\mathbb{S}_{\mathbf{0}}^{\mathbf{3}}\end{array} \quad\Leftrightarrow\quad D\in\mathbb{EDM}^{\mathbf{3}} \tag{515}$$

Yet the four axioms become insufficient when $N>3$.

4.12.2 Derivation of the fifth

Correspondence between the triangle inequality and the EDM was developed in §4.8.2 where a triangle inequality (458a) was revealed within the leading principal 2×2 submatrix of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ when positive semidefinite. Our choice of the leading principal submatrix was arbitrary; actually, a unique triangle inequality like (373) corresponds to any one of the $(N-1)!/(2!(N-1-2)!)$ principal 2×2 submatrices.[4.30] Assuming $D\in\mathbb{S}_{\mathbf{0}}^{\mathbf{4}}$

[4.30] There are fewer principal 2×2 submatrices in $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ than there are triangles made by four or more points because there are $N!/(3!(N-3)!)$ triangles made by point triples. The triangles corresponding to those submatrices all have vertex x_1. (*confer* §4.8.2.1) and $-V_{\mathcal{N}}^{T}DV_{\mathcal{N}}\in\mathbb{S}^{\mathbf{3}}$, then by the *positive (semi)definite principal submatrices theorem* (§A.3.1.0.4) it is sufficient to prove all d_{ij} are nonnegative, all triangle inequalities are satisfied, and $\det(-V_{\mathcal{N}}^{T}DV_{\mathcal{N}})$ is nonnegative. When $N=4$, in other words, that nonnegative determinant becomes the fifth and last Euclidean requirement for $D\in\mathbb{EDM}^N$. We now endeavor to ascribe geometric meaning to it.

4.12.2.1 Nonnegative determinant

By (379) when $D\in\mathbb{EDM}^{\mathbf{4}}$, $-V_{\mathcal{N}}^{T}DV_{\mathcal{N}}$ is equal to the inner product (374),

$$\Theta^T\Theta = \begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214} \\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314} \\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14} \end{bmatrix} \tag{516}$$

Because Euclidean space is an inner-product space, the more concise inner-product form of the determinant is admitted;

$$\det(\Theta^T\Theta) = -d_{12}d_{13}d_{14}\big(\cos^2\theta_{213}+\cos^2\theta_{214}+\cos^2\theta_{314}-2\cos\theta_{213}\cos\theta_{214}\cos\theta_{314}-1\big) \tag{517}$$

The determinant is nonnegative if and only if

$$\begin{array}{c}\cos\theta_{214}\cos\theta_{314}-\sqrt{\sin^2\theta_{214}\sin^2\theta_{314}}\;\leq\;\cos\theta_{213}\;\leq\;\cos\theta_{214}\cos\theta_{314}+\sqrt{\sin^2\theta_{214}\sin^2\theta_{314}}\\ \Leftrightarrow\\ \cos\theta_{213}\cos\theta_{314}-\sqrt{\sin^2\theta_{213}\sin^2\theta_{314}}\;\leq\;\cos\theta_{214}\;\leq\;\cos\theta_{213}\cos\theta_{314}+\sqrt{\sin^2\theta_{213}\sin^2\theta_{314}}\\ \Leftrightarrow\\ \cos\theta_{213}\cos\theta_{214}-\sqrt{\sin^2\theta_{213}\sin^2\theta_{214}}\;\leq\;\cos\theta_{314}\;\leq\;\cos\theta_{213}\cos\theta_{214}+\sqrt{\sin^2\theta_{213}\sin^2\theta_{214}}\end{array} \tag{518}$$

which simplifies, for $0\leq\theta_{i1\ell},\theta_{\ell1j},\theta_{i1j}\leq\pi$ and all $i\neq j\neq\ell\in\{2,3,4\}$, to

$$\cos(\theta_{i1\ell}+\theta_{\ell1j})\;\leq\;\cos\theta_{i1j}\;\leq\;\cos(\theta_{i1\ell}-\theta_{\ell1j}) \tag{519}$$

Analogously to triangle inequality (470), the determinant is 0 upon equality on either side of (519) which is tight. Inequality (519) can be equivalently written linearly as a "triangle inequality", but between relative angles [45, §1.4];

$$\begin{array}{c}|\theta_{i1\ell}-\theta_{\ell1j}|\;\leq\;\theta_{i1j}\;\leq\;\theta_{i1\ell}+\theta_{\ell1j}\\ \theta_{i1\ell}+\theta_{\ell1j}+\theta_{i1j}\;\leq\;2\pi\\ 0\leq\theta_{i1\ell},\theta_{\ell1j},\theta_{i1j}\leq\pi\end{array} \tag{520}$$

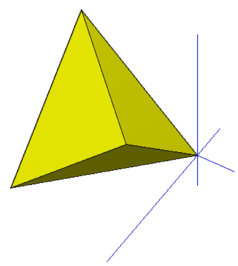


Figure 4.8: The *relative-angle inequality tetrahedron* (521) bounding $\mathbb{EDM}^4$ is regular; drawn in entirety. Each angle θ (371) must belong to the solid to be realizable.

Generalizing this:

Fifth Euclidean axiom - restatement. [86, §3.1] (*confer* §4.3.1) *Relative-angle inequality.* Augmenting the axioms of the Euclidean metric in $\mathbb{R}^n$, for all $i,j,\ell \neq k \in \{1 \ldots N\}$, $i<j<\ell$, and for $N \geq 4$ distinct points $\{x_k\}$, the inequalities

$$\begin{array}{cr} |\theta_{ik\ell} - \theta_{\ell kj}| \;\leq\; \theta_{ikj} \;\leq\; \theta_{ik\ell} + \theta_{\ell kj} & \text{(a)} \\ \theta_{ik\ell} + \theta_{\ell kj} + \theta_{ikj} \;\leq\; 2\pi & \text{(b)} \\ 0 \leq \theta_{ik\ell}\,, \theta_{\ell kj}\,, \theta_{ikj} \leq \pi & \text{(c)} \end{array} \tag{521}$$

where $\theta_{ikj} = \theta_{jki}$ is the angle between vectors at vertex x_k as defined in (371), must be satisfied at each point x_k regardless of affine dimension.

$\diamond$

Because point labelling is arbitrary, this fifth Euclidean metric requirement must apply to each of the N points as though each were in turn labelled x_1; hence the new index k in (521). Just as the triangle inequality is the ultimate test for realizability of only three points, the *relative-angle inequality* is the ultimate test for only four. For four distinct points, the triangle inequality remains a necessary although penultimate test;

$$\begin{array}{l} \text{Four Euclidean axioms (§4.2).} \\ \text{Angle } \theta \text{ inequality (328) or (521).} \end{array} \;\Leftrightarrow\; \begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^{\mathbf{4}} \end{array} \;\Leftrightarrow\; D = \mathbf{D}(\Theta) \in \mathbb{EDM}^{\mathbf{4}} \tag{522}$$

The *relative-angle inequality*, for this case, is illustrated in Figure **4.8**.

4.12.2.2 Beyond the fifth axiom

When the cardinality N exceeds 4, the four axioms of the Euclidean metric and the *relative-angle inequality* together become insufficient conditions for realizability. In other words, the Euclidean axioms and *relative-angle inequality* remain necessary but become a sufficient test of only the positive semidefiniteness of all the principal 3×3 submatrices in $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$. The *relative-angle inequality* can be considered a sufficient test of integrity at each point x_k for every purported tetrahedron.

When $N = 5$ in particular, the *relative-angle inequality* becomes the penultimate Euclidean requirement while nonnegativity of then unwieldy $\det(\Theta^T\Theta)$ corresponds (by the *positive (semi)definite principal submatrices theorem* in §A.3.1.0.4) to the sixth and last Euclidean requirement, and so on.

Yet for all values of N, only assuming nonnegative d_{ij}, the relative-angle matrix inequality in (472) is necessary and sufficient to certify realizability; (§4.4.3.1)

$$\begin{array}{l}\text{Euclidean axiom 1 (§4.2).}\\ \text{Angle matrix inequality } \Omega\succeq 0 \text{ (380).}\end{array} \;\Leftrightarrow\; \begin{array}{r}-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0\\ D\in\mathbb{S}_{\mathbf{0}}^N\end{array} \;\Leftrightarrow\; D=\mathbf{D}(\Omega\,,d)\in\mathbb{EDM}^N \tag{523}$$

Like matrix criteria (329), (352), and (472), the relative-angle matrix inequality and nonnegativity axiom subsume all the Euclidean axioms and further requirements.

4.12.3 Path not followed

An alternate and intuitively appealing way to augment the Euclidean axioms is to recognize, in the case $N=4$, the three-dimensional analogue to triangle & distance is tetrahedron & facet-area, while in the case $N=5$ the four-dimensional analogue to triangle & distance is polychoron & facet-volume, *ad infinitum.*

4.12.3.1 $N = 4$

Each of the four facets of a general tetrahedron is a triangle and its relative interior. Suppose we identify each facet of the tetrahedron by its area-squared:

c_1, c_2, c_3, c_4. Then analogous to axiom 4, we may write a tight[4.31] area inequality for the facets

$$\sqrt{c_i} \;\leq\; \sqrt{c_j} + \sqrt{c_k} + \sqrt{c_\ell}\,, \quad i\neq j\neq k\neq \ell\in\{1,2,3,4\} \tag{524}$$

which is a generalized "triangle" inequality [38, §1.1] that follows from

$$\sqrt{c_i} = \sqrt{c_j}\cos\varphi_{ij} + \sqrt{c_k}\cos\varphi_{ik} + \sqrt{c_\ell}\cos\varphi_{i\ell} \tag{525}$$

[101] [48, *Law of Cosines*] where φ_{ij} is the *dihedral* angle at the common edge between triangular facets i and j.

If D is the EDM corresponding to the whole tetrahedron, then area-squared of the i^{th} triangular facet has a convenient formula in terms of $D_i\in\mathbb{EDM}^{N-1}$ the EDM corresponding to that particular facet: From the *Cayley-Menger determinant*[4.32] for simplices, [48] [102] [84, §4] [22, §3.3] the i^{th} facet area-squared for $i\in\{1\ldots N\}$ is (§A.4.2)

$$\begin{aligned}
c_i \;&=\; \frac{-1}{2^{N-2}(N-2)!^2}\;\det\begin{bmatrix} -D_i & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} && (526)\\
&=\; \frac{(-1)^N}{2^{N-2}(N-2)!^2}\;\det D_i\left(\mathbf{1}^T D_i^{-1}\mathbf{1}\right) && (527)\\
&=\; \frac{(-1)^N}{2^{N-2}(N-2)!^2}\,\mathbf{1}^T\operatorname{cof}(D_i)^T\mathbf{1} && (528)
\end{aligned}$$

where D_i is the i^{th} principal $N-1\times N-1$ submatrix[4.33] of $D\in\mathbb{EDM}^N$, and $\operatorname{cof}(D_i)$ is the $N-1\times N-1$ matrix of *cofactors*[4.34] [26, §4] corresponding to D_i. The number of principal 3×3 submatrices in D is, of course, equal to the number of triangular facets in the tetrahedron; four $(N!/(3!(N-3)!))$ when $N=4$.

The triangle inequality (axiom 4) and area inequality (524) are conditions necessary for D to be an EDM; we do not prove their sufficiency in conjunction with the remaining three axioms.

[4.31] The upper bound is met when all angles in (525) are simultaneously 0; that occurs, for example, if one point is relatively interior to the convex hull of the three remaining.

[4.32] whose foremost characteristic is: the determinant vanishes if and only if affine dimension does not equal or exceed penultimate cardinality; *id est*, $\det\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} = 0 \Leftrightarrow r < N-1$, where D is any EDM (§4.7.3.0.1). Otherwise, the determinant is negative.

[4.33] Every principal submatrix of an EDM remains an EDM. [86, §4.1]

[4.34] Hence c_i is a linear function of the entries of D_i; even when D_i is singular.

4.12.3.2 $N = 5$

Moving to the next level, we might encounter a Euclidean object called polychoron, a bounded polyhedron in four dimensions.[4.35] The polychoron has five $(N!/(4!(N-4)!))$ facets, each of them a general tetrahedron whose volume-squared c_i is calculated using the same formula; (526) where D is the EDM corresponding to the polychoron, and D_i is the EDM corresponding to the i^{th} facet (the principal 4×4 submatrix of $D\in\mathbb{EDM}^N$ corresponding to the i^{th} tetrahedron). The analogue to triangle & distance is now polychoron & facet-volume. We could then write another generalized "triangle" inequality like (524) but in terms of facet volume; [103, §IV]

$$\sqrt{\mathrm{c}_i} \;\leq\; \sqrt{\mathrm{c}_j} + \sqrt{\mathrm{c}_k} + \sqrt{\mathrm{c}_\ell} + \sqrt{\mathrm{c}_m}\;, \quad i\neq j\neq k\neq \ell\neq m\in\{1\ldots 5\} \tag{529}$$

Now, for $N = 5$, the triangle (distance) inequality (§4.2) and the area inequality (524) and the volume inequality (529) are conditions necessary for D to be an EDM. We do not prove their sufficiency.

4.12.3.3 Volume of simplices

There is no known formula for the volume of a bounded convex polyhedron expressed either by halfspace or vertex-description. [4, §2.1] [104, p.173] [105] [75] [76] Volume is a concept germane to $\mathbb{R}^{\mathbf{3}}$; in higher dimensions it is called *content*. Applying the *EDM assertion* (§4.9.1) and a result given in [1, §8.3.1], a general nonempty simplex (§2.7.3) in $\mathbb{R}^{N-1}$ corresponding to an EDM $D\in\mathbb{S}_{\mathbf{0}}^N$ has content

$$\sqrt{\mathrm{c}} = \mathrm{content}(\mathcal{S})\;\det{}^{1/2}(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) \tag{530}$$

where the content-squared of the unit simplex $\mathcal{S}\subset\mathbb{R}^{N-1}$ is proportional to its Cayley-Menger determinant;

$$\mathrm{content}(\mathcal{S})^2 = \frac{-1}{2^{N-1}(N-1)!^2}\,\det\begin{bmatrix} -\mathbf{D}([\,\mathbf{0}\;\; e_1\;\; e_2\;\; \cdots\;\; e_{N-1}\,]) & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \tag{531}$$

where $e_i\in\mathbb{R}^{N-1}$ and the EDM definition used is $\mathbf{D}(X)$ (333).

[4.35] The simplest polychoron is called a pentatope [48]; a regular simplex hence convex. (A *pentahedron* is a three-dimensional object having five vertices.)

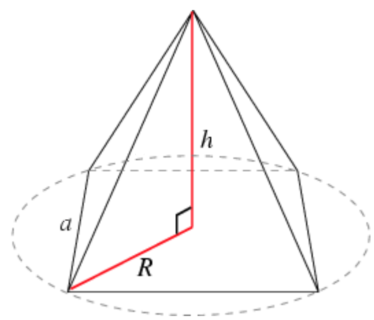


Figure 4.9: The length of one-dimensional face a equals the height $h = a = 1$ of this non-simplicial pyramid in $\mathbb{R}^3$ with square base inscribed in a circle of radius R centered at the origin. [48, *Pyramid*]

Example. *Pyramid.* A formula for volume of a pyramid is known;[4.36] it is 1/3 the product of its base area with its height. [57] The pyramid in Figure **4.9** has volume 1/3. To find its volume using EDMs, we must first decompose the pyramid into simplicial parts. Slicing it along the plane containing the line segments corresponding to radius R and height h we find the vertices of one simplex,

$$X = \begin{bmatrix} 1/2 & 1/2 & -1/2 & 0 \\ 1/2 & -1/2 & -1/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{n \times N} \tag{532}$$

where $N = n+1$ for any nonempty simplex in $\mathbb{R}^n$. The volume of this simplex is half that of the entire pyramid; *id est*, $\sqrt{\mathrm{c}} = 1/6$ found by evaluating (530).

$\square$

With that, we conclude the digression of path.

[4.36] Pyramid volume is independent of the paramount vertex position as long as its height remains constant.

4.12.4 Affine dimension reduction in three dimensions

(*confer* §4.8.4) The determinant of any $M\times M$ matrix is equal to the product of its M eigenvalues. [26, §5.1] When $N=4$ and $\det(\Theta^T\Theta)$ is 0, that means one or more eigenvalues of $\Theta^T\Theta\in\mathbb{R}^{\mathbf{3\times3}}$ are 0. The determinant will go to 0 whenever equality is attained on either side of (328), (521a), or (521b), meaning that a tetrahedron has collapsed to a lower affine dimension; *id est*, $r=\operatorname{rank}\Theta^T\Theta=\operatorname{rank}\Theta$ is reduced below $N-1$ exactly by the number of 0 eigenvalues (§4.7.2).

Therefore, in solving completion problems of any size N where one or more entries of an EDM are unknown, the dimension r of the affine hull required to contain the unknown points is potentially reduced by selecting distances to attain equality in (328) or (521a) or (521b).

4.12.4.1 *Exemplum redux*

We now apply the *fifth Euclidean axiom* to an earlier problem:

Example. *Small completion problem*, III. Returning again to the Example on page 132 that pertains to Figure **4.2** where $N=4$ (*confer* §4.9.3), d_{14} is ascertainable from the fifth Euclidean metric requirement. Because all distances in (326) are known except $\sqrt{d_{14}}$, $\cos\theta_{123}=0$ and $\theta_{324}=0$ result from identity (371). Applying (328),

$$\begin{array}{rcccl}\cos(\theta_{123}+\theta_{324}) & \leq & \cos\theta_{124} & \leq & \cos(\theta_{123}-\theta_{324})\\ 0 & \leq & \cos\theta_{124} & \leq & 0\end{array}\tag{533}$$

It follows from (371) that d_{14} can only be 2. Because equality is attained in (533), the affine dimension r cannot exceed $N-2$, as explained. $\square$

4.13 EDM-entry composition

Results of Schoenberg from 1938 can be used to show that certain nonlinear compositions of individual EDM entries yield more EDMs; Laurent [86, §2.3] claims, in particular,

$$D\in\mathbb{EDM}^N \;\Leftrightarrow\; 1-e^{-\alpha D}\triangleq[1-e^{-\alpha d_{ij}}]\in\mathbb{EDM}^N \quad \forall\,\alpha>0\tag{534}$$

(a)

(b)

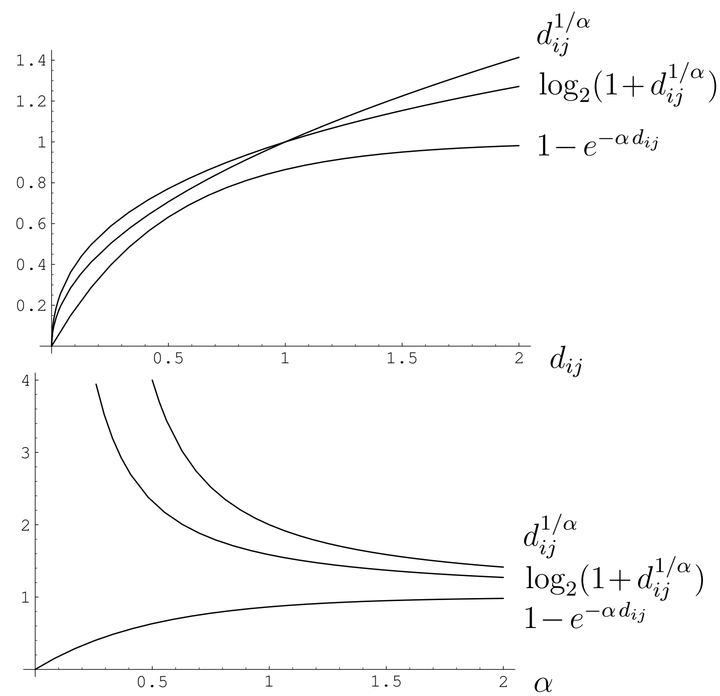


Figure 4.10: Some entry-wise EDM compositions: **(a)** $\alpha = 2$. Concave nondecreasing in d_{ij}. **(b)** Trajectory convergence in α for $d_{ij} = 2$.

Schoenberg's results suggest that certain finite positive roots of EDM entries produce another EDM; [106, §6, thm.5] (*confer* [38, p.108-109]) specifically,

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; D^{1/\alpha} \triangleq [d_{ij}^{1/\alpha}] \in \mathbb{EDM}^N \quad \forall\, \alpha > 1 \tag{535}$$

The special case $\alpha = 2$ is of interest because it corresponds to absolute distance.

Assuming that points constituting a corresponding list X are distinct (453) and because $D \in \mathbb{S}_{\mathbf{0}}^N$, then it follows:

$$\lim_{\alpha\to\infty} D^{1/\alpha} = \lim_{\alpha\to\infty} 1 - e^{-\alpha D} = -E \triangleq \mathbf{1}\mathbf{1}^T - I \tag{536}$$

Negative elementary matrix $-E$ (§B.3) is interior to the EDM cone (§5.4) and terminal to the respective trajectories (534) and (535) as functions of α. Both trajectories never leave the EDM cone; in engineering terms, the EDM cone is an *invariant set* [107] to either trajectory. Further, if D is not an EDM but for some particular α_p it becomes an EDM, then for all greater values of α it will remain an EDM.

These preliminary findings lead one to speculate whether any concave nondecreasing composition of individual EDM entries d_{ij} on $\mathbb{R}_+$ will produce another EDM; *e.g.*, empirical evidence suggests that given EDM D, for each fixed $\alpha \geq 1$ [*sic*] the composition $[\log_2(1 + d_{ij}^{1/\alpha})]$ is also an EDM. Figure **4.10** illustrates its concavity in d_{ij} together with functions (534) and (535).

4.14 EDM indefiniteness

By the known result in §A.7.1 regarding a 0-valued entry on the main diagonal of a symmetric positive semidefinite matrix, there can be no positive nor negative semidefinite EDM except the $\mathbf{0}$ matrix because $\mathbb{EDM}^N \subseteq \mathbb{S}_{\mathbf{0}}^N$ (332) and

$$\mathbb{S}_{\mathbf{0}}^N \cap \mathbb{S}_+^N = \mathbf{0} \tag{537}$$

the origin. So when $D \in \mathbb{EDM}^N$, there can be no factorization $D = A^T A$ nor $-D = A^T A$. [26, §6.3] Hence the eigenvalues of an EDM are neither all nonnegative or all nonpositive; an EDM is indefinite and possibly invertible.

4.14.1 EDM eigenvalues, congruence transformation

For any symmetric $-D$, we can characterize its eigenvalues by congruence transformation: [26, §6.3]

$$-W^TDW = -\begin{bmatrix} V_{\mathcal{N}}^T \\ \mathbf{1}^T \end{bmatrix} D\,[\,V_{\mathcal{N}} \quad \mathbf{1}\,] = -\begin{bmatrix} V_{\mathcal{N}}^T D V_{\mathcal{N}} & V_{\mathcal{N}}^T D\mathbf{1} \\ \mathbf{1}^T D V_{\mathcal{N}} & \mathbf{1}^T D\mathbf{1} \end{bmatrix} \tag{538}$$

Because

$$W \triangleq [\,V_{\mathcal{N}} \quad \mathbf{1}\,] \in \mathbb{R}^{N\times N} \tag{539}$$

is full-rank, then (891)

$$\operatorname{inertia}(-D) = \operatorname{inertia}\big(-W^TDW\big) \tag{540}$$

the congruence (538) has the same number of positive, zero, and negative eigenvalues as $-D$. Further, if we denote by σ_i, $i=1\ldots N-1$, the eigenvalues of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$, and the eigenvalues of the congruence $-W^TDW$ by ζ_i, $i=1\ldots N$, and if we arrange each respective set of eigenvalues in nonincreasing order, then by theory of *interlacing eigenvalues for bordered symmetric matrices*, [28, §4.3] [26, §6.4] [99, §IV.4.1]

$$\zeta_N \leq \sigma_{N-1} \leq \zeta_{N-1} \leq \sigma_{N-2} \leq \cdots \leq \sigma_2 \leq \zeta_2 \leq \sigma_1 \leq \zeta_1 \tag{541}$$

When $D\in\mathbb{EDM}^N$, $\sigma_i \geq 0$ for all i (845) because $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ as we now know. That means the congruence must have $N-1$ nonnegative eigenvalues; $\zeta_i \geq 0$, $i=1\ldots N-1$. The remaining eigenvalue ζ_N cannot be nonnegative because then $-D$ would be positive semidefinite, an impossibility; so $\zeta_N < 0$. By congruence, nontrivial $-D$ must therefore have one and only one negative eigenvalue;[4.37] [50, §2.4.5]

$$D \in \mathbb{EDM}^N \Rightarrow \begin{cases} \lambda(-D)_i \geq 0\,, \quad i=1\ldots N-1 \\ \sum\limits_{i=1}^{N} \lambda(-D)_i = 0 \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{cases} \tag{542}$$

[4.37] All the entries of the corresponding eigenvector must have the same sign with respect to each other because that eigenvector is the *Perron vector* corresponding to the spectral radius; [28, §8.2.6] the predominant characteristic of negative [*sic*] matrices.

where the $\lambda(-D)_i$ are eigenvalues of $-D$ whose sum must be 0 only because $\operatorname{tr} D = 0$. [26, §5.1] Yet this condition is insufficient to determine whether some given $H \in \mathbb{S}^N_{\mathbf{0}}$ is an EDM, as shown by counter-example.[4.38]

4.14.2 Spectral cone

Here we draw heavily from Chapter 2 with regard to polyhedral cones and their duals.

Denoting the eigenvalues of $\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \in \mathbb{S}^{N+1}$ by

$$\lambda\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}\right) \in \mathbb{R}^{N+1} \tag{543}$$

we have the Cayley-Menger form (*confer* §4.12.3.1) of necessary and sufficient conditions for $D \in \mathbb{EDM}^N$ from the literature; [97, §3][4.39] [108, §3] (*confer* (352) (329))

$$D \in \mathbb{EDM}^N \Leftrightarrow \left\{ \begin{array}{l} \lambda\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}\right)_i \geq\, 0\,, \quad i=1\ldots N \\[2ex] \lambda\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}\right)^T \mathbf{1} = 0 \\[2ex] D \in \mathbb{S}^N_{\mathbf{0}} \end{array} \right. \tag{544}$$

When D is an EDM, the eigenvalues $\lambda\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}\right)$ belong to the particular orthant in $\mathbb{R}^{N+1}$ having the $N+1^{\text{th}}$ coordinate as the sole negative coordinate;[4.40]

$$\mathbb{R}^{N+1}_{N+1-} \triangleq \text{cone}\{e_1\,,\ e_2\,,\ \cdots\ e_N\,,\ -e_{N+1}\} \tag{545}$$

[4.38] When $N=3$, for example, the symmetric hollow matrix

$$H = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 5 \\ 1 & 5 & 0 \end{bmatrix} \in \mathbb{S}^N_{\mathbf{0}}$$

is not an EDM, although $\lambda(-H) = \{5,\ 0.3723,\ -5.3723\}$ conforms to (542).

[4.39] Recall that for $D \in \mathbb{S}^N_{\mathbf{0}}$, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ subsumes nonnegativity axiom 1 (§4.8.1).

[4.40] We observe, empirically, all except one entry of the corresponding eigenvector have the same sign with respect to each other.

When the eigenvalues are ordered, the constraints (544) specify membership to a pointed polyhedral *spectral cone* for $\begin{bmatrix} -\mathbb{EDM}^N & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}$:

$$\begin{aligned} \mathcal{K}_\lambda &= \{\zeta \in \mathbb{R}^{N+1} \mid \zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_N \geq 0 \geq \zeta_{N+1}\ ,\ \mathbf{1}^T\zeta = 0\} \\ &= \mathcal{K}_\mathcal{M} \cap \mathbb{R}^{N+1}_{N+1\text{-}} \cap \partial\mathcal{H} \\ &= \lambda\left(\begin{bmatrix} -\mathbb{EDM}^N & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}\right) \end{aligned} \tag{546}$$

where

$$\partial\mathcal{H} = \{\zeta \in \mathbb{R}^{N+1} \mid \mathbf{1}^T\zeta = 0\} \tag{547}$$

is a hyperplane through the origin, and $\mathcal{K}_\mathcal{M}$ is the monotone cone (§2.9.2.2.2) which has nonempty interior but is not pointed;

$$\mathcal{K}_\mathcal{M} \stackrel{\Delta}{=} \{\zeta \in \mathbb{R}^{N+1} \mid \zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_{N+1}\} \tag{251}$$

$$\mathcal{K}^*_\mathcal{M} = \{\, [\, e_1 - e_2 \;\; e_2 - e_3 \;\; \cdots \;\; e_N - e_{N+1} \,]\, a \mid a \succeq 0 \,\} \subset \mathbb{R}^{N+1} \tag{252}$$

So,

$$\dim \operatorname{aff} \mathcal{K}_\lambda \;=\; \dim \partial\mathcal{H} \;=\; N \tag{548}$$

indicating $\mathcal{K}_\lambda$ has empty interior. Defining

$$A \stackrel{\Delta}{=} \begin{bmatrix} e_1^T - e_2^T \\ e_2^T - e_3^T \\ \vdots \\ e_N^T - e_{N+1}^T \end{bmatrix} \in \mathbb{R}^{N \times N+1}\,, \qquad B \stackrel{\Delta}{=} \begin{bmatrix} e_1^T \\ e_2^T \\ \vdots \\ e_N^T \\ -e_{N+1}^T \end{bmatrix} \in \mathbb{R}^{N+1 \times N+1} \tag{549}$$

we have the halfspace-description:

$$\mathcal{K}_\lambda \stackrel{\Delta}{=} \{\zeta \in \mathbb{R}^{N+1} \mid A\zeta \succeq 0\,,\ B\zeta \succeq 0\,,\ \mathbf{1}^T\zeta = 0\} \tag{550}$$

From (550) and (259) we get a vertex-description for the pointed spectral cone having empty interior:

$$\mathcal{K}_\lambda = \left\{ \tilde{V}_\mathcal{N}\left(\begin{bmatrix} \hat{A} \\ \hat{B} \end{bmatrix} \tilde{V}_\mathcal{N}\right)^{\dagger} b \mid b \succeq 0 \right\} \tag{551}$$

where $\tilde{V}_{\mathcal{N}} \in \mathbb{R}^{N+1\times N}$ and where $\hat{B} = e_N^T \in \mathbb{R}^{\mathbf{1}\times N+1}$ and

$$\hat{A} = \begin{bmatrix} e_1^T - e_2^T \\ e_2^T - e_3^T \\ \vdots \\ e_{N-1}^T - e_N^T \end{bmatrix} \in \mathbb{R}^{N-1\times N+1} \tag{552}$$

hold those rows of A and B corresponding to conically independent rows in $\begin{bmatrix} A \\ B \end{bmatrix} \tilde{V}_{\mathcal{N}}$. The vertex-description of the non-pointed dual spectral cone having nonempty interior is, (179)

$$\begin{aligned} \mathcal{K}_\lambda^* &= \overline{\mathcal{K}_{\mathcal{M}}^* + \mathbb{R}_{N+1\text{-}}^{N+1^*} + \partial\mathcal{H}^*} \subseteq \mathbb{R}^{N+1} \\ &= \left\{ \begin{bmatrix} A^T & B^T & \mathbf{1} & -\mathbf{1} \end{bmatrix} b \mid b \succeq 0 \right\} = \left\{ \begin{bmatrix} \hat{A}^T & \hat{B}^T & \mathbf{1} & -\mathbf{1} \end{bmatrix} a \mid a \succeq 0 \right\} \end{aligned} \tag{553}$$

From (551) and (260) we get a halfspace-description:

$$\mathcal{K}_\lambda^* = \{ y \in \mathbb{R}^{N+1} \mid (\tilde{V}_{\mathcal{N}}^T [\, \hat{A}^T \;\; \hat{B}^T \,])^\dagger \tilde{V}_{\mathcal{N}}^T y \succeq 0 \} \tag{554}$$

The polyhedral dual spectral cone $\mathcal{K}_\lambda^*$ is closed, convex, has nonempty interior because $\mathcal{K}_\lambda$ is pointed, but is not pointed because $\mathcal{K}_\lambda$ has empty interior.

For eigenvalues arranged in nonincreasing order, (544) can be restated

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \left\{ \begin{array}{l} \lambda\left(\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \right) \in \mathcal{K}_\lambda \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array} \right. \tag{555}$$

4.14.3 Eigenvalues of $-VDV$ *versus* $-V_{\mathcal{N}}^\dagger D V_{\mathcal{N}}$

Suppose for $D \in \mathbb{EDM}^N$ we are given eigenvectors $v_i \in \mathbb{R}^N$ of $-VDV$ and corresponding eigenvalues $\lambda \in \mathbb{R}^N$ so that

$$-VDVv_i = \lambda_i v_i \,, \quad i = 1 \ldots N \tag{556}$$

where $V = V_{\mathcal{N}} V_{\mathcal{N}}^\dagger = V_{\mathcal{W}} V_{\mathcal{W}}^T \in \mathbb{S}^N$ is the auxiliary geometric centering matrix (§B.4). From these we can determine the eigenvectors and eigenvalues of $-V_{\mathcal{N}}^\dagger D V_{\mathcal{N}}$ and $-V_{\mathcal{W}}^T D V_{\mathcal{W}}$: Define

$$\nu_i \triangleq V_{\mathcal{N}}^\dagger v_i \,, \quad \lambda_i \neq 0 \tag{557}$$

Then we have

$$-\,VDV_{\mathcal{N}}V_{\mathcal{N}}^{\dagger}\,v_i = \lambda_i\,v_i \tag{558}$$
$$-V_{\mathcal{N}}^{\dagger}VDV_{\mathcal{N}}\,\nu_i = \lambda_i V_{\mathcal{N}}^{\dagger}\,v_i \tag{559}$$
$$-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}\,\nu_i = \lambda_i\,\nu_i \tag{560}$$

the eigenvectors of $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$ are given by (557) while its corresponding nonzero eigenvalues are identical to those of $-VDV$ although $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$ is not necessarily positive semidefinite.

Similarly we can show the eigenvectors of $-V_{\mathcal{W}}^{T}DV_{\mathcal{W}}$ are $V_{\mathcal{W}}^{T}v_i$ corresponding to its nonzero eigenvalues which are identical to those of $-VDV$.

4.15 DFT

The discrete Fourier transform (DFT) is a staple of the digital signal processing community. [109] In essence, the DFT is a correlation of a rectangularly windowed sequence (or *discrete signal*) with exponentials whose frequencies are equispaced on the unit circle.[4.41] The DFT of the sequence $f \triangleq [f_i\,,\ i=0\ldots n-1]\in\mathbb{C}^n$ is, in traditional form[4.42] for $k\in\{0\ldots n-1\}$,

$$F_k = \sum_{i=0}^{n-1} f_i\, e^{-\jmath\, i2\pi k/n} \tag{561}$$

where $\jmath \triangleq \sqrt{-1}$. Sequence $F \triangleq [F_k\,,\ k=0\ldots n-1]\in\mathbb{C}^n$ is considered a frequency spectral analysis of the signal sequence f; *id est*, the F_k are amplitudes of exponentials which, when combined, give back the original sequence,

$$f_i = \frac{1}{n}\sum_{k=0}^{n-1} F_k\, e^{\jmath\, i2\pi k/n} \tag{562}$$

Index k in F_k references the discrete frequencies $2\pi k/n$ of the exponential $e^{\jmath\, i2\pi k/n}$ in the synthesis equation (562).

The matrix form of the DFT is written

$$F = W^H f \tag{563}$$

[4.41] on the unit circle in the z plane; $z = e^{sT}$ where $s = \sigma + \jmath\omega$ is the traditional Laplace frequency, ω is the Fourier frequency in radians, and T is the sample period in seconds.

[4.42] The convention is: lowercase for the sequence and uppercase for its transform.

where the *DFT matrix* is[4.43]

$$W \triangleq \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & e^{\jmath 2\pi/n} & e^{\jmath 4\pi/n} & \cdots & e^{\jmath(n-1)2\pi/n} \\ 1 & e^{\jmath 4\pi/n} & e^{\jmath 8\pi/n} & \cdots & e^{\jmath(n-1)4\pi/n} \\ 1 & e^{\jmath 6\pi/n} & e^{\jmath 12\pi/n} & \cdots & e^{\jmath(n-1)6\pi/n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & e^{\jmath(n-1)2\pi/n} & e^{\jmath(n-1)4\pi/n} & \cdots & e^{\jmath(n-1)^2 2\pi/n} \end{bmatrix} \in \mathbb{C}^{n\times n} \tag{564}$$

characterized by

$$W^T = W \tag{565}$$

$$W^{-1} = \frac{1}{n}\, W^H \tag{566}$$

where superscript $_H$ denotes conjugate transpose. Similarly, the IDFT is

$$f = \frac{1}{n} W F \tag{567}$$

Direct computation of (563) or (567) would require $O(n^2)$ operations for large n. Optimization of computational intensity for the DFT culminated in the development of the fast Fourier transform (FFT) algorithm whose intensity is $O(n\log_2(n))$, as is well known. [110]

4.15.1 DFT via EDM

There is a relationship between EDMs and the DFT. The norm of the difference of any two complex vectors $x, y \in \mathbb{C}^n$ is

$$\|x-y\|^2 \;=\; (x-y)^H(x-y) \;=\; \|\mathrm{Re}(x-y)\|^2 + \|\mathrm{Im}(x-y)\|^2 \tag{568}$$

Consider applying this Euclidean metric to a list comprising the Fourier exponentials and the signal sequence; *id est*, to $\{x_\ell \in \mathbb{C}^n,\ \ell = 1 \ldots N\}$ where

$$\begin{aligned} x_\ell &= \left[e^{-\jmath\, i 2\pi(\ell-1)/n},\ i = 0 \ldots n-1\right] \in \mathbb{C}^n\,, \quad \ell \in \{1 \ldots N-1\} \\ x_N &= [f_i\,,\ i = 0 \ldots n-1] \in \mathbb{C}^n \end{aligned} \tag{569}$$

where

$$N = n+1 \tag{570}$$

[4.43] conjugate to that of some other authors.

The EDM

$$D \triangleq \left[\, \|x_\ell - x_m\|^2 ,\;\; \ell\,, m\!=\!1\ldots N \times 1\ldots N \,\right] \tag{571}$$

is then constituted, for $\ell\,, m\!=\!1\ldots N\!-\!1 \times 1\ldots N\!-\!1$, by

$$\begin{aligned}\|\mathrm{Re}(x_\ell - x_m)\|^2 &= \sum_{i=0}^{n-1} \big(\cos(i2\pi(\ell\!-\!1)/n) \;-\; \cos(i2\pi(m\!-\!1)/n)\big)^2\\ \|\mathrm{Im}(x_\ell - x_m)\|^2 &= \sum_{i=0}^{n-1} \big(\sin(i2\pi(\ell\!-\!1)/n) \;-\; \sin(i2\pi(m\!-\!1)/n)\big)^2\end{aligned} \tag{572}$$

$$d_{\ell m} = 2\left(n - \sum_{i=0}^{n-1} \cos(2i(\ell - m)\pi/n)\right) = \begin{cases} 2n\,, & \ell \neq m\\ 0\,, & \text{otherwise}\end{cases} \tag{573}$$

while the last row is constituted, for $m\!=\!1\ldots N\!-\!1$, by

$$\begin{aligned}\|\mathrm{Re}(x_N - x_m)\|^2 &= \sum_{i=0}^{n-1} \big(\mathrm{Re}f_i \;-\; \cos(i2\pi(m\!-\!1)/n)\big)^2\\ &= \sum_{i=0}^{n-1} (\mathrm{Re}f_i)^2 \;-\; 2\mathrm{Re}f_i \cos(i2\pi(m\!-\!1)/n) \;+\; \cos^2(i2\pi(m\!-\!1)/n)\\ &= \tfrac{1}{4n}\sum_{k=0}^{n-1} |F_k + F_{n-k}^*|^2 - \mathrm{Re}(F_{m-1} + F_{n-m+1}^*) + \sum_{i=0}^{n-1} \cos^2(i2\pi(m\!-\!1)/n)\end{aligned} \tag{574}$$

$$\begin{aligned}\|\mathrm{Im}(x_N - x_m)\|^2 &= \sum_{i=0}^{n-1} \big(\mathrm{Im}f_i \;+\; \sin(i2\pi(m\!-\!1)/n)\big)^2\\ &= \sum_{i=0}^{n-1} (\mathrm{Im}f_i)^2 \;+\; 2\mathrm{Im}f_i \sin(i2\pi(m\!-\!1)/n) \;+\; \sin^2(i2\pi(m\!-\!1)/n)\\ &= \tfrac{1}{4n}\sum_{k=0}^{n-1} |F_k - F_{n-k}^*|^2 + \mathrm{Re}(F_{m-1} - F_{n-m+1}^*) + \sum_{i=0}^{n-1} \sin^2(i2\pi(m\!-\!1)/n)\end{aligned} \tag{575}$$

$$d_{Nm} = \frac{1}{4n}\sum_{k=0}^{n-1} |F_k + F_{n-k}^*|^2 + |F_k - F_{n-k}^*|^2 - 2\mathrm{Re}F_{n-m+1} + n \tag{576}$$

where $F_n \triangleq F_0$ due to transform periodicity, and where Parseval's relation[4.44] [111] [43] is substituted as well as sine and cosine transforms [112] of real and imaginary signals[4.45] [109, §8.8]. Thus exists the relationship between EDM

[4.44]The Fourier summation $\sum |F_k|^2/n$ is equivalent to $\sum |f_i|^2$.

[4.45]The complex conjugate of F is indicated by F^*. Some physical systems, such as Magnetic Resonance Imaging (MRI) devices [113] [114], naturally produce signals originating in the Fourier domain.

and DFT. Only the last row and column of the EDM depends on the sequence f itself. The remaining entries (573) depend only on sequence length n.

4.15.1.0.1 Example. *IDFT.* To relate the DFT to its associated EDM D in a useful way, consider finding the inverse discrete Fourier transform (IDFT). Assuming the signal is real, then we have

$$D = \begin{bmatrix} (\mathbf{1}\mathbf{1}^T - I)2n & [d_{Nm}\,,\ m=1\ldots N-1] \\ [d_{Nm}\,,\ m=1\ldots N-1]^T & 0 \end{bmatrix} \in \mathbb{EDM}^N \tag{577}$$

where

$$d_{Nm} = \frac{1}{n}\sum_{k=0}^{n-1}|F_k|^2 - 2\mathrm{Re}F_{m-1} + n \tag{578}$$

Assume $n=4$, $N=5$, and we are given the DFT $F=[4\ \ 0\ \ 0\ \ 0]^T$. Then

$$D = \begin{bmatrix} 0 & 8 & 8 & 8 & 0 \\ 8 & 0 & 8 & 8 & 8 \\ 8 & 8 & 0 & 8 & 8 \\ 8 & 8 & 8 & 0 & 8 \\ 0 & 8 & 8 & 8 & 0 \end{bmatrix} \tag{579}$$

We seek to recover the signal vector $x_5=f$. Cholesky factorization (§F.1.1.5) $\Theta^T\Theta \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{R}^{N-1\times N-1}$ yields (377);

$$\Theta = \begin{bmatrix} 2\sqrt{2} & \sqrt{2} & \sqrt{2} & 0 \\ 0 & \sqrt{6} & \sqrt{2/3} & 0 \\ 0 & 0 & 4/\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \triangleq [\,\tilde{x}_2 - \tilde{x}_1 \quad \tilde{x}_3 - \tilde{x}_1 \quad \tilde{x}_4 - \tilde{x}_1 \quad \tilde{x}_5 - \tilde{x}_1\,] \tag{580}$$

In this circumstance, x_1 through x_4 are always known from (569); *id est*, we always know, for any length-4 DFT,

$$[\,x_2 - x_1 \quad x_3 - x_1 \quad x_4 - x_1\,] = \begin{bmatrix} 0 & 0 & 0 \\ -1-\jmath & -2 & -1+\jmath \\ -2 & 0 & -2 \\ -1+\jmath & -2 & -1-\jmath \end{bmatrix} \tag{581}$$

The idea is to rotate the first three columns of Θ so as to become aligned with (581) using the Procrustes technique in §C.2, and to then apply that same rotation to the last column of Θ. Having found the optimal rotation, all that is left is to add x_1 to the rotated fourth column of Θ to recover x_5; in this particular case, rotation of the fourth column is superfluous because it is $\mathbf{0}$. Matrix Θ indicates $x_5 = x_1 = [1 \;\; 1 \;\; 1 \;\; 1]^T$ which is, in fact, the IDFT. □

Finding an inverse DFT via Cholesky factorization may appear to involve more computation than the FFT. Yet for D as in (577), we always have the block matrix

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} = \left[\begin{array}{cccc|c} & & & & \frac{1}{2}(d_{1N}-d_{2N})+n \\ & & & & \frac{1}{2}(d_{1N}-d_{3N})+n \\ & & (\mathbf{1}\mathbf{1}^T + I)n & & \frac{1}{2}(d_{1N}-d_{4N})+n \\ & & & & \vdots \\ \frac{1}{2}(d_{1N}-d_{2N})+n & \frac{1}{2}(d_{1N}-d_{3N})+n & \frac{1}{2}(d_{1N}-d_{4N})+n & \cdots & d_{1N} \end{array}\right] \tag{582}$$

whose first principal submatrix in $\mathbb{R}^{n-1\times n-1}$ is fixed whenever n is. We speculate this structure reduces normally cubic computational intensity to at most $O(n^2)$.

4.16 Self similarity...

The self similarity function $A(\ell)$ is related to the autocorrelation function $R(\ell)$; in fact, self-similarity is the progenitor of autocorrelation. When $n\rightarrow\infty$, $A(\ell) = \kappa - 2R(\ell)$ where, for some constant κ. Both functions are used to determine periodicity.

Given the length-M real sequence $[f_i\,,\; i=0\ldots M-1] \in \mathbb{R}^M$, we define the *self-similarity function*;

$$A(\ell) \triangleq \frac{1}{2}\sum_{i=0}^{n-1}(f_i - f_{i-\ell})^2 \tag{583}$$

where $n\leq M$ is the window length.

$$x_{i+1} \triangleq f(i) \in \mathbb{R} \tag{584}$$

$$d_{ij} = \begin{cases} (x_i - x_j)^2, & 1 \leq i,j \leq M \\ 0 & \text{otherwise} \end{cases} \tag{585}$$

$$A(\ell) = \frac{1}{2}\sum_{i=1}^{n} d_{i,i-\ell} \tag{586}$$

which is a sum of some diagonal of the EDM D. To select the ij^{th} entry of matrix Δ,

$$\sqrt{d_{ij}} \stackrel{\Delta}{=} e_i^T \Delta e_j \;=\; e_j^T \Delta e_i \;=\; \operatorname{tr}(e_j e_i^T \Delta) = \;\langle e_i e_j^T ,\, \Delta\rangle \tag{587}$$

where here,

$$D \stackrel{\Delta}{=} \Delta \circ \Delta \tag{588}$$

and where $\circ$ denotes the Hadamard (entry-wise) product. Each scaled entry

$$\sqrt{2d_{ij}} = \sqrt{2}\,\operatorname{tr}(e_j e_i^T \Delta) = \frac{1}{\sqrt{2}}\operatorname{tr}\big((e_i e_j^T + e_j e_i^T)\Delta\big) \tag{589}$$

is a coefficient of orthogonal projection of Δ (§E.6.4) on the range of a vectorized (§2.1.1) member of the orthonormal basis for the vector space $\mathbb{S}_{\mathbf{0}}^M$:

$$E_{ij} = \frac{1}{\sqrt{2}}\big(e_i e_j^T + e_j e_i^T\big)\,, \qquad 1 \le i < j \le M \tag{53}$$

The self-similarity function is therefore equivalent to the Parseval relation, [43] [109] [110] [111] giving a total energy of projection:

$$A(\ell) \;=\; \sum_{\substack{i=1\\ i>\ell}}^{n} \operatorname{tr}(e_i e_{i-\ell}^T D) \;=\; \operatorname{tr} \sum_{\substack{i=1\\ i>\ell}}^{n} e_i e_{i-\ell}^T\, D \tag{590}$$

Chapter 5

EDM cone

For $N>3$, the cone of EDMs is no longer a circular cone and the geometry becomes complicated. . .

−Hayden, Wells, Liu, & Tarazaga (1991) [49, §3]

From (537), we know the EDM cone does not intersect the positive semidefinite (PSD) cone $\mathbb{S}_+^N$ except at the origin, their only vertex; there can be no positive nor negative semidefinite EDM.

$$\mathbb{EDM}^N \cap \mathbb{S}_+^N = \mathbf{0} \tag{591}$$

Even so, the two cones can be related. In §7.3.1.1.1 we prove the resemblance to EDM definition (333):

$$\mathbb{EDM}^N = \mathbb{S}_{\mathbf{0}}^N \cap \left(\mathbb{S}_g^{N\perp} - \mathbb{S}_+^N\right) \tag{779}$$

where $\mathbb{S}_{\mathbf{0}}^N$ is the symmetric hollow subspace and $\mathbb{S}_g^{N\perp} = \{u\mathbf{1}^T + \mathbf{1}u^T \mid u \in \mathbb{R}^N\}$ is the orthogonal complement of the geometric center subspace (§E.7.1.0.2).

For now we invoke the popular matrix criterion (356) to illustrate the traditional correspondence between the EDM and PSD cones, both belonging to the same ambient space of symmetric matrices:

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \left\{ \begin{array}{c} -VDV \in \mathbb{S}_+^N \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array} \right. \tag{356}$$

The set of all EDMs of dimension $N \times N$ forms a closed convex cone $\mathbb{EDM}^N$ in $\mathbb{S}_{\mathbf{0}}^N$, a subspace of $\mathbb{S}^N$, because any pair of EDMs satisfies definition (111); *videlicet*, for all $\zeta_1, \zeta_2 \geq 0$, (§A.3.1.0.2)

$$\begin{array}{c} \zeta_1 VD_1V + \zeta_2 VD_2V \succeq 0 \\ \zeta_1 D_1 + \zeta_2 D_2 \in \mathbb{S}_{\mathbf{0}}^N \end{array} \;\Leftarrow\; \begin{array}{cc} VD_1V \succeq 0\,, & VD_2V \succeq 0 \\ D_1 \in \mathbb{S}_{\mathbf{0}}^N\,, & D_2 \in \mathbb{S}_{\mathbf{0}}^N \end{array} \tag{592}$$

5.0.0.0.1 Definition. *Cone of Euclidean distance matrices.*
(*confer* (402)) In the subspace of symmetric hollow matrices $\mathbb{S}_{\mathbf{0}}^N$ (45), the set of all Euclidean distance matrices $\mathbb{EDM}^N$ forms a unique immutable pointed closed convex cone called the EDM cone. For $N > 0$ (§4.8.3),

$$\begin{aligned} \mathbb{EDM}^N &\triangleq \left\{ D \in \mathbb{S}_{\mathbf{0}}^N \mid -VDV \in \mathbb{S}_+^N \right\} \\ &= \bigcap_{\substack{z \in \mathcal{N}(\mathbf{1}^T) \\ i=1\ldots N}} \left\{ D \in \mathbb{S}^N \mid \langle zz^T, -D\rangle \geq 0\,,\; \langle e_i e_i^T, D\rangle = 0 \right\} \end{aligned} \tag{593}$$

the EDM cone in isomorphic $\mathbb{R}^{N^2}$ is the intersection in variable $D = [d_{ij}]$ of an infinite number of halfspaces about the origin and a finite number of hyperplanes through the origin. Hence $\mathbb{EDM}^N$ has empty interior with respect to $\mathbb{S}^N$. $\triangle$

The EDM cone is more easily visualized in the isomorphic vector subspace $\mathbb{R}^{N(N-1)/2}$. In the case $N = 1$, the EDM cone is the origin in $\mathbb{R}^{\mathbf{0}}$. In the case $N = 2$, the EDM cone is the nonnegative real line in $\mathbb{R}$ illustrated in Figure **5.4**. In the case $N = 3$ points, the Euclidean axioms are necessary and sufficient tests to certify realizability of triangles; (515). Hence the triangle inequality (axiom 4) describes three halfspaces (459) whose intersection makes a polyhedral cone of realizable $\sqrt{d_{ij}}$ in $\mathbb{R}^{\mathbf{3}}$; an isomorphic subspace representation of $\mathbb{EDM}^{\mathbf{3}}$ in the natural coordinates illustrated in Figure **5.1**(b).

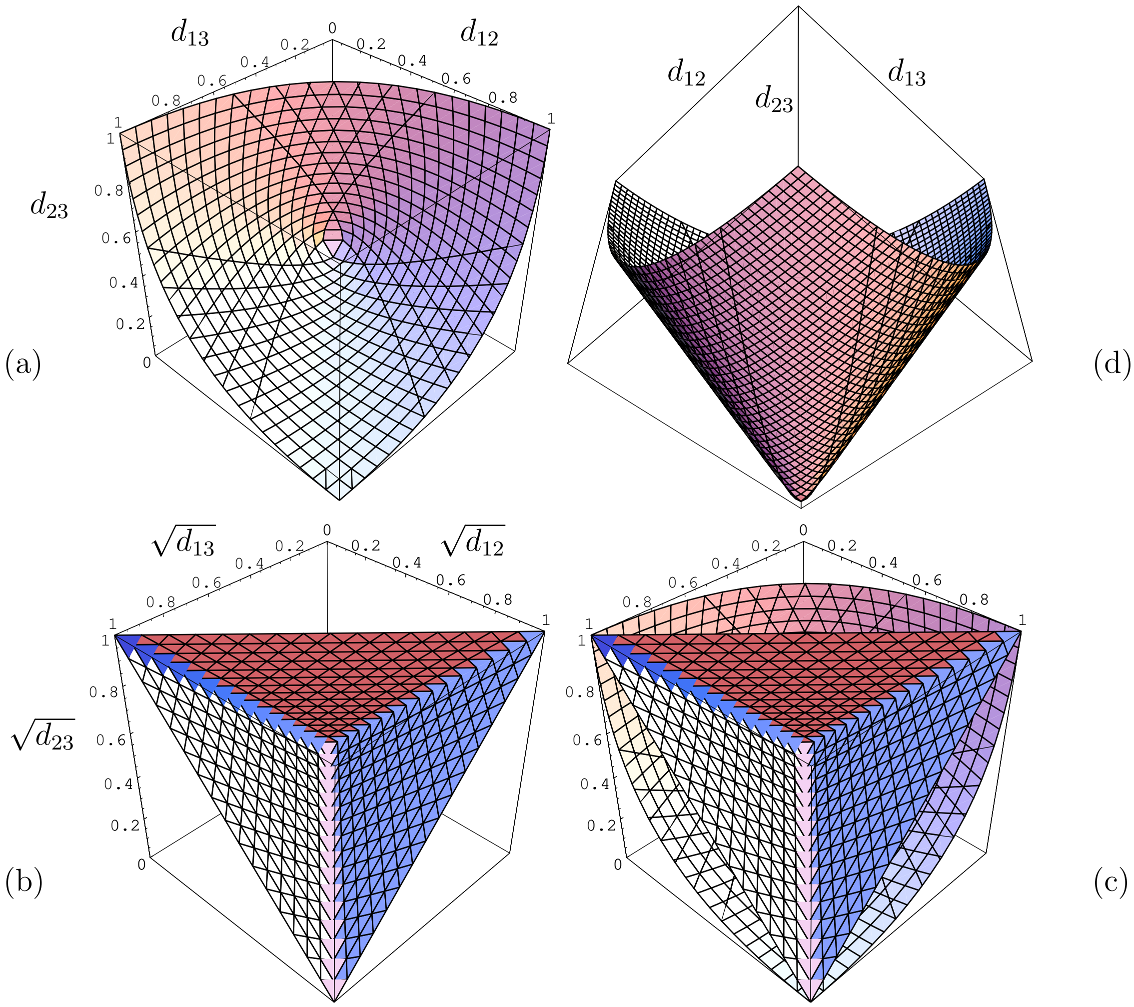


Figure 5.1: Relative boundary (tiled) of cone of Euclidean distance matrices $\mathbb{EDM}^N$ ($N=3$) drawn truncated in isomorphic subspace $\mathbb{R}^{\mathbf{3}}$; *id est*, $\text{dvec}\,\partial\mathbb{EDM}^{\mathbf{3}}$. **(a)** EDM cone drawn in usual distance-square coordinates d_{ij}. View is from inside looking toward origin. (Imagine it continuing out of page.) Unlike positive semidefinite cone, EDM cone is neither self-dual or proper in $\mathbb{S}^N$; dual EDM cone for this example belongs to ambient space of symmetric matrices in isomorphic $\mathbb{R}^{\mathbf{6}}$. **(b)** Drawn in its natural coordinates $\sqrt{d_{ij}}$ (absolute distance), cone remains convex; intersection of three halfspaces (459) whose partial boundaries each contain origin. Cone geometry becomes complicated (non-polyhedral) in higher dimension. [49, §3] **(c)** Two coordinate systems artificially superimposed. Coordinate transformation from d_{ij} to $\sqrt{d_{ij}}$ is apparently a topological contraction. **(d)** Sitting on its vertex, pointed $\mathbb{EDM}^{\mathbf{3}}$ is a *circular cone* having axis of revolution $\text{dvec}(-E) = \text{dvec}(\mathbf{11}^T - I)$ ((52), §4.13). Rounded vertex is artifact of plot.

5.1 Polyhedral bounds

Because the EDM cone comprises the intersection of an infinite number of independent halfspaces, the convex cone of EDMs is non-polyhedral in d_{ij} for $N>2$; [*sic*] (*e.g.*, Figure **5.1**(a)).

Albeit relative angles θ_{ikj} (371) are nonlinear functions of the d_{ij} , still we found polyhedral relations bounding the set of all EDMs for $N=1,2,3,4$: In the case $N=2$ we found the EDM cone to be a half-line (the polyhedron illustrated in Figure **5.4**), while for $N=3$ we have the polyhedral cone in Figure **5.1**(b). In the case $N=4$, *relative-angle inequality* (521) together with the four Euclidean axioms are necessary and sufficient tests for realizability of tetrahedra. (522) The *relative-angle inequality* provides a regular tetrahedron in $\mathbb{R}^{\mathbf{3}}$ [*sic*] bounding angles θ_{ikj} at vertex x_k belonging to $\mathbb{EDM}^{\mathbf{4}}$ (Figure **4.8**, p.184).[5.1]

Yet if we were to employ the procedure outlined in §4.12.3 for making generalized triangle inequalities, then there we would find all the d_{ij}-transformations necessary for generating polyhedral objects bounding EDMs of any higher dimension; $N>4$.

5.2 EDM definition in $\mathbf{11}^T$

Any EDM D corresponding to affine dimension r has representation (*confer* (333))

$$\mathbf{D}(V_{\mathcal{X}}\,,\,y) \triangleq y\mathbf{1}^T + \mathbf{1}y^T - 2V_{\mathcal{X}}V_{\mathcal{X}}^T + \frac{\lambda}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{EDM}^N \tag{594}$$

where $\mathcal{R}(V_{\mathcal{X}} \in \mathbb{R}^{N\times r}) \subseteq \mathcal{N}(\mathbf{1}^T)$ and $V_{\mathcal{X}}^T V_{\mathcal{X}}$ a diagonal matrix having no zeros along the main diagonal defines $V_{\mathcal{X}}$,

$$\lambda \triangleq 2\|V_{\mathcal{X}}\|_{\mathrm{F}}^2 \quad , \quad \text{and} \quad y \triangleq \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) - \frac{\lambda}{2N}\mathbf{1} \tag{595}$$

where $y=\mathbf{0}$ if and only if $\mathbf{1}$ is an eigenvector of EDM D . [49, §2] Scalar λ becomes an eigenvalue when corresponding eigenvector $\mathbf{1}$ exists; *e.g.*, when

[5.1] Still, the axiom-4 triangle inequalities corresponding to each principal 3×3 submatrix of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ demand that the corresponding $\sqrt{d_{ij}}$ belong to a polyhedral cone like that in Figure **5.1**(b).

$X = I$ in EDM definition (333).

Formula (594) can be validated by substituting (595); we find

$$\mathbf{D}(V_{\mathcal{X}}) \triangleq \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)\mathbf{1}^T + \mathbf{1}\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)^T - 2V_{\mathcal{X}} V_{\mathcal{X}}^T \in \mathbb{EDM}^N \tag{596}$$

is simply the standard EDM definition (333) where X^TX has been replaced with the subcompact singular value decomposition (§A.6.2)[5.2]

$$V_{\mathcal{X}} V_{\mathcal{X}}^T \equiv V^T X^T X V \tag{597}$$

Then the inner product $V_{\mathcal{X}}^T V_{\mathcal{X}}$ is an $r \times r$ diagonal matrix Σ of nonzero singular values. Next we validate eigenvector $\mathbf{1}$ and eigenvalue λ.
($\Longrightarrow$) Suppose $\mathbf{1}$ is an eigenvector of EDM D. Then because

$$V_{\mathcal{X}}^T \mathbf{1} = \mathbf{0} \tag{598}$$

it follows

$$\begin{aligned} D\mathbf{1} \;=\; \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)\mathbf{1}^T\mathbf{1} + \mathbf{1}\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)^T\mathbf{1} \;&=\; N\,\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) + \|V_{\mathcal{X}}\|_{\mathrm{F}}^2\mathbf{1} \\ &\Rightarrow \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \propto \mathbf{1} \end{aligned} \tag{599}$$

$\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)^T\mathbf{1} = N\kappa = \operatorname{tr}(V_{\mathcal{X}}^T V_{\mathcal{X}}) = \|V_{\mathcal{X}}\|_{\mathrm{F}}^2 \;\Rightarrow\; \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) = \kappa\mathbf{1}$ and $y = \mathbf{0}$.
($\Longleftarrow$) Now suppose $\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) = \frac{\lambda}{2N}\mathbf{1}$; *id est*, $y = \mathbf{0}$. Then

$$D = \frac{\lambda}{N}\mathbf{11}^T - 2V_{\mathcal{X}} V_{\mathcal{X}}^T \in \mathbb{EDM}^N \tag{600}$$

$\mathbf{1}$ is an eigenvector with corresponding eigenvalue λ. ♦

[5.2]Subcompact SVD: $V_{\mathcal{X}} V_{\mathcal{X}}^T \triangleq Q\Sigma^{1/2}\,\Sigma^{1/2}Q^T \equiv V^T X^T X V$. So $V_{\mathcal{X}}^T$ is not necessarily XV (§4.5.1.0.1), although affine dimension $r = \operatorname{rank}(V_{\mathcal{X}}^T) = \operatorname{rank}(XV)$. (436)

5.2.1 Range of EDM D

From §B.1.1 pertaining to linear independence of dyad sums: if the transpose halves of all the dyads in the sum (596)[5.3] make a linearly independent set, then the non-transpose halves constitute a basis for the range of EDM D. We have, for $D\in\mathbb{EDM}^N$,

$$\begin{array}{lcl}\mathcal{R}(D)=\mathcal{R}\big([\,\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\quad \mathbf{1}\quad V_{\mathcal{X}}\,]\big) & \Leftarrow & \operatorname{rank}\big([\,\mathbf{1}\quad \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\quad V_{\mathcal{X}}\,]\big)=2+r \\ \mathcal{R}(D)=\mathcal{R}\big([\,\mathbf{1}\quad V_{\mathcal{X}}\,]\big) & \Leftarrow & \text{otherwise}\end{array} \tag{601}$$

To show that, we need the condition under which the rank equality is satisfied: We know $\mathcal{R}(V_{\mathcal{X}})\perp\mathbf{1}$, but what is the relative geometric orientation of $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$? $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\succeq 0$ because $V_{\mathcal{X}}V_{\mathcal{X}}^T\succeq 0$, and $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\propto\mathbf{1}$ remains possible (599); this means $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\notin\mathcal{N}(\mathbf{1}^T)$ simply because it has no negative entries. (Figure **5.2**) If the projection of $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$ on $\mathcal{N}(\mathbf{1}^T)$ does not belong to $\mathcal{R}(V_{\mathcal{X}})$, then that is a necessary and sufficient condition for linear independence (l.i.) of $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$ with respect to $\mathcal{R}\big([\,\mathbf{1}\quad V_{\mathcal{X}}\,]\big)$; *id est*,

$$\begin{array}{rl}V\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) & \neq V_{\mathcal{X}}\,a \quad \text{for any } a\in\mathbb{R}^r \\ (I-\frac{1}{N}\mathbf{1}\mathbf{1}^T)\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) & \neq V_{\mathcal{X}}\,a \\ \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)-\frac{1}{N}\|V_{\mathcal{X}}\|_{\mathrm{F}}^2\mathbf{1} & \neq V_{\mathcal{X}}\,a \\ \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)-\frac{\lambda}{2N}\mathbf{1}=y & \neq V_{\mathcal{X}}\,a \;\Leftrightarrow\; \{\mathbf{1},\;\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T),\;V_{\mathcal{X}}\}\text{ is l.i.}\end{array} \tag{602}$$

On the other hand when this condition is violated (when (595) $y=V_{\mathcal{X}}\,a_p$), then from (594) we have

$$\begin{aligned}\mathcal{R}\big(D=y\mathbf{1}^T+\mathbf{1}y^T-2V_{\mathcal{X}}V_{\mathcal{X}}^T+\tfrac{\lambda}{N}\mathbf{1}\mathbf{1}^T\big) &= \mathcal{R}\big((V_{\mathcal{X}}\,a_p+\tfrac{\lambda}{N}\mathbf{1})\mathbf{1}^T+(\mathbf{1}a_p^T-2V_{\mathcal{X}})V_{\mathcal{X}}^T\big) \\ &= \mathcal{R}\big([V_{\mathcal{X}}\,a_p+\tfrac{\lambda}{N}\mathbf{1}\quad \mathbf{1}a_p^T-2V_{\mathcal{X}}\,]\big) \\ &= \mathcal{R}\big([\,\mathbf{1}\quad V_{\mathcal{X}}\,]\big)\end{aligned} \tag{603}$$

An example of such a violation is (600) where, in particular, $a_p=\mathbf{0}$. ♦

[5.3] Identifying the columns $V_{\mathcal{X}}\triangleq[\,v_1\cdots v_r\,]$, then $V_{\mathcal{X}}V_{\mathcal{X}}^T=\sum_i v_iv_i^T$ is a sum of dyads.

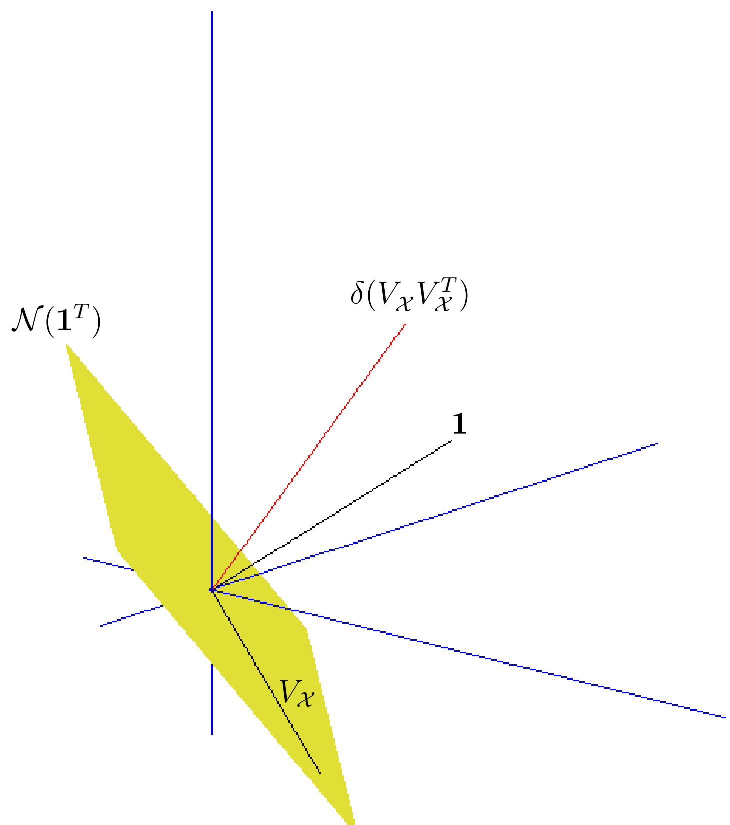


Figure 5.2: Example of $V_{\mathcal{X}}$ selection to make an EDM corresponding to cardinality $N=3$ and affine dimension $r=1$; $V_{\mathcal{X}}$ is a vector in $\mathcal{N}(\mathbf{1}^T) \subset \mathbb{R}^{\mathbf{3}}$. Nullspace of $\mathbf{1}^T$ (containing $V_{\mathcal{X}}$) is hyperplane in $\mathbb{R}^{\mathbf{3}}$ (drawn truncated) having normal $\mathbf{1}$. Vector $\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)$ may or may not be in plane spanned by $\{\mathbf{1}, V_{\mathcal{X}}\}$, but belongs to nonnegative orthant which is strictly supported by $\mathcal{N}(\mathbf{1}^T)$.

A statement parallel to (601) is therefore, for $D \in \mathbb{EDM}^N$, (Theorem 4.7.3.0.1)

$$\begin{array}{l} \operatorname{rank}(D) = r+2 \;\Leftrightarrow\; y \notin \mathcal{R}(V_{\mathcal{X}}) \;\; \left(\Leftrightarrow\; \mathbf{1}^T D^\dagger \mathbf{1} = 0\right) \\ \operatorname{rank}(D) = r+1 \;\Leftrightarrow\; y \in \mathcal{R}(V_{\mathcal{X}}) \;\; \left(\Leftrightarrow\; \mathbf{1}^T D^\dagger \mathbf{1} \neq 0\right) \end{array} \tag{604}$$

5.2.2 Faces of EDM cone

Expression (596) has utility constructing the set of all EDMs corresponding to affine dimension r :

$$\begin{aligned} &\left\{D \in \mathbb{EDM}^N \mid \operatorname{rank}(VDV) = r\right\} \\ = &\left\{\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)\mathbf{1}^T + \mathbf{1}\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)^T - 2V_{\mathcal{X}} V_{\mathcal{X}}^T \mid V_{\mathcal{X}} \in \mathbb{R}^{N\times r},\; V_{\mathcal{X}}^T V_{\mathcal{X}} = \delta^2(V_{\mathcal{X}}^T V_{\mathcal{X}}),\; \mathcal{R}(V_{\mathcal{X}}) \subseteq \mathcal{N}(\mathbf{1}^T)\right\} \end{aligned} \tag{605}$$

whereas $\{D \in \mathbb{EDM}^N \mid \operatorname{rank}(VDV) \leq r\}$ is just the closure of this same set;

$$\left\{D \in \mathbb{EDM}^N \mid \operatorname{rank}(VDV) \leq r\right\} = \overline{\left\{D \in \mathbb{EDM}^N \mid \operatorname{rank}(VDV) = r\right\}} \tag{606}$$

None of these are necessarily convex sets.

When cardinality $N = 3$ and affine dimension $r = 2$, for example, the interior $\operatorname{rel\,int} \mathbb{EDM}^{\mathbf{3}}$ is realized via (605). (§5.4)

When $N = 3$ and $r = 1$, the relative boundary of the EDM cone $\operatorname{dvec} \partial\mathbb{EDM}^{\mathbf{3}}$ is realized in isomorphic $\mathbb{R}^{\mathbf{3}}$ as in Figure **5.1**(d). This figure could be constructed via (606) by spiraling vector $V_{\mathcal{X}}$ tightly about the origin in $\mathcal{N}(\mathbf{1}^T)$; as can be imagined with aid of Figure **5.2**. Vectors close to the origin in $\mathcal{N}(\mathbf{1}^T)$ are correspondingly close to the origin in $\mathbb{EDM}^N$. As vector $V_{\mathcal{X}}$ orbits the origin in $\mathcal{N}(\mathbf{1}^T)$, the corresponding EDM orbits the axis of revolution while remaining on the boundary of the circular cone $\operatorname{dvec} \partial\mathbb{EDM}^{\mathbf{3}}$. (Figure **5.3**)

5.2.2.1 Isomorphic faces

In high cardinality N, any set of EDMs constructed via (605) or (606) with particular affine dimension r is isomorphic with any set constructed in lower cardinality that admits the same affine dimension. We do not prove that here.

(a)

(b)

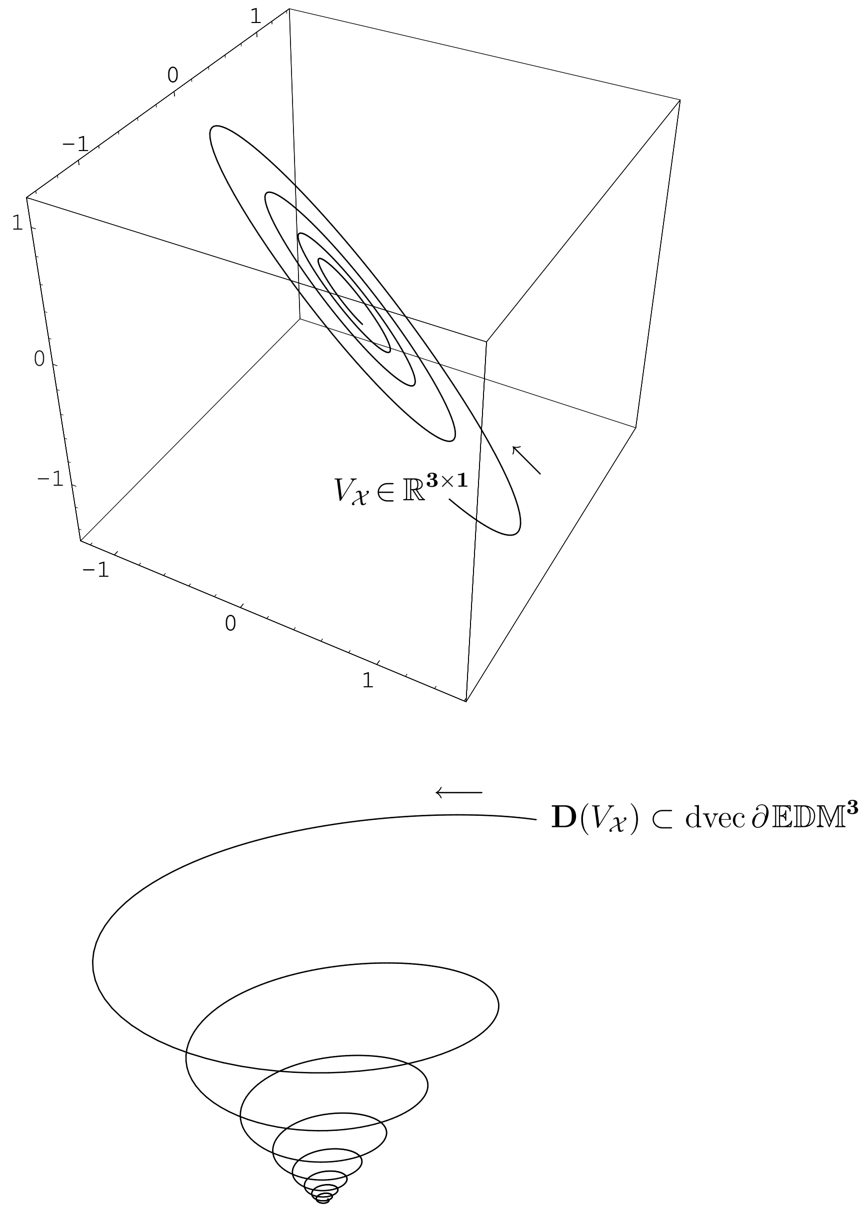


Figure 5.3: **(a)** Vector $V_{\mathcal{X}}$ from Figure **5.2** spirals in $\mathcal{N}(\mathbf{1}^T) \subset \mathbb{R}^{\mathbf{3}}$ decaying toward origin. (Spiral is two-dimensional in vector-space $\mathbb{R}^{\mathbf{3}}$.) **(b)** Corresponding trajectory $\mathbf{D}(V_{\mathcal{X}})$ on EDM cone relative boundary creates a vortex also decaying toward origin. There are two complete orbits on EDM cone boundary about axis of revolution for every single revolution of $V_{\mathcal{X}}$ about origin. (Vortex is three-dimensional in isometrically isomorphic $\mathbb{R}^{\mathbf{3}}$.)

In particular, extreme directions of $\mathbb{EDM}^N$ correspond to affine dimension $r=1$ and are simply represented: for any particular N and each and every $z\in\mathbb{R}^N$ in $\mathcal{N}(\mathbf{1}^T)$,

$$\Gamma = (z\circ z)\mathbf{1}^T + \mathbf{1}(z\circ z)^T - 2zz^T \tag{607}$$

is an extreme direction corresponding to a one-dimensional face of the EDM cone $\mathbb{EDM}^N$ that is a ray in isomorphic $\mathbb{R}^{N(N-1)/2}$.

Now suppose we are given a particular EDM $D_p\in\mathbb{EDM}^N$ corresponding to affine dimension r and parameterized by $V_{\mathcal{X}_p}$ in (596). The smallest face of $\mathbb{EDM}^N$ containing D_p is

$$\mathcal{F}\big(\mathbb{EDM}^N\ni D_p\big) = \overline{\left\{\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\mathbf{1}^T + \mathbf{1}\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)^T - 2V_{\mathcal{X}}V_{\mathcal{X}}^T \mid V_{\mathcal{X}}\in\mathbb{R}^{N\times r},\, V_{\mathcal{X}}^TV_{\mathcal{X}} = \delta^2(V_{\mathcal{X}}^TV_{\mathcal{X}}),\, \mathcal{R}(V_{\mathcal{X}})\subseteq\mathcal{R}(V_{\mathcal{X}_p})\right\}} \tag{608}$$

which is isomorphic[5.4] with the convex cone $\mathbb{EDM}^{r+1}$, hence of dimension

$$\dim\mathcal{F}\big(\mathbb{EDM}^N\ni D_p\big) = (r+1)r/2 \tag{609}$$

in isomorphic $\mathbb{R}^{N(N-1)/2}$. Not all dimensions are represented; *e.g.*, the EDM cone has no two-dimensional faces.

When cardinality $N=4$, and affine dimension $r=2$ so that $\mathcal{R}(V_{\mathcal{X}_p})$ is any two-dimensional subspace of three-dimensional $\mathcal{N}(\mathbf{1}^T)$ in $\mathbb{R}^{\mathbf{4}}$, for example, then the corresponding face of $\mathbb{EDM}^{\mathbf{4}}$ is isometrically isomorphic with: (606)

$$\mathbb{EDM}^{\mathbf{3}} = \{D\in\mathbb{EDM}^{\mathbf{3}} \mid \operatorname{rank}(VDV)\leq 2\} \simeq \mathcal{F}\big(\mathbb{EDM}^{\mathbf{4}}\ni\mathbf{D}(V_{\mathcal{X}_p})\big) \tag{610}$$

Each two-dimensional subspace of $\mathcal{N}(\mathbf{1}^T)$ corresponds to another three-dimensional face.

Because each and every principal submatrix of an EDM in $\mathbb{EDM}^N$ (§4.12.3) is another EDM [86, §4.1], for example, then each principal submatrix belongs to a particular face of $\mathbb{EDM}^N$.

5.2.2.2 Open question

This result (609) is analogous to that for the positive semidefinite cone in §2.6.6.3, although the question remains open whether all faces of $\mathbb{EDM}^N$ are exposed like they are for the PSD cone.

[5.4] The fact that the smallest face is isomorphic with another (perhaps smaller) EDM cone is implicit in [49, §2].

5.3 EDM cone by inverse image...

Use technique of §2.6.6.3.4...

5.4 Correspondence to PSD cone $\mathbb{S}_+^{N-1}$

Hayden & Wells *et alii* [49, §2] assert a one-to-one correspondence with matrices positive semidefinite on $\mathcal{N}(\mathbf{1}^T)$. Because $\operatorname{rank}(VDV) \leq N-1$ (§4.7.2), the corresponding positive semidefinite cone can only be $\mathbb{S}_+^{N-1}$. [95, §18.2.1]

To demonstrate that correspondence more clearly, we follow the inner-product form EDM definition (375): Any EDM may be expressed

$$\mathbf{D}(\Phi) \triangleq \begin{bmatrix} 0 \\ \delta(\Phi) \end{bmatrix} \mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & \delta(\Phi)^T \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Phi \end{bmatrix} \in \mathbb{EDM}^N \\ \Leftrightarrow \\ \Phi \succeq 0 \tag{611}$$

where this $\mathbf{D}$ is a *surjective* linear operator (onto $\mathbb{EDM}^N$), injective because it has no nullspace [92, §A.1] on domain $\mathbb{S}_+^{N-1}$. (*confer* §4.6) Then the EDM cone may be expressed,

$$\mathbb{EDM}^N = \left\{\mathbf{D}(\Phi) \mid \Phi \in \mathbb{S}_+^{N-1}\right\} \tag{612}$$

Hayden & Wells' assertion can therefore be equivalently stated in terms of the inner-product form EDM definition,

$$\mathbf{D}(\mathbb{S}_+^{N-1}) = \mathbb{EDM}^N \tag{613}$$

$$-V_{\mathcal{N}}^T\,\mathbb{EDM}^N V_{\mathcal{N}} = \mathbb{S}_+^{N-1} \tag{614}$$

because $\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$.

In terms of affine dimension r, Hayden & Wells claim particular correspondence between the PSD and EDM cones:

$r = N-1$: Symmetric hollow matrices D negative definite on $\mathcal{N}(\mathbf{1}^T)$ correspond to points relatively interior to the EDM cone.

$r < N-1$: Symmetric hollow matrices D negative semidefinite on $\mathcal{N}(\mathbf{1}^T)$, where $V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has at least one 0 eigenvalue, correspond to points on the relative boundary of the EDM cone.

$r = 1$: Symmetric hollow nonnegative matrices rank-one on $\mathcal{N}(\mathbf{1}^T)$ correspond to extreme directions of the EDM cone; *id est*, for some vector u, (§A.3.1.0.7)

$$\left.\begin{array}{c} \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} = 1 \\ D \in \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N} \end{array}\right\} \Leftrightarrow \begin{array}{c} D \in \mathbb{EDM}^N \\ D \text{ is an extreme direction} \end{array} \Leftrightarrow \left\{\begin{array}{c} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \equiv uu^T \\ D \in \mathbb{S}_{\mathbf{0}}^N \end{array}\right. \tag{615}$$

5.4.0.2.1 Example. *Extreme rays* versus *rays on the boundary.*
The EDM $D = \begin{bmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{bmatrix}$ is an extreme direction of $\mathbb{EDM}^{\mathbf{3}}$ where $u = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ in (615). Because $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has eigenvalues $\{0,5\}$, the ray whose direction is D also lies on the relative boundary of $\mathbb{EDM}^{\mathbf{3}}$.

In contrast, EDM $D = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ is an extreme direction of $\mathbb{EDM}^{\mathbf{2}}$ but $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has only one eigenvalue: $\{1\}$. Because $\mathbb{EDM}^{\mathbf{2}}$ is a ray whose relative boundary (§2.5.1.3.1) is the origin, this conventional boundary does not include D. $\square$

5.4.1 Gram-form correspondence to $\mathbb{S}_+^{N-1}$

Equivalence (614) coincides with[5.5]

$$-V_{\mathcal{W}}^T \,\mathbb{EDM}^N V_{\mathcal{W}} = \mathbb{S}_+^{N-1} \tag{616}$$

yielding

$$-V\,\mathbb{EDM}^N V = V_{\mathcal{W}}\,\mathbb{S}_+^{N-1} V_{\mathcal{W}}^T \tag{617}$$

where $V_{\mathcal{W}} \in \mathbb{R}^{N\times N-1}$ is an auxiliary V-matrix (§B.4.3) having properties $V_{\mathcal{W}} V_{\mathcal{W}}^T = V$, $V_{\mathcal{W}}^T V_{\mathcal{W}} = I$, $\mathcal{R}(V_{\mathcal{W}}) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$, $\mathcal{N}(V_{\mathcal{W}}^T) = \mathcal{R}(\mathbf{1})$. With respect to the linear Gram-form EDM definition

$$\mathbf{D}(G) \;=\; \delta(G)\mathbf{1}^T + \mathbf{1}\delta(G)^T - 2G \tag{344}$$

the mutual inverse relation (414) produces [93, §2.1] [94, §2] [95, §18.2.1] [96, §2.6]

$$\begin{aligned} \mathbb{EDM}^N \;&=\; \mathbf{D}\big(\mathbf{V}(\mathbb{EDM}^N)\big) \\ &=\; \mathbf{D}\big(-V\,\mathbb{EDM}^N V\tfrac{1}{2}\big) \\ &=\; \mathbf{D}\big(V_{\mathcal{W}}\,\mathbb{S}_+^{N-1} V_{\mathcal{W}}^T \tfrac{1}{2}\big) \;\equiv\; \mathbf{D}\big(V_{\mathcal{N}}\,\mathbb{S}_+^{N-1} V_{\mathcal{N}}^T \tfrac{1}{2}\big) \end{aligned} \tag{618}$$

a one-to-one correspondence between $\mathbb{EDM}^N$ and $\mathbb{S}_+^{N-1}$.

[5.5] The isomorphism $T(Y) = V_{\mathcal{N}}^T V_{\mathcal{W}} Y V_{\mathcal{W}}^T V_{\mathcal{N}}$ relates this necessarily positive semidefinite map to (614).

5.4.2 Monotonicity

Consider the linear function $g : \mathbb{S}^N \rightarrow \mathbb{S}^{N-1}$,

$$g(D) = -V_{\mathcal{N}}^T D V_{\mathcal{N}} \tag{619}$$

having $\operatorname{dom} g = \mathbb{S}_{\mathbf{0}}^N$ and *superlevel sets* (*confer* (315))

$$\mathcal{L}_\nu = \{D \in \mathbb{S}_{\mathbf{0}}^N \mid -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq \nu I\} \tag{620}$$

that are simply translations in isomorphic $\mathbb{R}^{N(N+1)/2}$ of the EDM cone that belongs to subspace $\mathbb{R}^{N(N-1)/2}$; *videlicet*, for each and every $\nu \in \mathbb{R}$,

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq \nu I \;\Leftrightarrow\; -V_{\mathcal{N}}^T (D - \nu V_{\mathcal{N}}^{\dagger T} V_{\mathcal{N}}^{\dagger}) V_{\mathcal{N}} \succeq 0 \tag{621}$$

Because g is concave,[5.6] all its superlevel sets are convex.

The difference $D_2 - D_1$ belongs to the EDM cone if and only if $-V_{\mathcal{N}}^T(D_2 - D_1)V_{\mathcal{N}} \succeq 0$ by (352);[5.7] *id est*,

$$D_1 \underset{\mathbb{EDM}^N}{\preceq} D_2 \;\Leftrightarrow\; \left\{\begin{array}{c} -V_{\mathcal{N}}^T D_1 V_{\mathcal{N}} \underset{\mathbb{S}_+^{N-1}}{\preceq} -V_{\mathcal{N}}^T D_2 V_{\mathcal{N}} \\ \\ D_2 - D_1 \in \mathbb{S}_{\mathbf{0}}^N \end{array}\right. \tag{622}$$

This correspondence between the EDM cone and the positive semidefinite cone connotes monotonicity [25] of g (619); in particular, $g(D)$ is a nondecreasing linear function on domain $\mathbb{S}_{\mathbf{0}}^N$.

5.5 Vectorization projection interpretation

In §E.7.1.0.2 we learn that $-VDV$ can be interpreted as orthogonal projection [94, §2] of $-D \in \mathbb{S}_{\mathbf{0}}^N$ on the subspace of geometrically centered symmetric matrices

$$\begin{aligned} \mathbb{S}_g^N &\triangleq \{Y \in \mathbb{S}^N \mid Y\mathbf{1} = \mathbf{0}\} \\ &= \{Y \in \mathbb{S}^N \mid \mathcal{N}(Y) \supseteq \mathbf{1}\} = \{Y \in \mathbb{S}^N \mid \mathcal{R}(Y) \subseteq \mathcal{N}(\mathbf{1}^T)\} && (1292) \\ &= \{VXV \mid X \in \mathbb{S}^N\} \subset \mathbb{S}^N && (1293) \end{aligned}$$

[5.6] Any linear function must, of course, be simultaneously concave and convex. (The sublevel sets of g are simply translations of the negative EDM cone.)

[5.7] From (329), any matrix V in place of $V_{\mathcal{N}}$ will satisfy (622) if $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$.

because elementary auxiliary matrix V is an orthogonal projector (§B.4.1). Yet there is another useful projection interpretation:

Revising the fundamental matrix criterion for membership to the EDM cone (329),[5.8]

$$\left.\begin{array}{r}\langle zz^T, -D\rangle \geq 0 \quad \forall\, zz^T \mid \mathbf{1}\mathbf{1}^T zz^T = \mathbf{0} \\ D \in \mathbb{S}^N_{\mathbf{0}}\end{array}\right\} \Leftrightarrow \; D \in \mathbb{EDM}^N \tag{623}$$

When $D \in \mathbb{EDM}^N$, this correspondence means $-z^T D z$ is proportional to a nonnegative coefficient of orthogonal projection (§E.6.4.2) of $-D$ in isometrically isomorphic $\mathbb{R}^{N(N+1)/2}$ on the range of each and every vectorized (§2.1.2.1) symmetric dyad (§B.1) in the nullspace of $\mathbf{1}\mathbf{1}^T$;[5.9] *id est*, on each and every member of

$$\begin{aligned}\mathcal{T} &= \left\{\operatorname{svec}(zz^T) \mid z \in \mathcal{N}(\mathbf{1}\mathbf{1}^T) = \mathcal{R}(V_{\mathcal{N}})\right\} \subset \operatorname{svec} \partial \mathbb{S}^N_+ \\ &= \left\{\operatorname{svec}(V_{\mathcal{N}} \upsilon \upsilon^T V_{\mathcal{N}}^T) \mid \upsilon \in \mathbb{R}^{N-1}\right\}\end{aligned} \tag{624}$$

whose dimension is

$$\dim \mathcal{T} = N(N-1)/2 \tag{625}$$

The set of all symmetric dyads $\{zz^T \mid z \in \mathbb{R}^N\}$ constitute the extreme directions of the positive semidefinite cone (§2.6.4, §2.6.6) $\mathbb{S}^N_+$, hence lie on its boundary. Yet only those dyads in $\mathcal{R}(V_{\mathcal{N}})$ are included in the test (623), thus only a subset $\mathcal{T}$ of all vectorized extreme directions of $\mathbb{S}^N_+$ is observed.

In the particularly simple case $D \in \mathbb{EDM}^{\mathbf{2}} = \{D \in \mathbb{S}^{\mathbf{2}}_{\mathbf{0}} \mid d_{12} \geq 0\}$, for example, there is only one extreme direction of the PSD cone involved (illustrated in Figure **5.4**):

$$zz^T = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{626}$$

[5.8] $\mathcal{N}(\mathbf{1}\mathbf{1}^T) = \mathcal{N}(\mathbf{1}^T)$ and $\mathcal{R}(zz^T) = \mathcal{R}(z)$.

[5.9] The range of the vectorized dyads (624) cannot be isomorphic with subspace $\mathcal{R}(V_{\mathcal{N}})$ simply because operator $T(z \in \mathcal{R}(V_{\mathcal{N}})) \triangleq \operatorname{svec}(zz^T)$ is nonlinear in z. [38, §2.8-8] Orthogonal projection on $\mathcal{T}$ cannot, therefore, be orthogonal on $\mathcal{R}(V_{\mathcal{N}})$.

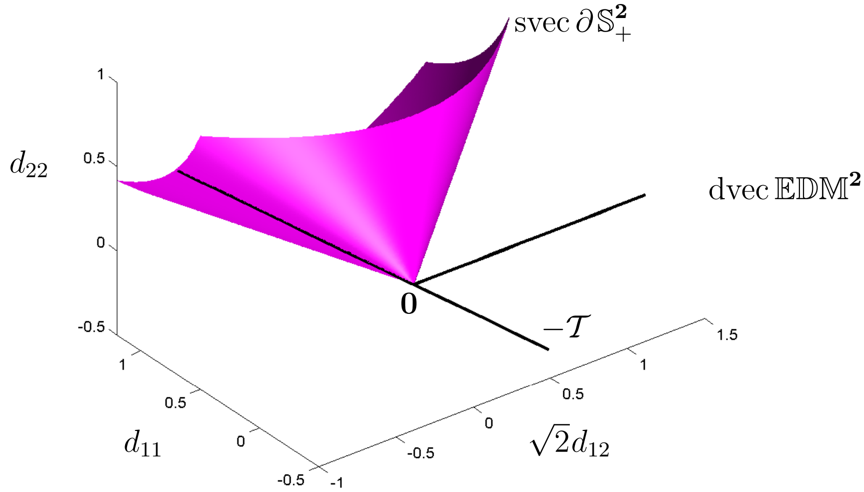


Figure 5.4: Truncated boundary of positive semidefinite cone $\mathbb{S}^2_+$ in isometrically isomorphic $\mathbb{R}^3$ (via svec (35)) is, in this dimension, constituted solely by its extreme directions. Truncated cone of Euclidean distance matrices $\mathbb{EDM}^2$ in isometrically isomorphic subspace $\mathbb{R}$. Relative boundary of EDM cone is constituted solely by matrix $\mathbf{0}$. Half-line $\mathcal{T} = \{\zeta\,[\,1 \quad -\sqrt{2} \quad 1\,]^T \mid \zeta \geq 0\}$ on PSD cone boundary depicts that lone extreme ray (626) on which orthogonal projection of $-D$ must be positive semidefinite if D is to belong to $\mathbb{EDM}^2$. Dual EDM cone is halfspace in $\mathbb{R}^3$ whose partially bounding hyperplane has inward-normal dvec $\mathbb{EDM}^2$.

5.5.1 Face of PSD cone $\mathbb{S}_+^N$ containing V

In any case, set $\mathcal{T}$ (624) constitutes the vectorized extreme directions of an $N(N-1)/2$-dimensional face of the PSD cone $\mathbb{S}_+^N$ containing auxiliary matrix V and isomorphic with $\mathbb{S}_+^{N-1} = \mathbb{S}_+^{\operatorname{rank} V}$ (§2.6.6.3).

To show this, we must first find the smallest face containing auxiliary matrix V and then determine its extreme directions. From (126),

$$\begin{aligned}\mathcal{F}\big(\mathbb{S}_+^N \ni V\big) &= \{W \in \mathbb{S}_+^N \mid \mathcal{N}(W) \supseteq \mathcal{N}(V)\}\\ &= \{W \in \mathbb{S}_+^N \mid \mathcal{N}(W) \supseteq \mathcal{R}(\mathbf{1})\}\\ &= \{V_{\mathcal{W}} A V_{\mathcal{W}}^T \mid A \in \mathbb{S}_+^{N-1}\} = \overline{\{V_{\mathcal{W}} A V_{\mathcal{W}}^T \mid A \in \operatorname{int} \mathbb{S}_+^{N-1}\}} \equiv \{V_{\mathcal{N}} B V_{\mathcal{N}}^T \mid B \in \mathbb{S}_+^{N-1}\}\\ &\simeq \mathbb{S}_+^{\operatorname{rank} V} = -V_{\mathcal{N}}^T \, \mathbb{EDM}^N V_{\mathcal{N}} \qquad (614)\end{aligned} \tag{627}$$

Because $V_{\mathcal{W}} V_{\mathcal{W}}^T = V_{\mathcal{N}} V_{\mathcal{N}}^\dagger = V$ (§B.4.3), then V belongs to $\mathcal{F}\big(\mathbb{S}_+^N \ni V\big)$. The isomorphism $T(X) = V_{\mathcal{N}} V_{\mathcal{W}}^T X V_{\mathcal{W}} V_{\mathcal{N}}^T$ is an injective map from $\mathbb{S}_g^N$ onto $\mathbb{S}_g^N$ relating $\{V_{\mathcal{W}} A V_{\mathcal{W}}^T\}$ to $\{V_{\mathcal{N}} B V_{\mathcal{N}}^T\}$. Every rank-one matrix belonging to this face is therefore of the form:

$$V_{\mathcal{N}} \upsilon \upsilon^T V_{\mathcal{N}}^T \mid \upsilon \in \mathbb{R}^{N-1} \tag{628}$$

Because $\mathcal{F}\big(\mathbb{S}_+^N \ni V\big)$ is isomorphic with a positive semidefinite cone $\mathbb{S}_+^{N-1}$, then $\mathcal{T}$ constitutes the extreme directions of $\mathcal{F}$, the origin constitutes the extreme points of $\mathcal{F}$, and auxiliary matrix V is some convex combination of those extreme points and directions by the *extremes theorem* (§2.6.4.0.1). ♦

In fact, the smallest face of the PSD cone $\mathbb{S}_+^N$ containing auxiliary matrix V is the intersection with the geometric center subspace (1292) (1293);

$$\begin{aligned}\mathcal{F}\big(\mathbb{S}_+^N \ni V\big) &= \operatorname{cone}\big\{V_{\mathcal{N}} \upsilon \upsilon^T V_{\mathcal{N}}^T \mid \upsilon \in \mathbb{R}^{N-1}\big\}\\ &= \mathbb{S}_g^N \cap \mathbb{S}_+^N \qquad (\text{confer } (632))\end{aligned} \tag{629}$$

In isometrically isomorphic $\mathbb{R}^{N(N+1)/2}$,

$$\mathcal{F}\big(\mathbb{S}_+^N \ni V\big) = \operatorname{cone} \mathcal{T} \tag{630}$$

5.6 Dual EDM cone

5.6.1 Ambient $\mathbb{S}^N$

We consider finding the ordinary dual EDM cone in ambient space $\mathbb{S}^N$ where $\mathbb{EDM}^N$ is pointed, closed, and convex, but has empty interior. The set of all EDMs in subspace $\mathbb{S}^N$ is a closed convex cone because it is the intersection of infinitely many halfspaces about the origin in variable D :

$$\mathbb{EDM}^N = \bigcap_{\substack{z\in\mathcal{N}(\mathbf{1}^T)\\ i=1\ldots N}} \left\{D \in \mathbb{S}^N \mid \langle e_i e_i^T, D\rangle \geq 0\,,\; \langle e_i e_i^T, D\rangle \leq 0\,,\; \langle zz^T, -D\rangle \geq 0\right\} \tag{631}$$

By definition (170), a dual cone $\mathcal{K}^*$ comprises all vectors inward-normal to each and every hyperplane $\partial\underline{\mathcal{H}}_+$ (§2.3.2.4.1) supporting (at the origin) or containing convex $\mathcal{K}$. The dual EDM cone in the ambient space of symmetric matrices is therefore expressible as the aggregate of every conic combination of inward-normals from (631): [1, exer.2.36]

$$\begin{aligned}
\mathbb{EDM}^{N^*} &= \{\sum_{i=1}^N \zeta_i e_i e_i^T - \sum_{j=1}^N \xi_j e_j e_j^T \mid \zeta_i\,, \xi_j \geq 0\} \,-\, \operatorname{cone}\{zz^T \mid \mathbf{1}\mathbf{1}^T zz^T\!=\!0\}\\
&= \{\delta(u) \mid u\in\mathbb{R}^N\} - \operatorname{cone}\left\{V_{\mathcal{N}}\upsilon\upsilon^T V_{\mathcal{N}}^T \mid \upsilon\in\mathbb{R}^{N-1},\ (\|v\|\!=\!1)\right\} \subset \mathbb{S}^N\\
&= \mathbb{S}_{\mathbf{0}}^{N\perp} - \mathbb{S}_g^N \cap \mathbb{S}_+^N \qquad\qquad \text{(confer (779))}
\end{aligned} \tag{632}$$

The EDM cone is not self-dual in ambient $\mathbb{S}^N$ because its affine hull belongs to a proper subspace

$$\operatorname{aff}\mathbb{EDM}^N = \mathbb{S}_{\mathbf{0}}^N \tag{633}$$

The ordinary dual EDM cone cannot, therefore, be pointed.

When $N=1$, for example, the EDM cone is the point at the origin in $\mathbb{R}$. The auxiliary matrix $V_{\mathcal{N}}$ is empty $[\,\emptyset\,]$, and the dual cone $\mathbb{EDM}^*$ is the real line.

When $N=2$, the EDM cone is a nonnegative real line in isometrically isomorphic $\mathbb{R}^{\mathbf{3}}$. $\mathbb{EDM}^{\mathbf{2}^*}$ is the halfspace whose partial boundary has inward-normal $\mathbb{EDM}^{\mathbf{2}}$. The diagonal matrices $\{\delta(u)\}$ are represented by a hyperplane through the origin $\{\underline{d} \mid [\,0\;1\;0\,]\underline{d}\!=\!0\}$ while the term $\operatorname{cone}\{V_{\mathcal{N}}\upsilon\upsilon^T V_{\mathcal{N}}^T\}$ is represented by the half-line $\mathcal{T}$ in Figure **5.4** belonging to the PSD cone. The dual EDM cone is formed by translating the hyperplane along the negative semidefinite half-line; the union of each and every translation. (*confer* §2.3.2.3.2)

5.6.2 Ambient $\mathbb{S}_{\mathbf{0}}^N$

When instead we consider the ambient space of symmetric hollow matrices (633), then still we find the EDM cone is not self-dual for $N>2$. This is proven as follows:

Given the minimal set of generators $\{\Gamma\}$ (607) for the pointed closed convex EDM cone, the *discrete membership theorem* in §2.8.2.1.3 asserts that members of the dual EDM cone in the ambient space of symmetric hollow matrices can be discerned by testing a discretized generalized inequality:

$$\begin{aligned}\mathbb{EDM}^{N^*}\cap\mathbb{S}_{\mathbf{0}}^N &\triangleq \{D^*\in\mathbb{S}_{\mathbf{0}}^N \mid \langle\Gamma\,,\,D^*\rangle\geq 0 \quad \forall\,\Gamma\in\mathcal{G}(\mathbb{EDM}^N)\}\\ &= \{D^*\in\mathbb{S}_{\mathbf{0}}^N \mid \langle(z\circ z)\mathbf{1}^T+\mathbf{1}(z\circ z)^T-2zz^T\,,\;D^*\rangle\geq 0\,,\;z\in\mathcal{N}(\mathbf{1}^T)\}\\ &= \{D^*\in\mathbb{S}_{\mathbf{0}}^N \mid (z\circ z)^TD^*\mathbf{1}-z^TD^*z\geq 0\,,\;z\in\mathcal{N}(\mathbf{1}^T)\}\end{aligned}\tag{634}$$

The term $(z\circ z)^TD^*\mathbf{1}$ foils any hope, for $N>2$, of self-duality in ambient $\mathbb{S}_{\mathbf{0}}^N$.

♦

The first adverse case $N=3$, for example, may be deduced from Figure **5.1**; a circular cone corresponding to no rotation of the Lorentz cone (the self-dual circular cone).

To find the dual EDM cone in ambient $\mathbb{S}_{\mathbf{0}}^N$ per §2.9.2.2 we prune aggregate (632) describing the ordinary dual EDM cone, removing any member having nonzero main diagonal:

$$\begin{aligned}\mathbb{EDM}^{N^*}\cap\mathbb{S}_{\mathbf{0}}^N &= \operatorname{cone}\big\{\delta\big(V_{\mathcal{N}}\upsilon\upsilon^TV_{\mathcal{N}}^T\big)-V_{\mathcal{N}}\upsilon\upsilon^TV_{\mathcal{N}}^T \mid \upsilon\in\mathbb{R}^{N-1}\big\}\\ &= \big(\mathbb{S}_{\mathbf{0}}^{N\perp}-\mathbb{S}_g^N\cap\mathbb{S}_+^N\big)\cap\mathbb{S}_{\mathbf{0}}^N\end{aligned}\tag{635}$$

When $N=1$, for example, the EDM cone and its dual in ambient $\mathbb{S}_{\mathbf{0}}^N$ each comprise the origin in isomorphic $\mathbb{R}^{\mathbf{0}}$ by convention (110).

When $N=2$, the EDM cone is the nonnegative real line in isomorphic $\mathbb{R}$. (Figure **5.4**) $\mathbb{EDM}^{\mathbf{2}^*}$ is identical, thus self-dual in this dimension. This result is in agreement with (634), verified directly: for all $\kappa\in\mathbb{R}$, $z=\kappa\begin{bmatrix}1\\-1\end{bmatrix}$ and $z\circ z=\kappa^2\begin{bmatrix}1\\1\end{bmatrix} \Rightarrow d_{12}\geq 0$.

5.6.2.1 Schoenberg criterion is discretized membership relation

Criterion (623) is a discretized membership relation (§2.8.2); *id est*, the classic Schoenberg criterion

$$\left.\begin{array}{r}-V_{\mathcal{N}}^{T} D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_{\mathbf{0}}^{N}\end{array}\right\} \Leftrightarrow \; D \in \mathbb{EDM}^{N} \tag{352}$$

is the same as

$$\left.\begin{array}{r}\langle z z^{T}, -D\rangle \geq 0 \quad \forall\, z z^{T} \mid \mathbf{1 1}^{T} z z^{T}=\mathbf{0} \\ D \in \mathbb{S}_{\mathbf{0}}^{N}\end{array}\right\} \Leftrightarrow \; D \in \mathbb{EDM}^{N} \tag{623}$$

which, by (624), is the same as

$$\left.\begin{array}{r}\langle z z^{T}, -D\rangle \geq 0 \quad \forall\, z z^{T} \in \left\{V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T} \mid \upsilon \in \mathbb{R}^{N-1}\right\} \\ D \in \mathbb{S}_{\mathbf{0}}^{N}\end{array}\right\} \Leftrightarrow \; D \in \mathbb{EDM}^{N} \tag{636}$$

where the zz^T constitute a set of generators for the face of the positive semidefinite cone containing auxiliary matrix V; $\mathcal{F}\big(\mathbb{S}_+^N \ni V\big)$ (§5.5.1). Criterion (636) is equivalent to the following constrained membership relation like (243), assuming $Z, D \in \operatorname{aff} \mathbb{EDM}^N$,

$$\begin{array}{l}\langle Z\,,\,D\rangle \geq 0 \quad \forall\, Z \in \mathbb{EDM}^{N^*} \cap\, \mathbb{S}_{\mathbf{0}}^{N} \;\Leftrightarrow\; D \in \mathbb{EDM}^{N} \\ \langle Z\,,\,D\rangle \geq 0 \quad \forall\, Z \in \operatorname{cone}\left\{\delta\left(V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T}\right)-V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T} \mid \upsilon \in \mathbb{R}^{N-1}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^{N}\end{array} \tag{637}$$

This membership relation must, of course, hold more broadly; specifically, over the ordinary dual cone breaching $\operatorname{aff} \mathbb{EDM}^N$ into the larger ambient space $\mathbb{S}^N$: For $D \in \mathbb{S}_{\mathbf{0}}^N$,

$$\begin{array}{l}\langle Z\,,\,D\rangle \geq 0 \quad \forall\, Z \in \mathbb{EDM}^{N^*} \Leftrightarrow\; D \in \mathbb{EDM}^{N} \\ \langle Z\,,\,D\rangle \geq 0 \quad \forall\, Z \in\{\delta(u) \mid u \in \mathbb{R}^{N}\}-\operatorname{cone}\left\{V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T} \mid \upsilon \in \mathbb{R}^{N-1}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^{N} \\ \langle Z\,,\,D\rangle \geq 0 \quad \forall\, Z \in-\operatorname{cone}\left\{V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T} \mid \upsilon \in \mathbb{R}^{N-1}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^{N}\end{array} \tag{638}$$

because $\langle \delta(u)\,,\,D\rangle = 0$. When discretized (§2.8.2.1.3), this membership relation becomes

$$\langle z z^{T}, -D\rangle \geq 0 \quad \forall\, z z^{T} \in\left\{V_{\mathcal{N}} \upsilon \upsilon^{T} V_{\mathcal{N}}^{T} \mid \upsilon \in \mathbb{R}^{N-1}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^{N} \tag{639}$$

the same as the classic Schoenberg criterion.

Hitherto a correspondence between the EDM cone and a face of the PSD cone, the Schoenberg criterion is now accurately interpreted as a discretized membership relation between the EDM cone and its ordinary dual.

5.6.3 Theorem of the alternative

Theorem. *EDM alternative.* [91, §1]
Given $D \in \mathbb{S}_{\mathbf{0}}^N$,

$$D \notin \mathbb{EDM}^N \;\Leftrightarrow\; \exists\, z \text{ such that } \left\{\begin{array}{l} \mathbf{1}^T z = 1 \\ Dz = \mathbf{0} \end{array}\right. \tag{640}$$

In words, either $\mathcal{N}(D)$ intersects hyperplane $\{z \mid \mathbf{1}^T z = 1\}$ or D is an EDM; the alternatives are incompatible. ⋄

When D is an EDM, on the other hand, [115, §2]

$$\mathcal{N}(D) \subset \mathcal{N}(\mathbf{1}^T) = \{z \mid \mathbf{1}^T z = 0\} \tag{641}$$

Because [91, §2] (§E.0.1)

$$\begin{array}{c} DD^\dagger \mathbf{1} = \mathbf{1} \\ \mathbf{1}^T D^\dagger D = \mathbf{1}^T \end{array} \tag{642}$$

then

$$\mathcal{R}(\mathbf{1}) \subset \mathcal{R}(D) \tag{643}$$

Chapter 6

Convex optimization

> *Prior to 1984*,[6.1] *linear and nonlinear programming, one a subset of the other, had evolved for the most part along unconnected paths, without even a common terminology.* (*The use of "programming" to mean "optimization" serves as a persistent reminder of these differences.*)
>
> −Forsgren, Gill, & Wright (2002) [116]

It may seem puzzling, at first, why given some application the search for its solution ends abruptly with a formalized statement of the problem as a constrained optimization. The explanation is: typically, we do not seek analytical solution because there are few; rather, if the problem can be expressed in *convex form*, then there exist computer programs providing efficient numerical global solution. [11] [117] [118] [4]

[6.1] nascence of *interior-point methods*, The goal, then, becomes conversion of a given problem to convex form:[6.2] Given convex objective function g and convex *feasible set*[6.3] $\mathcal{C}$, we have the generic convex optimization problem

$$\begin{array}{ll} \underset{X}{\text{minimize}} & g(X) \\ \text{subject to} & X \in \mathcal{C} \end{array} \tag{644}$$

where constraints are abstract in the membership of variable X to $\mathcal{C}$. Inequality constraint functions of a convex optimization problem are convex, while equality constraint functions are conventionally affine. [2, §1] [1, §4.2.1] The problem remains convex for maximization of a concave objective function (but not for maximization of a convex function). As conversion to convex form is not always possible, there is much ongoing research to determine what classes of problem have convex expression or relaxation. [7] [3] [5] [6] [119] [8]

6.1 Semidefinite programming

Still, we are surprised to see the relatively small number of submissions to semidefinite programming (SDP) solvers, as this is an area of significant current interest to the optimization community. We speculate that semidefinite programming is simply experiencing the fate of most new areas: Users have yet to understand how to pose their problems as semidefinite programs, and the lack of support for SDP solvers in popular modelling languages likely discourages submissions.

−*SIAM News*, 2002. [120, p.9]

[6.2] This means, essentially, the original problem statement might be a minimization of a constrained objective having many local minima. The equivalent or relaxed convex problem possesses one minimum, a unique global minimum ideally corresponding to a solution of the original problem; *e.g.*, §C.2.1.1.

[6.3] The feasible set of an optimization problem is the set of all variable values (belonging to the objective function domain) satisfying all the constraints.

6.1.1 Conic problem

Consider a prototypical *conic problem* (p) and its dual (d): [67, §3.3.1] [52, §2.1]

$$(\text{p}) \quad \begin{array}{ll} \underset{x}{\text{minimize}} & c^T x \\ \text{subject to} & x \in \mathcal{K} \\ & Ax = b \end{array} \qquad \begin{array}{ll} \underset{y,s}{\text{maximize}} & b^T y \\ \text{subject to} & s \in \mathcal{K}^* \\ & A^T y + s = c \end{array} \quad (\text{d}) \tag{173}$$

where $\mathcal{K}$ is a closed convex cone, $\mathcal{K}^*$ is its dual, matrix A is fixed, and the remaining quantities are vectors.

When $\mathcal{K}$ is a polyhedral cone (§2.7.1), then each conic problem becomes a *linear program.* More generally, each optimization problem is convex when $\mathcal{K}$ is a closed convex cone. Unlike the optimal objective value, a solution to each is not necessarily unique; in other words, the optimal solution set $\{x^\star\}$ or $\{y^\star, s^\star\}$ may each comprise more than a single point although the corresponding optimal objective value is unique when the feasible set is nonempty.

When $\mathcal{K}$ is the self-dual cone of positive semidefinite matrices in the subspace of symmetric matrices, then each conic problem is called a *semidefinite program*; primal problem (P) having matrix variable $X \in \mathbb{S}^n$ while corresponding dual (D) has matrix *slack variable* $S \in \mathbb{S}^n$ and vector variable $y \in \mathbb{R}^m$: [4, §1.3.8]

$$(\text{P}) \quad \begin{array}{ll} \underset{X}{\text{minimize}} & \langle C\,,\,X\rangle \\ \text{subject to} & X \succeq 0 \\ & A \operatorname{vec} X = b \end{array} \qquad \begin{array}{ll} \underset{y,S}{\text{maximize}} & \langle b\,,\,y\rangle \\ \text{subject to} & S \succeq 0 \\ & \operatorname{vec}^{-1}(A^T y) + S = C \end{array} \quad (\text{D}) \tag{645}$$

where matrix $C \in \mathbb{S}^n$ and vector $b \in \mathbb{R}^m$ are fixed, as is

$$A \triangleq \begin{bmatrix} \operatorname{vec}(A_1)^T \\ \vdots \\ \operatorname{vec}(A_m)^T \end{bmatrix} \in \mathbb{R}^{m \times n^2} \tag{646}$$

where $A_i \in \mathbb{S}^n$, $i=1 \ldots m$, are given. Thus

$$\begin{aligned} A \operatorname{vec} X &= \begin{bmatrix} \langle A_1\,,\,X\rangle \\ \vdots \\ \langle A_m\,,\,X\rangle \end{bmatrix} \\ \operatorname{vec}^{-1}(A^T y) &= \sum_{i=1}^m y_i A_i \end{aligned} \tag{647}$$

The vector inner product for matrices is defined in the Euclidean/Frobenius sense in the isomorphic vector space $\mathbb{R}^{n^2}$; *id est*, $\langle C\,, X\rangle \overset{\Delta}{=} \operatorname{tr}(C^TX) = \operatorname{vec}(C)^T \operatorname{vec} X$ where $\operatorname{vec} X$ (18) denotes vectorization by stacking columns in the natural order.

It has been shown that *interior-point methods* [1, §11] [42] [121] [6] can converge to a solution of maximal *complementarity*; [122] (§6.1.2.3.1) in that case, not a vertex-solution but a solution of high cardinality or rank. [4, §2.5.3]

We desire a simple algorithm for construction of a primal optimal solution $X^\star$ to (P) satisfying a least upper bound on rank governed by Proposition 2.6.6.4.1 (Barvinok) that asserts existence of low-rank feasible solutions. [23, §II.13.1] Specifically, the proposition asserts an extreme point (§2.5) of the primal feasible set $\mathcal{A} \cap \mathbb{S}^n_+$ satisfies least upper bound

$$\operatorname{rank} X \leq \left\lfloor \frac{\sqrt{8m+1}-1}{2} \right\rfloor \tag{148}$$

where

$$\mathcal{A} \overset{\Delta}{=} \{X \in \mathbb{S}^n \mid A \operatorname{vec} X = b\} \tag{648}$$

is the affine set from primal problem (P). Barvinok showed [60, §2.2] when given a positive definite matrix C and an arbitrarily small neighborhood of C comprising positive definite matrices, there exists a matrix $\tilde{C}$ from that neighborhood such that optimal solution $X^\star$ to (P) $\big($substituting $\tilde{C}\big)$ is an extreme point of $\mathcal{A} \cap \mathbb{S}^n_+$ and satisfies least upper bound (148).[6.4]

This means given arbitrary positive definite C, there is no guarantee an optimal solution $X^\star$ to (P) (using C) satisfies (148).

To prove that by example: (Ye) Assume dimension n to be an even positive number. Then the particular instance of problem (P),

$$\begin{array}{cl} \underset{X}{\text{minimize}} & \left\langle \begin{bmatrix} I & \mathbf{0} \\ \mathbf{0} & 2I \end{bmatrix}, X \right\rangle \\ \text{subject to} & X \succeq 0 \\ & \langle I\,, X\rangle = n \end{array} \tag{649}$$

has optimal solution

$$X^\star = \begin{bmatrix} 2I & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \in \mathbb{S}^n \tag{650}$$

[6.4] Further, the set of all such $\tilde{C}$ in that neighborhood is open and dense.

with an equal number of ones and zeros along the main diagonal. Indeed, optimal solution (650) is the terminal solution along the *central path* taken by the interior-point method as implemented in [4, §2.5.3]. Clearly, rank of this primal optimal solution exceeds by far the rank 1 solution predicted by least upper bound (148). ♦

This rational example (649) illustrates the need for a more generally applicable and simple algorithm to identify an optimal solution $X^\star$ satisfying the proposition. We will review such an algorithm in §6.1.3, but first we provide some background.

6.1.2 Framework

6.1.2.1 Feasible sets

Respectively denote by $\mathcal{F}_p$ and $\mathcal{F}_d$ the sets of primal and dual points satisfying the primal and dual constraints, each assumed nonempty;

$$\begin{aligned}
\mathcal{F}_p &= \left\{ X \in \mathbb{S}^n_+ \mid \begin{bmatrix} \langle A_1\,,\,X\rangle \\ \vdots \\ \langle A_m\,,\,X\rangle \end{bmatrix} = b \right\} \\
\mathcal{F}_d &= \left\{ S \in \mathbb{S}^n_+\,,\; y \in \mathbb{R}^m \mid \sum_{i=1}^m y_i A_i + S = C \right\}
\end{aligned} \tag{651}$$

These are the primal and dual *feasible sets* in the domain intersection of the respective constraint functions. Geometrically, primal feasible $\mathcal{F}_p$ represents an intersection of the positive semidefinite cone with an affine subset of the subspace of symmetric matrices $\mathbb{S}^n$ in isometrically isomorphic $\mathbb{R}^{n(n+1)/2}$. The affine subset has dimension $n(n+1)/2-m$ when the A_i are linearly independent. Dual feasible $\mathcal{F}_d$ is the Cartesian product of the positive semidefinite cone with its inverse image (§2.1.0.10.2) under affine transformation $C-\sum y_i A_i$.[6.5] Hence both sets are closed and convex, and (P) and (D) are convex optimization problems.

[6.5] The inequality $C-\sum y_i A_i \succeq 0$ follows directly from (D) and is known as a *linear matrix inequality.* (§2.8.2.4.1) Because $\sum y_i A_i \preceq C$, matrix S is known as a *slack variable* (a term borrowed from linear programming [63]) since its inclusion raises this inequality to equality.

6.1.2.2 Duals

The dual *objective function* evaluated at any feasible point represents a lower bound on the primal optimal objective value. We can see this by direct substitution: Assume the feasible sets $\mathcal{F}_p$ and $\mathcal{F}_d$ are nonempty. Then it is always true that

$$\begin{aligned} \langle C\,,\,X\rangle &\geq \langle b\,,y\rangle \\ \left\langle \sum_i y_i A_i + S\,,\,X\right\rangle &\geq [\,\langle A_1\,,\,X\rangle \;\cdots\; \langle A_m\,,\,X\rangle\,]\;y \\ \langle S\,,\,X\rangle &\geq 0 \end{aligned} \tag{652}$$

The converse also follows because

$$X \succeq 0\,,\;\; S \succeq 0 \;\;\Rightarrow\;\; \langle S, X\rangle \geq 0 \tag{862}$$

The optimal value of the dual objective thus represents the greatest lower bound on the primal. This fact is known as the *weak duality theorem* for semidefinite programming, [4, §1.3.8] and can be used to detect convergence in any primal/dual numerical method of solution.

6.1.2.3 Classical optimality conditions

When any primal feasible point exists interior to $\mathcal{F}_p$ in $\mathbb{S}^n$, or when any dual feasible point exists interior to $\mathcal{F}_d$ in $\mathbb{S}^n \times \mathbb{R}^m$, then by *Slater's condition* [1, §5.2.3] these two problems (645)(P) and (D) become *strong duals.* In other words, the primal optimal objective value becomes equivalent to the dual optimal objective value: there is no duality gap; *id est*, if $\exists\, X \in \operatorname{int} \mathcal{F}_p$ or $\exists\, S, y \in \operatorname{int} \mathcal{F}_d$, then

$$\begin{aligned} \langle C\,,\,X^\star\rangle &= \langle b\,,y^\star\rangle \\ \left\langle \sum_i y_i^\star A_i + S^\star,\,X^\star\right\rangle &= [\,\langle A_1\,,\,X^\star\rangle \;\cdots\; \langle A_m\,,\,X^\star\rangle\,]\;y^\star \\ \langle S^\star,\,X^\star\rangle &= 0 \end{aligned} \tag{653}$$

where $S^\star$, $y^\star$ denote the dual optimal solution.[6.6] We summarize this:

[6.6] The optimality condition $\langle S^\star, X^\star\rangle = 0$ is called the *complementary slackness condition* in keeping with the tradition of linear programming. [63]

6.1.2.3.1 Corollary. *Strong duality and optimality.* [69, §3.1] [4, §1.3.8] For semidefinite programs (645)(P) and (D), assume primal and dual feasible sets $\mathcal{F}_p \subset \mathbb{S}^n$ and $\mathcal{F}_d \subset \mathbb{S}^n \times \mathbb{R}^m$ (651) are nonempty. Then

- $X^\star$ is optimal for (P)
- $S^\star$, $y^\star$ are optimal for (D)
- the duality gap $\langle C\,, X^\star\rangle - \langle b\,, y^\star\rangle$ is 0

if and only if

i) $\exists\, X \in \operatorname{int} \mathcal{F}_p$ **or** $\exists\, S\,,\ y \in \operatorname{int} \mathcal{F}_d$

and

ii) $\langle S^\star, X^\star\rangle = 0$ ◇

For symmetric positive semidefinite matrices, requirement **ii** is equivalent to the complementarity (§A.7.3)

$$S^\star X^\star = X^\star S^\star = \mathbf{0} \tag{654}$$

Because these two optimal symmetric matrices are simultaneously diagonalizable due to their commutativity,

$$\operatorname{rank} X^\star + \operatorname{rank} S^\star \leq\ n \tag{655}$$

To see that, the product of the symmetric optimal matrices $X^\star, S^\star \in \mathbb{S}^n$ must itself be symmetric because of commutativity. (856) The symmetric product has diagonalization

$$S^\star X^\star = X^\star S^\star = Q \Lambda_{S^\star} \Lambda_{X^\star} Q^T = \mathbf{0} \quad \Leftrightarrow \quad \Lambda_{X^\star} \Lambda_{S^\star} = \mathbf{0} \tag{656}$$

where Q is an orthogonal matrix. The product of the nonnegative diagonal Λ matrices can be $\mathbf{0}$ if their diagonal zeros are complementary or coincide. Due only to symmetry, $\operatorname{rank} X^\star = \operatorname{rank} \Lambda_{X^\star}$ and $\operatorname{rank} S^\star = \operatorname{rank} \Lambda_{S^\star}$ for these optimal primal and dual solutions. (846) So, because of the complementarity, the total number of nonzero diagonal entries from both Λ cannot exceed n .
♦

When equality is attained in (655),

$$\operatorname{rank} X^\star + \operatorname{rank} S^\star = n \tag{657}$$

there are no coinciding diagonal zeros in $\Lambda_{X^\star}\Lambda_{S^\star}$, and then we have what is called *strict complementarity.* Logically it follows that a necessary and sufficient condition for strict complementarity of the optimal primal and dual solution is

$$X^\star + S^\star \succ 0 \tag{658}$$

The beauty of Corollary 6.1.2.3.1 is its symmetry; *id est*, one can solve either the primal or dual problem and then find a solution to the other via the optimality conditions. When the dual optimal solution is known, for example, the primal optimal solution belongs to the hyperplane $\{X \mid \langle S^\star, X\rangle = 0\}$.

6.1.3 Rank-reduced solution

Recall, there is an extreme point of $\mathcal{A}\cap\mathbb{S}^n_+$ (648) satisfying least upper bound (148) on rank. [60, §2.2] It is therefore sufficient to locate an extreme point whose primal objective value (645)(P) is optimal:[6.7]

For affine set $\mathcal{A}$ as in (648), given any optimal solution $X^\star$ to (645)(P)

$$(\mathrm{P}) \qquad \begin{array}{cl} \underset{X}{\text{minimize}} & \langle C\,,\,X\rangle \\ \text{subject to} & X \in \mathcal{A}\cap\mathbb{S}^n_+ \end{array} \tag{659}$$

whose rank does not satisfy least upper bound (148), we posit the existence of a set of perturbations

$$\{t_j B_j \mid t_j \in \mathbb{R}\,,\ B_j \in \mathbb{S}^n,\ j = 1 \ldots n\} \tag{660}$$

such that for some $0 \le i \le n$

$$X^\star + \sum_{j=1}^{i} t_j B_j \tag{661}$$

becomes an extreme point of $\mathcal{A}\cap\mathbb{S}^n_+$ and remains an optimal solution of (P). Membership of $X^\star + \sum\limits_{j=1}^{i} t_j B_j$ to affine set $\mathcal{A}$ is secured for the i^{th}

[6.7] Similar strategies can be found in [50, §31.5.3] [52, §2.4] [93, §3] [123]. There is no known construction for Barvinok's tighter result (153).

perturbation by demanding

$$\langle B_i\,, A_j\rangle = 0\,,\quad j\!=\!1\ldots m \tag{662}$$

Membership to the positive semidefinite cone $\mathbb{S}^n_+$ is insured by a small perturbation. (671) In this manner feasibility is insured. Optimality is proved in §6.1.3.2.

The following simple procedure has very low computational intensity and locates an optimal extreme point, assuming a nontrivial solution:

6.1.3.0.1 Rank reduction procedure

`initialize:` $B_i\!=\!\mathbf{0}\ \ \forall\, i$
`for` iteration `i=1...n`
{

1. `compute` a nonzero perturbation matrix B_i of $X^\star + \sum\limits_{j=1}^{i-1} t_j B_j$

2. `maximize` t_i such that $X^\star + \sum\limits_{j=1}^{i} t_j B_j \in \mathbb{S}^n_+$

}

The rank-reduced optimal solution is then

$$X^\star \leftarrow X^\star + \sum_{j=1}^{i} t_j B_j \tag{663}$$

6.1.3.0.2 Definition. *Matrix step function.*

Define the signum-like real function $\Psi : \mathbb{S}^n \to \mathbb{R}$,

$$\Psi(A) \triangleq \begin{cases} \;\;1\,, & A \succeq 0 \\ -1\,, & \text{otherwise} \end{cases} \tag{664}$$

The value -1 is taken for indefinite or nonzero negative semidefinite argument. △

6.1.3.1 Perturbation form

Deza & Laurent [50, §31.5.3] prove every perturbation matrix B_i , $i=1\ldots n$, is of the form,

$$B_i = -\Psi(Z_i) R_i Z_i R_i^T \tag{665}$$

where

$$X^\star + \sum_{j=1}^{i-1} t_j B_j \triangleq R_i R_i^T \tag{666}$$

where $R_i \in \mathbb{R}^{n\times\rho}$ is full-rank and skinny where

$$\rho \triangleq \operatorname{rank}\left(X^\star + \sum_{j=1}^{i-1} t_j B_j\right) \tag{667}$$

and where matrix $Z_i \in \mathbb{S}^\rho$ is found at each iteration i by solving a very simple feasibility problem: [6.8]

$$\begin{array}{cll} \text{find} & Z_i \in \mathbb{S}^\rho & \\ \text{subject to} & \langle Z_i\,,\, R_i^T A_j R_i\rangle = 0\,, & j=1\ldots m \end{array} \tag{668}$$

At iteration i ,

$$X^\star + \sum_{j=1}^{i-1} t_j B_j \;+\; t_i B_i \;=\; R_i\big(I - t_i \Psi(Z_i) Z_i\big) R_i^T \tag{669}$$

Maximization of each t_i in step 2 reduces the rank of (669) and locates a new point on the boundary $\partial(\mathcal{A}\cap\mathbb{S}_+^n)$ because, by fact (845),

$$\mathbf{1} - t_i \Psi(Z_i)\lambda(Z_i) \succeq 0 \;\Leftrightarrow\; X^\star + \sum_{j=1}^{i-1} t_j B_j \;+\; t_i B_i \succeq 0 \tag{670}$$

rank of a positive semidefinite matrix in $\mathbb{S}^n$ is diminished below n by the number of 0 eigenvalues (846), where $\lambda(Z_i)$ denotes eigenvalues of Z_i , and

[6.8] whose simplest method of solution projects a random nonzero point on the proper subspace of isomorphic $\mathbb{R}^{\rho(\rho+1)/2}$ specified by the constraints. (§E.5) The solution is nontrivial assuming the specified intersection of hyperplanes is not the origin; guaranteed by $\rho(\rho+1)/2 > m$. Indeed, this geometric intuition about forming the perturbation is what bounds the solution's rank from below; m is fixed by the number of equality constraints in (645)(P) while rank ρ decreases with each iteration i . Otherwise, we might iterate indefinitely.

because a positive semidefinite matrix having one or more 0 eigenvalues corresponds to a point on the PSD cone boundary (122). Necessity and sufficiency are due to the facts: R_i can be completed to a nonsingular matrix (§A.3.1.0.5), and $I - t_i\Psi(Z_i)Z_i$ can be padded with zeros while maintaining equivalence in (669). The maximization of t_i thereby has closed form;

$$(t_i^\star)^{-1} = \max\{\Psi(Z_i)\lambda(Z_i)_j \;,\; j=1\ldots\rho\} \tag{671}$$

When Z_i is indefinite, the direction of perturbation (determined by $\Psi(Z_i)$) is arbitrary. We may take an early exit from the Procedure under the circumstance

$$\operatorname{rank}\big[\operatorname{svec} R_i^T A_1 R_i \quad \operatorname{svec} R_i^T A_2 R_i \;\cdots\; \operatorname{svec} R_i^T A_m R_i\big] = \rho(\rho+1)/2 \tag{672}$$

which characterizes the rank ρ of any [*sic*] extreme point in $\mathcal{A}\cap\mathbb{S}_+^n$. [52, §2.4]

To see that, assuming the form of every perturbation matrix is indeed (665), then by (668)

$$\operatorname{svec} Z_i \perp \big[\operatorname{svec}(R_i^T A_1 R_i) \quad \operatorname{svec}(R_i^T A_2 R_i) \;\cdots\; \operatorname{svec}(R_i^T A_m R_i)\big] \tag{673}$$

By orthogonal complement we have

$$\operatorname{rank}\big[\operatorname{svec}(R_i^T A_1 R_i) \;\cdots\; \operatorname{svec}(R_i^T A_m R_i)\big]^\perp + \operatorname{rank}\big[\operatorname{svec}(R_i^T A_1 R_i) \;\cdots\; \operatorname{svec}(R_i^T A_m R_i)\big] = \rho(\rho+1)/2 \tag{674}$$

When Z_i can only be $\mathbf{0}$, then the perturbation is null because an extreme point has been found; thus

$$\big[\operatorname{svec}(R_i^T A_1 R_i) \;\cdots\; \operatorname{svec}(R_i^T A_m R_i)\big]^\perp = \mathbf{0} \tag{675}$$

from which the stated result (672) directly follows. ♦

6.1.3.2 Optimality of perturbed $X^\star$

We show that the optimal objective value is unaltered by perturbation (665); *id est*,

$$\langle C \;,\; X^\star + \sum_{j=1}^{i} t_j B_j\rangle \;=\; \langle C \;,\; X^\star\rangle \tag{676}$$

From Corollary 6.1.2.3.1 we have the necessary and sufficient relationship between optimal primal and dual solutions under the assumption of existence of an interior feasible point:

$$S^\star X^\star = S^\star R_1 R_1^T = X^\star S^\star = R_1 R_1^T S^\star = \mathbf{0} \tag{677}$$

This means $\mathcal{R}(R_1) \subseteq \mathcal{N}(S^\star)$ and $\mathcal{R}(S^\star) \subseteq \mathcal{N}(R_1^T)$. From (666) and (669) we get the sequence:

$$\begin{aligned}
&X^\star = R_1 R_1^T \\
&X^\star + t_1 B_1 = R_2 R_2^T = R_1\big(I - t_1\Psi(Z_1)Z_1\big)R_1^T \\
&X^\star + t_1 B_1 + t_2 B_2 = R_3 R_3^T = R_2\big(I - t_2\Psi(Z_2)Z_2\big)R_2^T = R_1\big(I - t_1\Psi(Z_1)Z_1\big)\big(I - t_2\Psi(Z_2)Z_2\big)R_1^T \\
&\vdots \\
&X^\star + \sum_{j=1}^{i} t_j B_j = R_1\left(\prod_{j=1}^{i}\big(I - t_j\Psi(Z_j)Z_j\big)\right)R_1^T
\end{aligned} \tag{678}$$

Substituting $C = \operatorname{vec}^{-1}(A^T y^\star) + S^\star$ from (645),

$$\begin{aligned}
\langle C\ ,\ X^\star + \sum_{j=1}^{i} t_j B_j\rangle &= \left\langle \operatorname{vec}^{-1}(A^T y^\star) + S^\star\ ,\ R_1\left(\prod_{j=1}^{i}\big(I - t_j\Psi(Z_j)Z_j\big)\right)R_1^T\right\rangle \\
&= \left\langle \sum_{k=1}^{m} y_k^\star A_k\ ,\ X^\star + \sum_{j=1}^{i} t_j B_j\right\rangle \\
&= \left\langle \sum_{k=1}^{m} y_k^\star A_k + S^\star\ ,\ X^\star\right\rangle = \langle C\ ,\ X^\star\rangle
\end{aligned} \tag{679}$$

because $\langle B_i\,, A_j\rangle = 0\ \ \forall\, i\,, j$ by design (662). ♦

6.2 Examples

6.2.0.0.1 Example. *Rank reduction.*
Given data

$$A = \begin{bmatrix} -1 & 1 & 8 & 1 & 1 \\ -3 & 2 & 8 & 1/2 & 1/3 \\ -9 & 4 & 8 & 1/4 & 1/9 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ 1/2 \\ 1/4 \end{bmatrix} \tag{680}$$

consider the convex optimization problem

$$\begin{array}{ll}\underset{X\in\mathbb{S}^5}{\text{minimize}} & \operatorname{tr} X\\ \text{subject to} & X\succeq 0\\ & A\delta(X)=b\end{array}\tag{681}$$

where the number of equality constraints is $m=3$. Rank-3 solution $X^\star=\delta(x_M)$ is optimal, where

$$x_M=\begin{bmatrix}\frac{2}{128}\\ 0\\ \frac{5}{128}\\ 0\\ \frac{90}{128}\end{bmatrix}\tag{682}$$

although least upper bound (148) predicts existence of at most a rank-$\left(\left\lfloor\frac{\sqrt{8m+1}-1}{2}\right\rfloor=2\right)$ feasible solution from three equality constraints. To find a lower rank ρ solution to (681) (barring combinatorics), we invoke Procedure 6.1.3.0.1:

`Initialize:`

$C=I\,,\ \ \rho=3,\ \ A_j\stackrel{\Delta}{=}\delta(A(j,:))\,,\ j=1,2,3,\ \ X^\star=\delta(x_M)\,,\ \ m=3,\ \ n=5.$

{

`Iteration:` $i=1$:

`Step 1:` $R_1=\begin{bmatrix}\sqrt{\frac{2}{128}} & 0 & 0\\ 0 & 0 & 0\\ 0 & \sqrt{\frac{5}{128}} & 0\\ 0 & 0 & 0\\ 0 & 0 & \sqrt{\frac{90}{128}}\end{bmatrix}.$

$$\begin{array}{ll}\text{find} & Z_1\in\mathbb{S}^3\\ \text{subject to} & \langle Z_1\,,\,R_1^TA_jR_1\rangle=0\,,\qquad j=1,2,3\end{array}\tag{683}$$

A nonzero random matrix Z_1 having $\mathbf{0}$ main diagonal is feasible and yields a nonzero perturbation matrix. Arbitrarily choose

$$Z_1=\mathbf{1}\mathbf{1}^T-I\in\mathbb{S}^3\tag{684}$$

then (rounding)

$$B_1 = \begin{bmatrix} 0 & 0 & 0.0247 & 0 & 0.1048 \\ 0 & 0 & 0 & 0 & 0 \\ 0.0247 & 0 & 0 & 0 & 0.1657 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1048 & 0 & 0.1657 & 0 & 0 \end{bmatrix} \tag{685}$$

`Step 2:` $t_1^\star = 1$ because $\lambda(Z_1) = [\,-1 \;\; -1 \;\;\; 2\,]^T$. So,

$$X^\star \leftarrow \delta(x_M) + B_1 = \begin{bmatrix} \frac{2}{128} & 0 & 0.0247 & 0 & 0.1048 \\ 0 & 0 & 0 & 0 & 0 \\ 0.0247 & 0 & \frac{5}{128} & 0 & 0.1657 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1048 & 0 & 0.1657 & 0 & \frac{90}{128} \end{bmatrix} \tag{686}$$

having rank $\rho \leftarrow 1$ and produces the same optimal objective value.

}

□

This example demonstrates the solution found by rank reduction can certainly be less than Barvinok's least upper bound (148).

6.2.0.0.2 Example. *Boolean.* [10] [7, §4.3.4] [119]
Consider another approach to finding a solution of Platonic linear problem

$$Ax = b \tag{687}$$

given data (680). Matrix A is full-rank having a two-dimensional nullspace (now different from A in the prototype (645)(P), as is b). The obvious and desired solution to this problem,

$$x^\star = e_4 \in \mathbb{R}^{\mathbf{5}} \tag{688}$$

has norm equal to 1 and minimum cardinality;[6.9] the minimum number of nonzero entries in x. A minimum cardinality solution answers the question: "Which fewest linear combination of columns in A most closely resembles

[6.9] $\dim x = 5$ while $\dim \mathcal{R}(x) = 1$.

vector b?" Such a problem has universal appeal, arising in many fields of science and across many disciplines. [124] [125]

Designing an efficient algorithm to optimize cardinality has proved difficult. Though solution (688) is obvious, the simplest method of solution is combinatorial in general. The MATLAB backslash command `x=A\b`, for example, finds x_M (682) having norm 0.7044. The pseudoinverse solution (rounded)

$$x_P = A^\dagger b = \begin{bmatrix} -0.0505 \\ -0.1975 \\ 0.0590 \\ 0.2796 \\ 0.3955 \end{bmatrix} \tag{689}$$

has minimum norm 0.5288. Certainly, none of the traditional methods provide $x^\star = e_4$.

Formulate the problem $Ax = b$ using $x \triangleq (\hat{x} + \mathbf{1})/2$, for $A \in \mathbb{R}^{m\times n}$:

$$\begin{array}{cl} \underset{\hat{x}}{\text{minimize}} & \|A(\hat{x}+\mathbf{1})\frac{1}{2} - b\|_2^2 \\ \text{subject to} & \delta(\hat{x})^2 = I \end{array} \tag{690}$$

which is the same as

$$\begin{array}{cl} \underset{\hat{x}}{\text{minimize}} & \hat{x}^T A^T A \hat{x} \frac{1}{2} - 2(A^T b - A^T A \mathbf{1}\frac{1}{2})^T \hat{x} \\ \text{subject to} & \delta(\hat{x})^2 = I \end{array} \tag{691}$$

Neither problem is convex because of the nonlinear equality constraints. Thus the problem is made difficult by the quantized variable, having two allowable states. By defining

$$X \triangleq \begin{bmatrix} \hat{x} \\ 1 \end{bmatrix} [\,\hat{x}^T \;\; 1\,] \in \mathbb{R}^{n+1\times n+1} \tag{692}$$

these two problems become equivalent to:

$$\begin{array}{cl} \underset{X\in\mathbb{S}^{n+1}}{\text{minimize}} & \operatorname{tr}\left(X \begin{bmatrix} A^T A \frac{1}{2} & A^T A \mathbf{1}\frac{1}{2} - A^T b \\ (A^T A \mathbf{1}\frac{1}{2} - A^T b)^T & 0 \end{bmatrix}\right) \\ \text{subject to} & \delta(X) = \mathbf{1} \\ & X \succeq 0 \\ & \operatorname{rank} X = 1 \end{array} \tag{693}$$

The rank constraint is non-convex. By eliminating it we get the convex optimization[6.10]

$$\begin{array}{ll}\underset{X\in\mathbb{S}^{n+1}}{\text{minimize}} & \operatorname{tr}\left(X\begin{bmatrix} A^TA\frac{1}{2} & A^TA\mathbf{1}\frac{1}{2}-A^Tb \\ (A^TA\mathbf{1}\frac{1}{2}-A^Tb)^T & 0\end{bmatrix}\right) \\ \text{subject to} & \delta(X)=\mathbf{1} \\ & X\succeq 0\end{array} \tag{694}$$

whose solution $X^\star$ is identical to that of the original problem (690) if and only if $\operatorname{rank}X^\star=1$; in that case, we are done. Otherwise we may invoke our rank reduction procedure which is guaranteed only to produce another optimal solution conforming to Barvinok's least upper bound (148); in the case $n=5$ with six constraints $\delta(X)=\mathbf{1}$, that upper bound on rank is 3.

Our semidefinite program solver produces $X^\star$ with the following eigenvalues (accurate to four decimal places):

$$\lambda(X^\star)=\{0.0000,\ 0.0000,\ 0.0000,\ 0.0001,\ 0.0010,\ 5.9989\} \tag{695}$$

$\square$

The rank reduction procedure will not produce solutions of arbitrarily low rank. To force a lower rank solution, spectral projection methods must be employed as in §7.

[6.10] This relaxed problem can also be derived via Lagrange duality; it is the dual of the dual program to (690). Therefore it must be convex.

6.2.0.0.3 Riemann mapping theorem... Techniques for reconstruction we studied ...thus far... essentially are methods for optimally embedding in a subspace of desired dimension an unknown list of points corresponding to given Euclidean distance data. While these techniques are themselves important and have found useful contemporary application, we turn now to optimal embedding of sampled non-affine manifolds in subspaces.

6.2.0.0.4 Manifold... A smooth manifold is...
A smooth manifold topologically *homeomorphic* with a vector space is embeddable in that vector space. [Whitney, H., "Differentiable Manifolds", Annals of Mathematics (1936)] Contemporary applications generally seek that embedding having lowest dimension because it is believed that obscured information is thereby revealed. [Saul]

6.2.0.0.5 Ye projection for dimension reduction...

6.2.0.0.6 Linear Complementarity Problem as SDP cite SIAM Review vol.46 no.2 June 2004...

Chapter 7

EDM proximity

In summary, we find that the solution to problem [(703.3) p.248] *is difficult and depends on the dimension of the space as the geometry of the cone of EDMs becomes more complex.*

−Hayden, Wells, Liu, & Tarazaga (1991) [49, §3]

A problem common to various sciences is to find the Euclidean distance matrix (EDM) $D\in\mathbb{EDM}^N$ closest in some sense to a given matrix of measurements H under the constraint that affine dimension $0\le r\le N-1$ (§2.2.1, §4.7.2) is predetermined; rather, constrained by upper bound ρ. That commonality was unified by de Leeuw and Heiser in 1982 [126] [73] who denoted by the term they coined *multidimensional scaling* [85] any reconstruction of a list X in Euclidean space from only inter-point distance information, possibly incomplete (§8) or ordinal (§4.11.2).

7.0.1 Lower bound

Most of the problems we will encounter in this chapter have the general form:

$$\underset{B\in\mathcal{C}}{\text{minimize}} \ \ \|B-A\|_{\mathrm{F}} \tag{696}$$

where $A\in\mathbb{R}^{m\times n}$ is given data. This particular objective denotes Euclidean projection of A on the set $\mathcal{C}$ (§E.3) which may or may not be convex. When $\mathcal{C}$ is convex, the projection is unique; when $\mathcal{C}$ is a subspace, then the projection is orthogonal.

Denoting by $A = U_A\Sigma_A Q_A^T$ and $B = U_B\Sigma_B Q_B^T$ their full singular value decompositions (§A.6), there exists a tight lower bound on the objective;

$$\|\Sigma_B-\Sigma_A\|_{\mathrm{F}} \ \leq \inf_{U_A,\,U_B,\,Q_A,\,Q_B} \|B-A\|_{\mathrm{F}} \tag{697}$$

This lower bound holds more generally for any orthogonally invariant norm on $\mathbb{R}^{m\times n}$ (§2.1.1.1) including the Frobenius. [28, §7.4.51]

7.0.2 Measurement matrix H

Ideally, we want a given measurement matrix $H\in\mathbb{R}^{N\times N}$ to conform with the first three Euclidean axioms (§4.2), to belong to the intersection of the orthant of nonnegative matrices $\mathbb{R}_+^{N\times N}$ with the symmetric hollow subspace $\mathbb{S}_{\mathbf{0}}^N$ (§2.1.2.2); *id est*, we want H to belong to the polyhedral cone (§2.7.1)

$$\mathcal{K} \triangleq \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N} \tag{698}$$

Yet in practice, H can possess significant measurement uncertainty.

Sometimes an optimization problem demands that its input, the given matrix H, possess some particular characteristics; perhaps symmetry and hollowness or nonnegativity. When that H given does not have the desired properties, then we must impose them upon H prior to optimization:

- When measurement matrix H is not symmetric or hollow, taking its symmetric hollow part is equivalent to orthogonal projection on the symmetric hollow subspace $\mathbb{S}_{\mathbf{0}}^N$.

- When measurements of distance in H are negative, zeroing negative entries effects *unique* (minimum distance) *projection* on the orthant of nonnegative matrices $\mathbb{R}_+^{N\times N}$ in isomorphic $\mathbb{R}^{N^2}$ (§E.8.1.2.1).

7.0.2.1 Order of imposition

Since convex cone $\mathcal{K}$ (698) is the intersection of an orthant with a subspace, we want to project on that subset of the orthant belonging to the subspace; on the nonnegative orthant in the symmetric hollow subspace that is, in fact, the intersection. For that reason alone, the unique projection of H on $\mathcal{K}$ (that member of $\mathcal{K}$ closest to H in $\mathbb{R}^{N^2}$ in the Euclidean sense) can be obtained by first taking its symmetric hollow part, and only then clipping negative entries of the result to 0; *id est*, there is only one correct *order of projection*, in general, on an orthant intersecting a subspace:

- project on the subspace, then project the result on the orthant. (§E.8.3)

In contrast, the order of projection on an intersection of subspaces is arbitrary.

That order-of-projection rule applies more generally, of course, to the intersection of any convex set $\mathcal{C}$ with any subspace.[7.1] Consider the *projective optimization*[7.2] over convex set $\mathbb{S}^N_{\mathbf{0}} \cap \mathcal{C}$ given nonsymmetric nonhollow H :

$$\begin{array}{cl}\underset{B\in\mathbb{S}^N_{\mathbf{0}}}{\text{minimize}} & \|B-H\|_{\mathrm{F}}^2\\ \text{subject to} & B\in\mathcal{C}\end{array}\tag{699}$$

Because the symmetric hollow subspace is orthogonal to the antisymmetric antihollow subspace (§2.1.2.2), then for $B\in\mathbb{S}^N_{\mathbf{0}}$,

$$\operatorname{tr}\left(B^T\left(\frac{1}{2}(H-H^T)+\delta^2(H)\right)\right)=0\tag{700}$$

so the objective function is equivalent to

$$\|B-H\|_{\mathrm{F}}^2 \equiv \left\|B-\left(\frac{1}{2}(H+H^T)-\delta^2(H)\right)\right\|_{\mathrm{F}}^2 + \left\|\frac{1}{2}(H-H^T)+\delta^2(H)\right\|_{\mathrm{F}}^2\tag{701}$$

[7.1] There are special cases where order of projection is arbitrary; *e.g.*, when all the faces of $\mathcal{C}$ are perpendicular to the intersecting subspace.

[7.2] There are two equivalent interpretations of projection (§E.3, §E.8): one finds the perpendicular, the other, minimum distance between a point and a set. In projective optimization we realize the latter view.

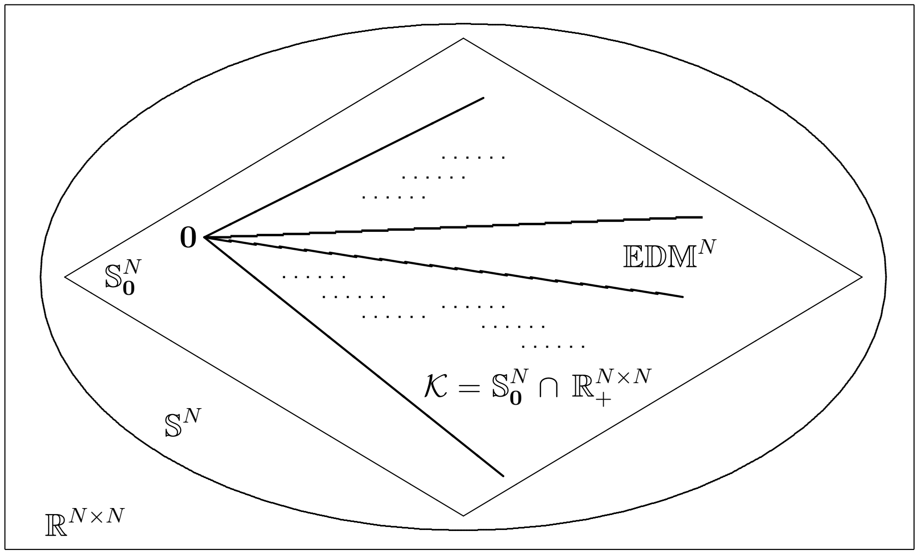


Figure 7.1: Pseudo-Venn diagram: The EDM cone belongs to the intersection of the symmetric hollow subspace with the nonnegative orthant; $\mathbb{EDM}^N \subseteq \mathcal{K}$ (332). $\mathbb{EDM}^N$ cannot exist outside $\mathbb{S}_0^N$, but $\mathbb{R}_+^{N\times N}$ does.

This means the antisymmetric antihollow part of given matrix H would be ignored by minimization with respect to symmetric hollow variable B under the Frobenius norm; *id est*, minimization proceeds as though given the symmetric hollow part of H .

This action of the Frobenius norm (701) is effectively a projection of H on the symmetric hollow subspace $\mathbb{S}_0^N$ prior to minimization. Thus the minimization proceeds inherently following the correct order for projection on $\mathbb{S}_0^N \cap \mathcal{C}$. Therefore we may assume $H \in \mathbb{S}_0^N$ or take its symmetric hollow part prior to optimization.

7.0.2.2 Egregious input error under nonnegativity demand

More pertinent to the optimization problems presented herein where

$$\mathcal{C} \triangleq \mathbb{EDM}^N \subseteq \mathcal{K} = \mathbb{S}_0^N \cap \mathbb{R}_+^{N\times N} \tag{702}$$

then should some particular realization of a projective optimization problem demand input H be nonnegative, and were we only to zero negative entries of

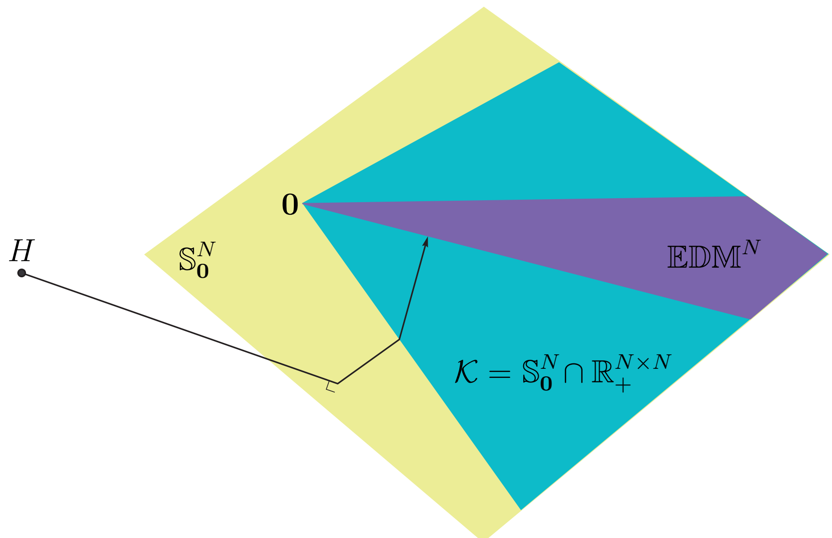


Figure 7.2: Pseudo-Venn diagram from Figure **7.1** showing elbow placed in path of projection of H on $\mathbb{EDM}^N \subset \mathbb{S}_{\mathbf{0}}^{N}$ by an optimization problem demanding nonnegative input matrix H. The first two line segments leading away from H result from correct order-of-projection required to provide nonnegative H prior to optimization. Were H nonnegative, then its projection on $\mathbb{S}_{\mathbf{0}}^{N}$ would instead belong to $\mathcal{K}$; making the elbow disappear. (*confer* Figure **E.3**)

a nonsymmetric nonhollow input H prior to optimization, then the ensuing projection on $\mathbb{EDM}^N$ would be guaranteed incorrect (out of order).

Now comes a surprising fact: Even were we to correctly follow the order-of-projection rule and provide $H \in \mathcal{K}$ prior to optimization, then the ensuing projection on $\mathbb{EDM}^N$ will still be incorrect whenever H has negative entries. This is best understood referring to Figure **7.1**: Suppose some projective optimization problem demands a nonnegative input H. Further suppose that same optimization problem correctly projects its input first on $\mathbb{S}_{\mathbf{0}}^{N}$ and then directly on $\mathcal{C} = \mathbb{EDM}^N$. Knowing this, then the demand for nonnegative input H effectively requires imposition of $\mathcal{K}$ on H prior to optimization so as to obtain correct order of projection; *id est*, $\mathbb{S}_{\mathbf{0}}^{N}$ first. Yet such an imposition prior to projection on $\mathbb{EDM}^N$ generally introduces an elbow into the path of projection (illustrated in Figure **7.2**) caused by the technique itself; a particular optimization problem formulation requiring nonnegative input.

Any procedure for imposition of nonnegativity on input H is incorrect in this circumstance. There is no resolution unless input H is guaranteed nonnegative with no tinkering. Otherwise, we have no choice but to employ a different optimization technique; one not demanding nonnegative input.

7.0.3 Three prevalent fundamental problems

There are three statements of the closest-EDM problem prevalent in the literature, the multiplicity due primarily to concessions for hard problems and vacillation between the distance-square variable d_{ij} *versus* absolute distance $\sqrt{d_{ij}}$; they are, (703.1), (703.2), and (703.3):

$$\begin{array}{llll}
(1) & \begin{array}{ll}\underset{D}{\text{minimize}} & \|-V(D-H)V\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} VDV \leq \rho\\ & D\in\mathbb{EDM}^N\end{array} & \begin{array}{ll}\underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} VDV \leq \rho\\ & D\in\mathbb{EDM}^N\end{array} & (2)\\
\\
(3) & \begin{array}{ll}\underset{D}{\text{minimize}} & \|D-H\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} VDV \leq \rho\\ & D\in\mathbb{EDM}^N\end{array} & \begin{array}{ll}\underset{D}{\text{minimize}} & \|-V(\sqrt{D}-H)V\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} VDV \leq \rho\\ & D\in\mathbb{EDM}^N\end{array} & (4)
\end{array} \tag{703}$$

where ρ is the upper bound on affine dimension and $D \triangleq [d_{ij}]$. Problem (703.2) has the associated moniker *stress* [127] ascribed by the mathematical community,[7.3] while (703.1) has the nickname *strain*; [100] [22] two nebulous mnemonics. Problem (703.4) is not posed in the literature because it has limited theoretical foundation (§4.13).

Generally speaking, each problem produces different results. Of the various auxiliary matrices (§B.4), the geometric centering matrix V (996) ap-

---

[7.3] *I have been interested in the concept of stress in a mathematical setting for some time. It is true that the way I use it is not exactly the same as what it means in physics or elasticity theory. But it is closely related. I did not want to take the time to motivate the word in this paper. I tend to use the word "stress" as the scalar coefficients for the squared distances in a energy functional, not as a force. The physical sense of stress could be used, but it is distracting from the simple mathematical ideas that are involved. Again one can translate, but my motivation is from geometry not engineering or even physics. Nevertheless, the idea is quite useful. Indeed, "stress matrices" explain a lot about the "rigidity" of many tensegrity structures, and they do it in a reasonable way, in my opinion.* —Robert Connelly pears in the literature most often although $V_{\mathcal{N}}$ (339) is the auxiliary matrix naturally consequent to Schoenberg's seminal exposition [87].

Substitution of $V_{\mathcal{N}}^T$ for left-hand V in (703.1) produces a different result because minimization of

$$\|-V(D-H)V\|_{\mathrm{F}}^2 \tag{704}$$

selects D to minimize the distance of $-VHV$ to the positive semidefinite cone in ambient $\mathbb{S}^N$, whereas minimization of

$$\|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_{\mathrm{F}}^2 \tag{705}$$

minimizes the distance of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ to the positive semidefinite cone in $\mathbb{S}^{N-1}$; quite different mappings.[7.4] But substitution of $V_{\mathcal{W}}^T$ (§B.4.3) or $V_{\mathcal{N}}^\dagger$ in (703.1) instead yields the same result because $V = V_{\mathcal{W}} V_{\mathcal{W}}^T = V_{\mathcal{N}} V_{\mathcal{N}}^\dagger$; *id est*,

$$\begin{aligned}\|-V(D-H)V\|_{\mathrm{F}}^2 &= \|-V_{\mathcal{W}}V_{\mathcal{W}}^T(D-H)V_{\mathcal{W}}V_{\mathcal{W}}^T\|_{\mathrm{F}}^2 = \|-V_{\mathcal{W}}^T(D-H)V_{\mathcal{W}}\|_{\mathrm{F}}^2 \\ &= \|-V_{\mathcal{N}}V_{\mathcal{N}}^\dagger(D-H)V_{\mathcal{N}}V_{\mathcal{N}}^\dagger\|_{\mathrm{F}}^2 = \|-V_{\mathcal{N}}^\dagger(D-H)V_{\mathcal{N}}\|_{\mathrm{F}}^2\end{aligned} \tag{706}$$

Problems (703.2) and (703.3) are convex optimization problems in the case $\rho = N-1$. When the rank constraint is removed from (703.2), we will see the convex problem remaining inherently minimizes affine dimension.

7.1 First prevalent problem: Projection on PSD cone

This first problem

$$\left.\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \le \rho \\ & D \in \mathbb{EDM}^N\end{array}\right\} \quad \text{Problem 1} \tag{707}$$

poses a projection [37, §3.12] of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ in subspace $\mathbb{S}^{N-1}$ on a non-convex subset (when $\rho < N-1$) of the positive semidefinite cone $\mathbb{S}_+^{N-1}$ whose elemental

[7.4] The isomorphism $T(Y) = V_{\mathcal{N}}^{\dagger T} Y V_{\mathcal{N}}^\dagger$ onto $\{VXV \mid X \in \mathbb{S}^N\}$ relates the latter map to the former, but is not an isometry. At this moment we see little compelling reason to prefer one particular auxiliary V-matrix (§B.4) over another. Each has its own coherent interpretations; *e.g.*, §4.4.2, §5.5.1...

matrices have rank no greater than desired affine dimension ρ . Problem 1 finds the closest EDM D in the sense of Schoenberg. (352) [87] This optimization problem is convex only when desired affine dimension (§4.7.2) is largest $\rho = N-1$ although its analytical solution is known [128] for all $\rho \leq N-1$, being first pronounced in the context of multidimensional scaling by Mardia [129] in 1978: We assume only that the given measurement matrix H is symmetric;[7.5]

$$H \in \mathbb{S}^N \tag{708}$$

Arranging the eigenvalues λ_i of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ in nonincreasing order for all i, $\lambda_i \geq \lambda_{i+1}$ with v_i the corresponding i^{th} eigenvector,

$$-V_{\mathcal{N}}^T H V_{\mathcal{N}} \triangleq \sum_{i=1}^{N-1} \lambda_i \, v_i v_i^T \tag{709}$$

then the optimal solution to Problem 1 is [73, §2]

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} = \sum_{i=1}^{\rho} \max\{0,\, \lambda_i\} v_i v_i^T \tag{710}$$

7.1.1 Closest EDM Problem 1, proof of (710), convex case

When desired affine dimension is largest, $\rho = N-1$, the rank function disappears from (707); *videlicet*

$$\begin{array}{cl} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_{\mathrm{F}}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N \end{array} \tag{711}$$

In those terms, assuming $D \in \mathbb{S}^N$ [*sic*], the necessary and sufficient conditions (§E.8.1.0.1) for unique projection in isomorphic $\mathbb{R}^{(N-1)^2}$ on the self-dual (199)

[7.5] Projection in Problem 1 is on a rank ρ subset (§7.1.2) of the positive semidefinite cone in the ambient space of symmetric matrices. It is wrong here to zero the main diagonal of given H because projecting first on the symmetric hollow subspace places an elbow in the path of projection (*confer* Figure **7.2**).

positive semidefinite cone are:[7.6] (943) (*confer* (1306))

$$\begin{array}{l} -V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} \succeq 0 \\ -V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} \left(-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} + V_{\mathcal{N}}^T H V_{\mathcal{N}}\right) = \mathbf{0} \\ -V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} + V_{\mathcal{N}}^T H V_{\mathcal{N}} \succeq 0 \end{array} \tag{712}$$

Symmetric $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ is diagonalizable hence decomposable in terms of its eigenvectors v and eigenvalues λ as in (709). Therefore, (*confer* (710))

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} = \sum_{i=1}^{N-1} \max\{0,\ \lambda_i\} v_i v_i^T \tag{713}$$

satisfies (712), optimally solving (711). To see that, recall: these eigenvectors constitute an orthogonal set and

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} + V_{\mathcal{N}}^T H V_{\mathcal{N}} = -\sum_{i=1}^{N-1} \min\{0,\ \lambda_i\} v_i v_i^T \tag{714}$$

♦

7.1.2 rank ρ subset

Prior to determination of $D^\star$, analytical solution (710) is equivalent to solution of the generic problem: given $A \in \mathbb{S}^{N-1}$ and desired affine dimension ρ,

$$\begin{array}{cl} \underset{B \in \mathbb{S}^{N-1}}{\text{minimize}} & \|B - A\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} B \leq \rho \\ & B \succeq 0 \end{array} \tag{715}$$

where $B \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{S}^{N-1}$ and $A \triangleq -V_{\mathcal{N}}^T H V_{\mathcal{N}} \in \mathbb{S}^{N-1}$. Once optimal $B^\star$ is found, the technique of §4.10 can be used to determine the optimal distance matrix

$$D^\star \in \mathbb{EDM}^N \tag{716}$$

Hence Problem 1 is truly a projection of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ on that non-convex subset of symmetric matrices, belonging to the positive semidefinite cone, having rank no greater than desired affine dimension[7.7] ρ ; called *rank ρ subset* of the positive semidefinite cone.

[7.6] These conditions for projection on a convex cone are identical to the Karush-Kuhn-Tucker (KKT) optimality conditions for problem (711).

[7.7] Recall that affine dimension is a lower bound on embedding (§2.2.1), equal to the dimension of the smallest affine set in which points from a list X corresponding to an EDM D can be embedded.

7.1.3 Closest EDM Problem 1, non-convex case

It is curious how non-convex Problem 1 has such a simple analytical solution (710). Solution to the generic problem (715) was presented in [128, thm.14.4.2] in 1979. In 1997 Trosset [73] first observed equivalence of this rank-constrained problem to spectral projection on the monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$. He generalized the problem and its solution by admitting projection on any convex subset of $\mathcal{K}_{\mathcal{M}+}$. The nature of Trosset's proof was algebraic. Here we derive the known solution (710) for a rank ρ subset of the positive semidefinite cone using instead a more geometric argument (subsuming the proof in §7.1.1):

7.1.3.0.1 Proof. (710), *non-convex case.*
With diagonalization of unknown

$$B \triangleq U\Upsilon U^T \in \mathbb{S}^{N-1} \tag{717}$$

given desired affine dimension $0 \le \rho \le N-1$ and diagonalizable

$$A \triangleq Q\Lambda Q^T \in \mathbb{S}^{N-1} \tag{718}$$

having eigenvalues arranged in Λ in nonincreasing order, problem (715) is equivalent to a spectral projection: (28)

$$\begin{array}{ll} \underset{U,\Upsilon}{\text{minimize}} & \|\Upsilon - U^T Q\Lambda Q^T U\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}+}^{\rho} \\ & U^{-1} = U^T \end{array} \tag{719}$$

where δ is the linear main-diagonal operator (§A.1), and where

$$\mathcal{K}_{\mathcal{M}+}^{\rho} \triangleq \{\upsilon \in \mathbb{R}^{N-1} \mid \upsilon_1 \ge \upsilon_2 \ge \cdots \ge \upsilon_\rho \ge \upsilon_{\rho+1} = \upsilon_{\rho+2} = \cdots = \upsilon_{N-1} = 0\} \subseteq \mathbb{R}_+^{\rho} \tag{720}$$

is a pointed polyhedral cone, a ρ-dimensional subset of the monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$ in $\mathbb{R}^{N-1}$ (§2.9.2.2.1),

$$\mathcal{K}_{\mathcal{M}+} = \{\upsilon \mid \upsilon_1 \ge \upsilon_2 \ge \cdots \ge \upsilon_{N-1} \ge 0\} \subseteq \mathbb{R}_+^{N-1} \tag{244}$$

where $\mathcal{K}_{\mathcal{M}+}^{N-1} \triangleq \mathcal{K}_{\mathcal{M}+}$. Problem (719) is equivalent to the problem sequence: [29, §0.1.2]

$$\begin{aligned}
&\begin{array}{ll}\underset{\Upsilon}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_F^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}+}^{\rho}\end{array} && \text{(a)} \\
&\begin{array}{ll}\underset{R}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_F^2 \\ \text{subject to} & R^{-1} = R^T\end{array} && \text{(b)}
\end{aligned} \tag{721}$$

where

$$R \triangleq Q^T U \tag{722}$$

is a *bijection* in U on the set of orthogonal matrices. Problem (721a) is a unique projection of $R^T\Lambda R$ on a convex subset of the monotone nonnegative cone; on $\delta(\mathcal{K}_{\mathcal{M}+}^{\rho})$ in isometrically isomorphic $\mathbb{R}^{(N-1)^2}$.[7.8] Projection can be accomplished by first projecting $R^T\Lambda R$ orthogonally on the ρ-dimensional subspace containing $\mathcal{K}_{\mathcal{M}+}^{\rho}$, and then projecting the result on $\mathcal{K}_{\mathcal{M}+}^{\rho}$ itself: (§E.8.3) Projection on that subspace amounts to zeroing all entries of $R^T\Lambda R$ off its main diagonal and the last $N-1-\rho$ entries along its main diagonal. Then we have the equivalent problem sequence:

$$\begin{aligned}
&\begin{array}{ll}\underset{\tilde{\Upsilon}}{\text{minimize}} & \|\delta(\tilde{\Upsilon}) - \delta(\tilde{R}^T\Lambda \tilde{R})\|^2 \\ \text{subject to} & \delta(\tilde{\Upsilon}) \in \tilde{\mathcal{K}}_{\mathcal{M}+}\end{array} && \text{(a)} \\
&\begin{array}{ll}\underset{\tilde{R}}{\text{minimize}} & \|\delta(\tilde{\Upsilon}) - \delta(\tilde{R}^T\Lambda \tilde{R})\|^2 \\ \text{subject to} & \tilde{R}^T\tilde{R} = I\end{array} && \text{(b)}
\end{aligned} \tag{723}$$

where

$$\delta(\tilde{\Upsilon}) \triangleq \delta(\Upsilon)_{1:\rho} \in \mathbb{R}^{\rho} \tag{724}$$

and $\delta(\Upsilon)_{\rho+1:N-1} = \mathbf{0}$, and where

$$\tilde{\mathcal{K}}_{\mathcal{M}+} \triangleq \{\upsilon \mid \upsilon_1 \geq \upsilon_2 \geq \cdots \geq \upsilon_\rho \geq 0\} \subseteq \mathbb{R}_+^{\rho} \tag{244}$$

[7.8]Isometry is a consequence of the fact, for diagonal $\Upsilon_1, \Upsilon_2 \in \mathbb{S}^{N-1}$, [38, §3.2]

$$\langle \delta(\Upsilon_1), \delta(\Upsilon_2)\rangle = \langle \Upsilon_1, \Upsilon_2\rangle$$

meaning, distances are preserved in the map from $\mathbb{R}^{\rho}$ to the vectorization in $\mathbb{R}^{(N-1)^2}$.

is dimensionally redefined hence a simplicial cone with respect to $\mathbb{R}^\rho$, and where

$$\tilde{R} \stackrel{\Delta}{=} [r_1\ r_2 \cdots r_\rho] \in \mathbb{R}^{N-1\times\rho} \tag{725}$$

constitutes the first ρ columns of orthogonal variable R. Because any permutation matrix is an orthogonal matrix, we may always assume $\delta(\tilde{R}^T\Lambda\tilde{R}) \in \mathbb{R}^\rho$ to be arranged in nonincreasing order; *id est*,

$$\delta(\tilde{R}^T\Lambda\tilde{R})_i \geq \delta(\tilde{R}^T\Lambda\tilde{R})_{i+1}\ , \quad i=1\ldots\rho-1 \tag{726}$$

Unique projection of vector $\delta(\tilde{R}^T\Lambda\tilde{R})$ on convex cone $\tilde{\mathcal{K}}_{\mathcal{M}+}$ requires: (§E.8.1.0.1, §2.9.2.2.1)

$$\begin{aligned} Y^\dagger\delta(\tilde{\Upsilon}^\star) &\succeq 0 \\ \delta(\tilde{\Upsilon}^\star)^T\Big(\delta(\tilde{\Upsilon}^\star) - \delta(\tilde{R}^T\Lambda\tilde{R})\Big) &= 0 \\ Y^T\Big(\delta(\tilde{\Upsilon}^\star) - \delta(\tilde{R}^T\Lambda\tilde{R})\Big) &\succeq 0 \end{aligned} \tag{727}$$

which are necessary and sufficient conditions, where

$$\begin{aligned} Y^{\dagger T} &\stackrel{\Delta}{=} [e_1-e_2 \quad e_2-e_3 \quad \cdots \quad e_\rho] \in \mathbb{R}^{\rho\times\rho} && (245) \\ Y &= [e_1 \quad e_1+e_2 \quad e_1+e_2+e_3 \quad \cdots \quad \mathbf{1}] \in \mathbb{R}^{\rho\times\rho} && (249) \end{aligned}$$

Any value $\tilde{\Upsilon}^\star$ that satisfies conditions (727) is optimal for (723a). Then the relationship

$$\delta(\Upsilon^\star)_i = \begin{cases} \max\{0\,,\ \delta(\tilde{R}^T\Lambda\tilde{R})_i\}\,, & i=1\ldots\rho \\ 0\,, & i=\rho+1\ldots N-1 \end{cases} \tag{728}$$

specifies an optimal solution. The lower bound on the objective with respect to R in (721b) is tight; (697) (§C.2.1.2.1)

$$\|\,|\Upsilon^\star| - |\Lambda|\,\|_F \;\leq\; \|\Upsilon^\star - R^T\Lambda R\|_F \tag{729}$$

where $|\cdot|$ denotes absolute entry-value. For selection of $\Upsilon^\star$ as in (728), this lower bound is achieved when

$$R^\star = I \tag{730}$$

the known solution. ♦

7.1.3.1 Significance...

The importance of this result cannot be overstated:

Firstly, the solution is closed form having been discovered only in 1979 (relatively late in the development of linear algebra that has its roots in the 17^{th} century [130]).

Secondly, the solution is equivalent to projection on a polyhedral cone in the spectral domain; a necessary and sufficient condition for membership to the positive semidefinite cone...

Thirdly, the solution at once includes projection on a rank ρ subset (part of the boundary of the positive semidefinite cone) from the exterior or interior of the cone. Projection on the boundary from the interior is a non-convex problem...

7.1.4 Problem 1 in spectral norm, convex case

When instead we pose the matrix 2-norm (*spectral norm*) in Problem 1 (707) for the convex case $\rho = N-1$, then the new problem

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_2\\ \text{subject to} & D\in\mathbb{EDM}^N\end{array}\tag{731}$$

is convex although its solution is not necessarily unique because the spectral norm is not a strictly convex function (§3.1);[7.9] giving rise to *oblique* projection (§E) on the positive semidefinite cone. Indeed, its solution set includes the Frobenius solution (710) for the convex case whenever $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ is a normal matrix. [97, §1] [131] [1, §8.1.1] *Singular value problem* (731) is equivalent to

$$\begin{array}{cl}\underset{\mu,D}{\text{minimize}} & \mu\\ \text{subject to} & -\mu I \preceq -V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}} \preceq \mu I\\ & D\in\mathbb{EDM}^N\end{array}\tag{732}$$

where

$$\mu^\star = \max_i\left\{\,\left|\lambda\big(-V_{\mathcal{N}}^T(D^\star-H)V_{\mathcal{N}}\big)_i\right|\;,\;\; i=1\ldots N-1\right\}\tag{733}$$

the maximum absolute eigenvalue (due to matrix symmetry).

[7.9] For each and every $|t|\leq 2$, for example, $\begin{bmatrix}2&0\\0&t\end{bmatrix}$ has the same spectral norm.

For lack of a unique solution here, we prefer the Frobenius rather than spectral norm.

7.2 Second prevalent problem: Projection on EDM cone in $\sqrt{d_{ij}}$

Let

$$\sqrt{D} \triangleq [\sqrt{d_{ij}}\,] \in \mathcal{K} \tag{734}$$

be an unknown matrix of absolute distance; *id est*,

$$D = [d_{ij}] \triangleq \sqrt{D} \circ \sqrt{D} \in \mathbb{EDM}^N \tag{735}$$

where $\circ$ denotes the Hadamard product. The second prevalent problem is a projection of H in the natural coordinates (absolute distance) on a nonconvex subset (when $\rho < N-1$) of the convex cone of Euclidean distance matrices $\mathbb{EDM}^N$ in subspace $\mathbb{S}_{\mathbf{0}}^N$: (*confer* Figure **5.1**(b))

$$\left.\begin{array}{ll}\underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq \rho\\ & D \in \mathbb{EDM}^N\end{array}\right\}\quad \text{Problem 2} \tag{736}$$

This statement of the second closest-EDM problem is considered difficult to solve because of the constraint on affine dimension ρ (445) and because the objective function

$$\|\sqrt{D}-H\|_{\mathrm{F}}^2 \;=\; \sum_{i,j}(\sqrt{d_{ij}}-h_{ij})^2 \tag{737}$$

is expressed distinctly in the natural coordinates with respect to the constraints.

Our solution to this second problem prevalent in the literature generally requires measurement matrix H to be nonnegative.

$$H = [h_{ij}] \in \mathbb{R}_+^{N\times N} \tag{738}$$

If the H given has negative entries, then the technique of solution presented here becomes invalid. As explained in §7.0.2, projection of H on $\mathcal{K}$ (698) prior to application of this proposed solution is incorrect.

7.2.1 Convex case

When $\rho = N-1$, the rank constraint vanishes and a convex problem appears: [132] [100, §13.6]

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \|\sqrt{D} - H\|_{\mathrm{F}}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \quad \Leftrightarrow \quad \begin{array}{ll}\underset{D}{\text{minimize}} & \sum\limits_{i,j} d_{ij} - 2h_{ij}\sqrt{d_{ij}} + h_{ij}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{739}$$

For any fixed i and j, the argument of summation is a convex function of d_{ij} because the negative square root is convex in nonnegative d_{ij} and h_{ij} and because $d_{ij} + h_{ij}^2$ is affine (convex). Because the sum of any number of convex functions in D remains convex [1, §3.2.1] and because the feasible set is convex in D, we have a convex problem. The existence of a unique (global) solution $D^\star$ for this second prevalent problem depends upon nonnegativity of H.

7.2.1.1 Equivalent semidefinite program, Problem 2, convex case

Convex problem (739) is solvable for its global minimum by any interior-point method [1, §11] [4] [121] [6] [42] and requires no further modification. Nevertheless, we translate (739) to an equivalent *semidefinite program* (SDP) for a pedagogical reason made clear in §7.2.2, and because there exist readily available and efficient computer programs for numerical solution. [69] [7] [11] [117] [118]

Substituting a new matrix variable $Y \triangleq [y_{ij}] \in \mathbb{R}^{N\times N}$,

$$y_{ij} \leftarrow h_{ij}\sqrt{d_{ij}} \tag{740}$$

we propose that (739) is equivalent to the SDP

$$\begin{array}{ll}\underset{D,Y}{\text{minimize}} & \sum\limits_{i,j} d_{ij} - 2y_{ij} + h_{ij}^2 \\ \text{subject to} & \begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0, \quad i,j = 1\ldots N \\ & D \in \mathbb{EDM}^N \end{array} \tag{741}$$

To see that, recall $d_{ij} \geq 0$ is implicit to $D \in \mathbb{EDM}^N$ (§4.8.1, (352)). So when

H is nonnegative as assumed,

$$\begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0 \;\Leftrightarrow\; h_{ij}\sqrt{d_{ij}} \geq \sqrt{y_{ij}^2} \tag{742}$$

Because negative y_{ij} will not minimize the objective function, nonnegativity of y_{ij} is implicit in (741). Further, minimization of the objective function implies maximization of y_{ij} that is bounded above. Hence, as desired, $y_{ij} \rightarrow h_{ij}\sqrt{d_{ij}}$ as optimization proceeds.

If the given matrix H is now assumed nonnegative and symmetric,

$$H = [h_{ij}] \in \mathbb{R}_+^{N\times N} \cap \mathbb{S}^N \tag{743}$$

then $Y = H \circ \sqrt{D}$ must belong to $\mathcal{K} = \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N}$ (698). Then because $Y \in \mathbb{S}_{\mathbf{0}}^N$, (§B.4.2 no.11)

$$\|\sqrt{D} - H\|_{\mathrm{F}}^2 \;=\; \sum_{i,j} d_{ij} - 2y_{ij} + h_{ij}^2 \;=\; -N\,\mathrm{tr}\Big(V_{\mathcal{N}}^\dagger (D - 2\,Y) V_{\mathcal{N}}\Big) + \sum_{i,j} h_{ij}^2 \tag{744}$$

convex problem (741) is equivalent to the SDP

$$\begin{array}{cl} \underset{D,Y}{\text{minimize}} & -\,\mathrm{tr}\Big(V_{\mathcal{N}}^\dagger (D - 2\,Y) V_{\mathcal{N}}\Big) \\ \text{subject to} & \begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0\,, \quad j > i = 1 \ldots N-1 \\ & Y \in \mathbb{S}_{\mathbf{0}}^N \\ & D \in \mathbb{EDM}^N \end{array} \tag{745}$$

where the constants h_{ij}^2 and N have been dropped arbitrarily from the objective.

7.2.2 Minimization of affine dimension in Problem 2

When desired affine dimension ρ is diminished, the rank function becomes reintroduced into problem (741) that is then rendered difficult to solve because the feasible set loses convexity in $\mathbb{S}_{\mathbf{0}}^N \times \mathbb{R}^{N\times N}$. Indeed, the rank function is quasiconcave on the positive semidefinite cone (§3.2.0.0.1).

7.2.2.1 Rank minimization heuristic

A remedy developed in [133] [72] [134] introduces the *convex envelope* (cenv) of the rank function:

Definition. *Convex envelope.* [135] The convex envelope of a function $f:\mathcal{C}\rightarrow\mathbb{R}$ is defined as the largest convex function g such that $g\leq f$ on convex domain $\mathcal{C}\subseteq\mathbb{R}^n$.[7.10] $\triangle$

- The convex envelope of the rank function is proportional to the trace function when its argument is constrained to be symmetric and positive semidefinite.

A properly scaled trace thus represents the best convex lower bound on rank. The idea, then, is to substitute the convex envelope for the rank of some variable $A\in\mathbb{S}_+^M$;

$$\operatorname{rank} A \;\leftarrow\; \operatorname{cenv}(\operatorname{rank} A) \;\propto\; \operatorname{tr} A \tag{746}$$

7.2.2.1.1 Applying the trace heuristic to Problem 2

Substituting the rank envelope for the rank function (445), for $D\in\mathbb{EDM}^N$,

$$\operatorname{cenv}\operatorname{rank}(-V_{\mathcal{N}}^TDV_{\mathcal{N}}) = \operatorname{cenv}\operatorname{rank}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \;\propto\; -\operatorname{tr}(V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \tag{747}$$

and for $\rho\leq N-1$ and nonnegative H we have the convex optimization problem

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm{F}}^2\\ \text{subject to} & -\operatorname{tr}(V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}})\leq\kappa\,\rho\\ & D\in\mathbb{EDM}^N\end{array} \tag{748}$$

[7.10] Provided $f\not\equiv+\infty$ and there exists an affine function $h\leq f$ on $\mathbb{R}^n$, then the convex envelope is equal to the convex conjugate (the *Legendre-Fenchel transform*) of the convex conjugate of f ; *id est*, the conjugate-conjugate function f^{**}. [29, §E.1] where $\kappa \in \mathbb{R}_+$ is a constant determined by cut and try.[7.11] The equivalent SDP makes κ variable: for nonnegative and symmetric H,

$$\begin{array}{cl}\underset{D,Y,\kappa}{\text{minimize}} & \kappa\,\rho + 2\operatorname{tr}(V_{\mathcal{N}}^{\dagger} Y V_{\mathcal{N}})\\ \text{subject to} & \left[\begin{array}{cc} d_{ij} & y_{ij}\\ y_{ij} & h_{ij}^2\end{array}\right] \succeq 0\,, \quad j > i = 1 \ldots N-1\\ & -\operatorname{tr}(V_{\mathcal{N}}^{\dagger} D V_{\mathcal{N}}) \leq \kappa\,\rho\\ & Y \in \mathbb{S}_{\mathbf{0}}^N\\ & D \in \mathbb{EDM}^N \end{array} \tag{749}$$

which is the same as (745). As the problem is stated, the desired affine dimension ρ yields to the variable scale factor κ; ρ is effectively ignored.

Yet the result is an illuminant for (745) and it equivalents; when the given measurement matrix H is nonnegative and symmetric, finding the closest EDM D as in problem (739), (741), or (745) implicitly entails minimization of affine dimension (*confer* §4.8.4, §4.12.4). In other words, those non rank-constrained problems are each inherently equivalent to cenv(rank)-minimization problem (749).

7.2.2.2 Heuristic insight

Minimization of affine dimension by using this trace heuristic tends to find the list configuration of least energy; rather, it tends to optimize compaction of the reconstruction by minimizing total distance. (357) It is best used where some physical equilibrium implies such an energy minimization.

In the case of Problem 2, the trace heuristic arose naturally in the objective. Our preference for $V_{\mathcal{N}}^{\dagger}$ over $V_{\mathcal{N}}^T$ spreads the energy over all available distances (§B.4.2 no.11, no.13) although the rank function itself is insensitive to the choice (445).

7.2.2.3 Rank minimization heuristic beyond convex envelope

Fazel, Hindi, & Boyd [134] propose a rank heuristic more potent than trace (747) for problems of rank minimization; the concave surrogate function

$$\log\det(Y + \varepsilon I) \;\leftarrow\; \operatorname{rank} Y \tag{750}$$

[7.11] $\operatorname{cenv}(\operatorname{rank} A)$ on $\|A \in \mathbb{S}_+^n\|_2 \leq \kappa \;=\; \operatorname{tr}(A)/\kappa$ [133]

in place of quasiconcave $\operatorname{rank} Y$ (§3.2.0.0.1) when $Y \in \mathbb{S}^n_+$ is variable and ε is a small positive constant. They propose minimization of the surrogate by substituting a sequence comprising infima of a linearized surrogate about the current estimate Y_i; *id est*, from the first-order Taylor series expansion about Y_i on some open interval of $\|Y\|$, (§D.1.6)

$$\log\det(Y + \varepsilon I) \approx \log\det(Y_i + \varepsilon I) + \operatorname{tr}\big((Y_i + \varepsilon I)^{-1}(Y - Y_i)\big) \tag{751}$$

we make the surrogate sequence of infima over bounded convex feasible set $\mathcal{C}$,

$$\arg\inf_{Y\in\mathcal{C}} \operatorname{rank} Y \;\leftarrow\; \lim_{i\to\infty} Y_{i+1} \tag{752}$$

where

$$Y_{i+1} = \arg\inf_{Y\in\mathcal{C}} \operatorname{tr}\big((Y_i + \varepsilon I)^{-1} Y\big) \tag{753}$$

Choosing $Y_0 = I$, the first iteration becomes equivalent to a minimization of $\operatorname{tr} Y$. (747) The intuition underlying (753) is the new term in the argument of trace; specifically, $(Y_i + \varepsilon I)^{-1}$ weights Y so that relatively small eigenvalues of Y found by the infimum are made even smaller.

To see that, substitute into (753) the non-increasingly ordered diagonalizations

$$\begin{aligned} Y_i + \varepsilon I &\triangleq Q(\Lambda + \varepsilon I)Q^T && \text{(a)} \\ Y &\triangleq U\Upsilon U^T && \text{(b)} \end{aligned} \tag{754}$$

Then from (1034) we have,

$$\begin{aligned} \inf_{\Upsilon\in U^{\star T}\mathcal{C}U^{\star}} \delta\big((\Lambda + \varepsilon I)^{-1}\big)^T \delta(\Upsilon) &= \inf_{\Upsilon\in U^T\mathcal{C}U}\; \inf_{R^T=R^{-1}} \operatorname{tr}\big((\Lambda + \varepsilon I)^{-1} R^T \Upsilon R\big) \\ &\le \inf_{Y\in\mathcal{C}} \operatorname{tr}((Y_i + \varepsilon I)^{-1} Y) \end{aligned} \tag{755}$$

where $R \triangleq Q^T U$ is a bijection in U on the set of orthogonal matrices. The role of ε is, therefore, to limit the maximum weight; the smallest diagonal entry of Υ gets the largest weight. ♦

7.2.2.3.1 Tightening this rank heuristic

This $\log\det$ technique is therefore inherently different from projection methods of rank constraint (such as §7.1.3) because the number of eigenvalues to be zeroed is not determined *a priori.* As it stands, there is no provision for meeting an upper bound ρ on rank. Yet since the eigenvalues of the sum are simply determined, $\lambda(Y_i + \varepsilon I) = \delta(\Lambda + \varepsilon I)$, we may certainly force selected weights to ε^{-1} by manipulating diagonalization (754a). Empirically we find this sometimes leads to better results, although affine dimension of a solution cannot be guaranteed.

7.3 Third prevalent problem: Projection on EDM cone in d_{ij}

Reformulating Problem 2 (p.256) in terms of EDM D changes the problem considerably:

$$\left.\begin{array}{ll}\underset{D}{\text{minimize}} & \|D - H\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq \rho \\ & D \in \mathbb{EDM}^N\end{array}\right\} \quad \text{Problem 3} \tag{756}$$

This third prevalent problem is a projection of H on a non-convex subset (when $\rho < N-1$) of the convex cone of Euclidean distance matrices $\mathbb{EDM}^N$ in subspace $\mathbb{S}_{\mathbf{0}}^N$ (Figure **5.1**(a)). Because the coordinates of projection are distance-square and H presumably now holds distance-square measurements, the solution to Problem 3 is generally different than that of Problem 2 .[7.12]

For the moment, we need make no assumptions regarding measurement matrix H .

7.3.1 Convex case

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \|D - H\|_{\mathrm{F}}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{757}$$

When the rank constraint disappears (for $\rho = N-1$), this third problem becomes obviously convex because the feasible set is then the entire EDM cone, and because the objective function

$$\|D - H\|_{\mathrm{F}}^2 = \sum_{i,j}(d_{ij} - h_{ij})^2 \tag{758}$$

[7.12]We speculate this third problem to be prevalent because it was once thought easier to solve than Problem 2.

is a strictly convex quadratic in D ;[7.13]

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \sum\limits_{i,j} d_{ij}^2 - 2h_{ij}\,d_{ij} \;+\; h_{ij}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{759}$$

7.3.1.1 Equivalent semidefinite programs, convex case

In the past, this convex problem was solved numerically by means of alternating projection. (Example 7.3.1.1.1) [136] [137] [49, §1] We translate (759) to an equivalent semidefinite program because we have a good SDP solver:

Now assume the given measurement matrix H to be positive, symmetric, and hollow;[7.14]

$$H = [h_{ij}] \in \mathbb{S}_{\mathbf{0}}^N \cap \operatorname{int}\mathbb{R}_+^{N\times N} \tag{760}$$

For $Y = [y_{ij}]$, and $\partial \triangleq [d_{ij}^2] = D \circ D$ distance-square squared, we substitute

$$y_{ij} \leftarrow h_{ij}\,d_{ij} \tag{761}$$

Similarly to the development in §7.2.1.1, we then propose: Problem (759) is equivalent to the SDP

$$\begin{array}{ll}\underset{\partial\,,\,Y}{\text{minimize}} & -\operatorname{tr}\Big(V_{\mathcal{N}}^{\dagger}(\partial - 2\,Y)V_{\mathcal{N}}\Big) \\ \text{subject to} & \left[\begin{array}{cc}\partial_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2\end{array}\right] \succeq 0\,, \quad j > i = 1\ldots N-1 \\ & \dfrac{Y}{H} \in \mathbb{EDM}^N \\ & \partial \in \mathbb{S}_{\mathbf{0}}^N \cap \mathbb{R}_+^{N\times N}\end{array} \tag{762}$$

where $Y/H \triangleq [y_{ij}/h_{ij}]$ for $i \neq j$, $h_{ij} \neq 0$ for $i \neq j$, and

$$\left[\begin{array}{cc}\partial_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2\end{array}\right] \succeq 0 \;\Leftrightarrow\; h_{ij}\,d_{ij} \geq \sqrt{y_{ij}^2}\;, \quad \partial_{ij} \geq 0 \tag{763}$$

[7.13] For nonzero $Y \in \mathbb{S}_{\mathbf{0}}^N$ and some open interval of $t \in \mathbb{R}$, (§3.1.2.4, §D.2.2.1)

$$\frac{d^2}{dt^2}\|(D + t\,Y) - H\|_{\mathrm{F}}^2 \;=\; 2\operatorname{tr} Y^T Y > 0$$

[7.14] If that H given has negative entries, then the technique of solution presented here becomes invalid. As explained in §7.0.2, projection of H on $\mathcal{K}$ (698) prior to application of this proposed solution is incorrect.

For the same reasons as before, $y_{ij} \to h_{ij}\, d_{ij}$ as optimization proceeds.

The similarity of problem (762) to (745) cannot go unnoticed, but the possibility of numerical instability due to division by small numbers here is troublesome.

7.3.1.1.1 Example. *Alternating projection on nearest EDM.*
By solving (762) we confirm the result from an example given by Glunt, Hayden, *et alii* [136, §6] who found an analytical solution to (757) for the particular cardinality $N=3$ by using the alternating projection method of von Neumann (§E.9):

$$H = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 9 \\ 1 & 9 & 0 \end{bmatrix}, \qquad D^\star = \begin{bmatrix} 0 & \frac{19}{9} & \frac{19}{9} \\ \frac{19}{9} & 0 & \frac{76}{9} \\ \frac{19}{9} & \frac{76}{9} & 0 \end{bmatrix} \tag{764}$$

Let the alternate convex sets be the two cones

$$\begin{aligned} \mathcal{K}_1 &= \mathbb{S}^N_{\mathbf{0}} \\ \mathcal{K}_2 &= \bigcap_{y\in\mathcal{N}(\mathbf{1}^T)} \left\{ A\in\mathbb{S}^N \mid \langle yy^T, -A\rangle \geq 0 \right\} \\ &= \left\{ A\in\mathbb{S}^N \mid -y^T VAVy \geq 0\,,\ \ \forall\, yy^T(\succeq 0) \right\} \\ &= \left\{ A\in\mathbb{S}^N \mid -VAV \succeq 0 \right\} \end{aligned} \tag{765}$$

where auxiliary matrix $V\in\mathbb{S}^N$ is the geometric centering matrix (996), so

$$\mathcal{K}_1 \cap \mathcal{K}_2 = \mathbb{EDM}^N \tag{766}$$

The dual cone $\mathcal{K}_1^* = \mathbb{S}^{N\perp}_{\mathbf{0}} \subseteq \mathbb{S}^N$ (51) is an orthogonal subspace, and from the dual EDM cone development in §5.6.1,

$$\mathcal{K}_2^* = -\operatorname{cone}\left\{ V_{\mathcal{N}} \upsilon\upsilon^T V_{\mathcal{N}}^T \mid \upsilon\in\mathbb{R}^{N-1} \right\} \subset \mathbb{S}^N \tag{767}$$

In [137, §5.3] Gaffke & Mathar observe that projection on $\mathcal{K}_1$ and $\mathcal{K}_2$ have simple closed forms: Projection on subspace $\mathcal{K}_1$ is easily performed by symmetrization and zeroing the main diagonal or *vice versa*, while projection of $H\in\mathbb{S}^N$ on $\mathcal{K}_2$ is

$$P_{\mathcal{K}_2} H = H - P_{\mathbb{S}^N_+}(VHV) \tag{768}$$

Thus the original problem (757) of projecting H on the EDM cone is transformed, basically, to an equivalent sequence of projections on the PSD cone.

Using ordinary alternating projections, input H goes to $D^\star$ with an accuracy of four decimal places in about 17 iterations. Obviation of semidefinite programming's computational expense is the principal advantage of this alternating projection technique.

To prove (768), first we observe membership of $H - P_{\mathbb{S}_+^N}(VHV)$ to $\mathcal{K}_2$ because

$$P_{\mathbb{S}_+^N}(VHV) - H = (P_{\mathbb{S}_+^N}(VHV) - VHV) + (VHV - H) \tag{769}$$

The term $P_{\mathbb{S}_+^N}(VHV) - VHV$ must belong to the (dual) positive semidefinite cone by Theorem E.8.1.0.1, and $V^2 = V$. Hence, $-V\Big(H - P_{\mathbb{S}_+^N}(VHV)\Big)V \succeq 0$ by Corollary A.3.1.0.5. Next, we require

$$\langle P_{\mathcal{K}_2} H - H\,,\, P_{\mathcal{K}_2} H\rangle = 0 \tag{770}$$

Expanding,

$$\langle -P_{\mathbb{S}_+^N}(VHV)\,,\, H - P_{\mathbb{S}_+^N}(VHV)\rangle = 0 \tag{771}$$
$$\langle P_{\mathbb{S}_+^N}(VHV)\,,\, (P_{\mathbb{S}_+^N}(VHV) - VHV) + (VHV - H)\rangle = 0 \tag{772}$$
$$\langle P_{\mathbb{S}_+^N}(VHV)\,,\, (VHV - H)\rangle = 0 \tag{773}$$

Product VHV belongs to the geometric center subspace; (§E.7.1.0.2)

$$VHV \in \mathbb{S}_g^N = \{Y \in \mathbb{S}^N \mid \mathcal{N}(Y) \supseteq \mathbf{1}\} \tag{774}$$

Diagonalize $VHV \overset{\Delta}{=} Q\Lambda Q^T$ (§A.5) whose nullspace is spanned by the eigenvectors corresponding to 0 eigenvalues by Theorem A.7.2.0.1. Projection of VHV on the PSD cone (§7.1) simply zeros negative eigenvalues in diagonal matrix Λ. Then

$$\mathcal{N}\big(P_{\mathbb{S}_+^N}(VHV)\big) \supseteq \mathcal{N}(VHV)\ \big(\supseteq \mathcal{N}(V)\big) \tag{775}$$

from which it follows:

$$P_{\mathbb{S}_+^N}(VHV) \in \mathbb{S}_g^N \tag{776}$$

so $P_{\mathbb{S}_+^N}(VHV) \perp (VHV - H)$ because $VHV - H \in \mathbb{S}_g^{N\perp}$. Finally, we must have $P_{\mathcal{K}_2} H - H = -P_{\mathbb{S}_+^N}(VHV) \in \mathcal{K}_2^*$. From §5.5.1 we know dual cone

$\mathcal{K}_2^* = -\mathcal{F}\big(\mathbb{S}_+^N \ni V\big)$ is the negative of the smallest face of the positive semidefinite cone containing auxiliary matrix V. Thus $P_{\mathbb{S}_+^N}(VHV) \in \mathcal{F}\big(\mathbb{S}_+^N \ni V\big) \Leftrightarrow \mathcal{N}(P_{\mathbb{S}_+^N}(VHV)) \supseteq \mathcal{N}(V)$ (§2.6.6.3) which was already established above. ♦

From the results in §E.7.1.0.2, we know VHV is an orthogonal projection of $H \in \mathbb{S}^N$ on the geometric center subspace $\mathbb{S}_g^N$. Thus we have

$$P_{\mathcal{K}_2} H = H - P_{\mathbb{S}_+^N} P_{\mathbb{S}_g^N} H \tag{777}$$

and by (1305) and (179) we get

$$\mathcal{K}_2 \;=\; -\big(\mathbb{S}_+^N \cap \mathbb{S}_g^N\big)^* \;=\; \mathbb{S}_g^{N\perp} - \mathbb{S}_+^N \tag{778}$$

Therefore

$$\mathbb{EDM}^N \;=\; \mathcal{K}_1 \cap \mathcal{K}_2 \;=\; \mathbb{S}_{\mathbf{0}}^N \cap \big(\mathbb{S}_g^{N\perp} - \mathbb{S}_+^N\big) \tag{779}$$

□

7.3.1.2 Schur-form semidefinite program, Problem 3

Potential instability in problem (762) motivates another formulation: Moving the objective function in (759) to the constraints makes an equivalent *second-order cone program*: for any measurement matrix H,

$$\begin{array}{cl}\underset{D,\,t}{\text{minimize}} & t\\ \text{subject to} & \|D-H\|_{\mathrm F} \le t\\ & D \in \mathbb{EDM}^N\end{array} \tag{780}$$

We can transform this problem to an equivalent Schur-form semidefinite program; (§A.4.1)

$$\begin{array}{cl}\underset{D,\,t}{\text{minimize}} & t\\ \text{subject to} & \begin{bmatrix} tI & \operatorname{vec}(D-H)\\ \operatorname{vec}^T(D-H) & t\end{bmatrix} \succeq 0\\ & D \in \mathbb{EDM}^N\end{array} \tag{781}$$

characterized by great sparsity and structure. The advantage of this SDP is the lack of requirements on input H; *e.g.*, nonpositive entries would invalidate the solution provided by (762). (§7.0.2.2)

7.3.2 Minimization of affine dimension in Problem 3

When the desired affine dimension ρ is diminished, Problem 3 (756) is difficult to solve [49, §3] because the feasible set in $\mathbb{R}^{N(N-1)/2}$ loses convexity. By substituting the rank envelope (747) into Problem 3, then for any given H we have the convex problem

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|D-H\|_{\mathrm{F}}^2\\ \text{subject to} & -\operatorname{tr}(V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \leq \kappa\,\rho\\ & D\in\mathbb{EDM}^N\end{array} \tag{782}$$

where $\kappa\in\mathbb{R}_+$ is a constant determined by cut and try. Problem (782) is a convex optimization problem in any affine dimension ρ; a convex approximation to projection on that non-convex subset of the EDM cone containing EDMs with corresponding affine dimension no greater than ρ.

The SDP equivalent to (782) does not move κ into the variables as before (p.259): for positive symmetric hollow input H,

$$\begin{array}{cl}\underset{\partial\,,\,Y}{\text{minimize}} & -\operatorname{tr}\Big(V_{\mathcal{N}}^{\dagger}(\partial-2\,Y)V_{\mathcal{N}}\Big)\\ \text{subject to} & \begin{bmatrix}\partial_{ij} & y_{ij}\\ y_{ij} & h_{ij}^2\end{bmatrix}\succeq 0\,,\quad j>i=1\ldots N-1\\ & -\operatorname{tr}(V_{\mathcal{N}}^{\dagger}\dfrac{Y}{H}V_{\mathcal{N}})\leq\kappa\,\rho\\ & \dfrac{Y}{H}\in\mathbb{EDM}^N\\ & \partial\in\mathbb{S}_{\mathbf{0}}^N\cap\mathbb{R}_+^{N\times N}\end{array} \tag{783}$$

That means we will not see equivalence of this cenv(rank)-minimization problem to the non rank-constrained problems (759) and (762) like we saw for its counterpart (749) in Problem 2.

7.3.3 Tightly constrained affine dimension, Problem 3

We use the Cayley-Menger form (§4.14.2) to solve a problem that is the same as Problem 3 (756):

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \left\|\begin{bmatrix}-D & \mathbf{1}\\ \mathbf{1}^T & 0\end{bmatrix}-\begin{bmatrix}-H & \mathbf{1}\\ \mathbf{1}^T & 0\end{bmatrix}\right\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank}V_{\mathcal{N}}^TDV_{\mathcal{N}}\leq\rho\\ & D\in\mathbb{EDM}^N\end{array} \tag{784}$$

a projection of H on a non-convex subset (when $\rho < N-1$) of the cone of Euclidean distance matrices $\mathbb{EDM}^N$. Relationship (555) provides necessary and sufficient conditions for membership of D to the whole EDM cone ($\rho = N-1$); expressed in terms of the spectral cone

$$\mathcal{K}_\lambda = \{\lambda \in \mathbb{R}^{N+1} \mid \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \geq 0 \geq \lambda_{N+1}\;,\; \mathbf{1}^T\lambda = 0\} \subset \mathbb{R}^{N+1} \tag{546}$$

for $\begin{bmatrix} -\mathbb{EDM}^N & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}$. When one desires affine dimension ρ diminished further below what can be achieved via cenv(rank)-minimization as in (783), spectral projection methods become attractive. Our strategy for low-rank solution is projection on that subset $\mathcal{K}_\lambda^{\rho+2}$ of the spectral cone corresponding to affine dimension not in excess of that desired; *id est*, on

$$\begin{aligned}\mathcal{K}_\lambda^{\rho+2} &\triangleq \{\lambda \in \mathbb{R}^{N+1} \mid \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{\rho+1} \geq \lambda_{\rho+2} = \lambda_{\rho+3} = \cdots = \lambda_N = 0 \geq \lambda_{N+1}\;,\; \mathbf{1}^T\lambda = 0\} \\ &= \mathcal{K}_{\mathcal{M}} \cap \mathbb{R}^{N+1}_{N+1-} \cap \partial\mathcal{H} \cap \{\lambda \mid e_i^T\lambda = 0\,,\; i = \rho+2 \ldots N\} \subset \mathbb{R}^{\rho+2}\end{aligned} \tag{785}$$

a pointed polyhedral cone having empty interior, to which membership subsumes the rank constraint;[7.15] a $(\rho+2)$-dimensional convex subset of the spectral cone $\mathcal{K}_\lambda$ in $\mathbb{R}^{N+1}$ where $\mathcal{K}_\lambda^{N+1} \triangleq \mathcal{K}_\lambda$.

Given desired affine dimension $0 \leq \rho \leq N-1$ with unknown EDM D in diagonalization

$$\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \triangleq U\Upsilon U^T \in \mathbb{S}^{N+1} \tag{786}$$

and symmetric H in diagonalization

$$\begin{bmatrix} -H & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \triangleq Q\Lambda Q^T \in \mathbb{S}^{N+1} \tag{787}$$

having eigenvalues arranged in nonincreasing order, then problem (784) is equivalent to:

$$\begin{array}{cl} \underset{\Upsilon,\,R}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_\lambda^{\rho+2} \\ & \delta(QR\Upsilon R^TQ^T) = \mathbf{0} \\ & R^TR = I \end{array} \tag{788}$$

[7.15] $\mathcal{K}_{\mathcal{M}}$ is the monotone cone (251), $\mathbb{R}^{N+1}_{N+1-}$ is that orthant whose members' sole negative coordinate is their $N+1^{\text{th}}$ (§2.1.0.7.1), and $\partial\mathcal{H} \triangleq \{\lambda \mid \mathbf{1}^T\lambda = 0\}$.

where

$$R \triangleq Q^T U \in \mathbb{R}^{N+1\times N+1} \tag{789}$$

is a bijection in U on the set of orthogonal matrices, and where (§4.7.3.0.1)

$$2 \;\leq\; \operatorname{rank}\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \leq\; \rho+2 \;\leq\; N+1 \tag{790}$$

The diagonal constraint $\delta(QR\Upsilon R^T Q^T) = \mathbf{0}$ makes problem (788) difficult to solve because it makes the two variables dependent. Without it, the problem could be solved exactly by (1168) reducing it to the following finite sequence (a) (b): Initialize R to the identity I,

$$\text{(a)}\quad \begin{array}{ll} \underset{\Upsilon}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_{\mathrm F}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\lambda}^{\rho+2} \cap \mathcal{K}_{\lambda\delta}^{*} \end{array}$$

$$\circlearrowleft \qquad H^\star = P_{\mathbb{S}_{\mathbf{0}}^{N+1}}(QR^\star\Upsilon^\star R^{\star T}Q^T) \qquad \text{(c)}$$

$$\text{(b)}\quad \begin{array}{ll} \underset{R}{\text{minimize}} & \|\Upsilon^\star - R^T\Lambda R\|_{\mathrm F}^2 \\ \text{subject to} & R^T R = I \end{array} \tag{791}$$

Ignoring $\mathcal{K}_{\lambda\delta}^{*}$ for a moment, subproblem (791a) is equivalent to unique projection of $R^T\Lambda R$ on $\delta(\mathcal{K}_{\lambda}^{\rho+2})$, a pointed polyhedral cone belonging to a $(\rho+2)$-dimensional subspace of isometrically isomorphic $\mathbb{R}^{(N+1)^{\mathbf{2}}}$.

Subproblem (791b) is a *Procrustes problem* whose analytical solution is known (§C.2.1); a minimization on the non-convex manifold of orthogonal matrices:

$$R^\star = \sqrt{\delta(\psi(\delta(\Lambda)))}^{H}\sqrt{\delta(\psi(\delta(\Upsilon^\star)))} \in \mathbb{C}^{N+1\times N+1} \tag{792}$$

a complex diagonal matrix, where the step function ψ is defined in (933). So

$$R^\star\Upsilon^\star R^{\star T} = \;\delta(\psi(\delta(\Lambda)))\,|\Upsilon^\star| \in \mathbb{S}^{N+1} \tag{793}$$

where the absolute value is entry-wise. Intersection of the feasible set in subproblem (a) with the *polyhedral cone of majorization* $\mathcal{K}_{\lambda\delta}^{*}$ (§A.1 no.23) insures the existence of a matrix $\begin{bmatrix} -D & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix}$ in $\mathbb{S}_{\mathbf{0}}^{N+1}$ having eigenvalues $\Upsilon^\star$ solving (a). We attempt to find that matrix by solving the sequence (a) (b), and then projecting the symmetric result on $\mathbb{S}_{\mathbf{0}}^{N+1}$ in subproblem (791c) by simply resetting all main diagonal entries of $QR^\star\Upsilon^\star R^{\star T}Q^T$ to 0 ; *id est*,

$$H^\star \triangleq \begin{array}{rl} \arg\underset{H\in\mathbb{S}^N}{\text{minimize}} & \left\|\begin{bmatrix} -H & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} - QR^\star\Upsilon^\star R^{\star T}Q^T\right\|_F^2 = QR^\star\Upsilon^\star R^{\star T}Q^T - \delta^2(QR^\star\Upsilon^\star R^{\star T}Q^T) \\ \text{subject to} & \delta(H) = \mathbf{0} \end{array} \tag{794}$$

This produces a new input H we call $H^\star$:

1. (791a) produces feasible $\Upsilon^\star$
2. (791b) calculates $R^\star$ in closed form
3. (791c) provides $H^\star$ by zeroing diagonal entries

7.3.3.1 Alternation convergence

We have no theoretical guarantee the alternation (791)(a) (b) (c) will converge, in the sense of §E.9, because Procrustes problem (791b) is a projection on a non-convex set. Because every matrix is orthogonally equivalent to a matrix having equal diagonal entries [28, §2.2, prob.3], an alternative but equally valid interpretation of subproblem (c) at convergence is a rotation (§B.5.2) of $QR^\star\Upsilon^\star R^{\star T}Q^T$ into $\mathbb{S}_{\mathbf{0}}^{N+1}$; an adjustment to the rotation found in (b). A test for convergence might therefore be detection of a fixed point $\Upsilon^\star$ of projection product.

7.3.3.2 (791a) conversion to SDP

Subproblem (791a) is easily converted to a semidefinite program with affine constraints. Since variable Υ is a diagonal matrix and $R^T\Lambda R$ fixed, only diagonal entries participate in the minimization because $\delta(\mathcal{K}_\lambda^{\rho+2})$ belongs to a subspace. (§E.8.3) Hence the objective is equivalently stated

$$\|\delta(\Upsilon) - \delta(R^T\Lambda R)\|_2^2 \tag{795}$$

and then converted to a Schur-form semidefinite program: (§A.4.1)

$$\begin{array}{rl} \underset{t,\Upsilon}{\text{minimize}} & t \\ \text{subject to} & \begin{bmatrix} tI & \delta(\Upsilon) - \delta(R^T\Lambda R) \\ (\delta(\Upsilon) - \delta(R^T\Lambda R))^T & t \end{bmatrix} \succeq 0 \\ & \delta(\Upsilon) \in \mathcal{K}_\lambda^{\rho+2} \cap \mathcal{K}_{\lambda\delta}^* \cdots \end{array} \tag{796}$$

Because any permutation matrix is an orthogonal matrix, we must insure $\delta(R^T\Lambda R) \in \mathcal{K}_{\mathcal{M}} \subset \mathbb{R}^{N+1}$ membership to the monotone cone (§2.9.2.2.2); arrangement in nonincreasing order.

7.3.3.2.1 Solution of (791)(b) and (c) by Lagrange multipliers...

Chapter 8

EDM completion

It is not known how to proceed if one wishes to restrict the dimension of the Euclidean space in which the configuration of points may be constructed.

−Michael W. Trosset, 2000 [47]

Intriguing is the question of whether the list in $X \in \mathbb{R}^{n\times N}$ (54) may be reconstructed given an incomplete EDM, and under what circumstances the reconstruction is unique. In this chapter we assume an EDM is only partially known, and the known entries are noiseless.[8.1] Due to translation invariance of an EDM (§4.5), we need only consider reconstruction in subspace $\mathbb{R}^r$ where r is affine dimension.

We examined this completion problem for small Example 4.3.0.0.2 (p.132); revisited in §4.9.3 and §4.12.4.1. When the cardinality N exceeds 4, it is no longer sufficient or convenient to use the *fifth Euclidean axiom* as we did in §4.12.4.1; we need a universal theory.

[8.1] Unknown entries may, for example, be constrained by upper and lower bounds; indeed, all the entries might be unknown having bound constraints.

(b) (c)

(a)

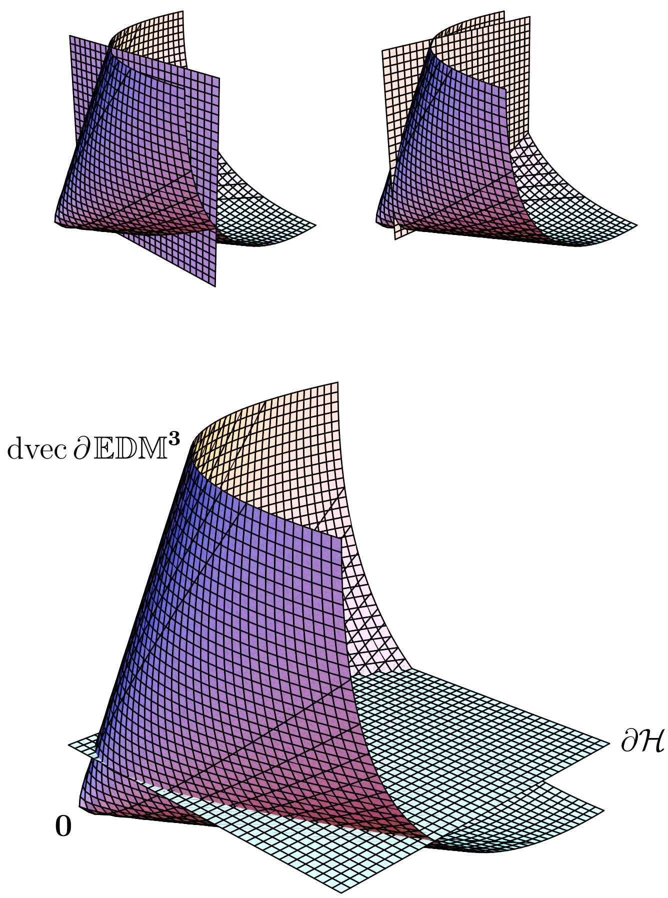


Figure 8.1: **(a)** Intersection of hyperplane $\partial\mathcal{H}$ (representing EDM entry $d_{23}=1/5$) with EDM cone $\mathbb{EDM}^{\mathbf{3}}$ in isomorphic $\mathbb{R}^{\mathbf{3}}$ (both drawn truncated). EDMs in this dimension corresponding to affine dimension 1 comprise the relative boundary of the EDM cone (§5.4) which, by itself, is not a convex set. Since the intersection illustrated includes a subset of the cone's relative boundary, then it is obvious there exist many EDM completions corresponding to affine dimension 1. (Rounded vertex of cone is artifact of plotting routine.) **(b)** $d_{13}=1/5$. **(c)** $d_{12}=1/5$.

8.1 Completion not necessarily unique

It remains somewhat of an open question as how to efficiently identify which matrices can be completed to positive semidefinite or Euclidean distance. [86] [54] [138] [139] Yet the semidefinite version of *Farkas' lemma*, originally regarding only linear inequalities (polyhedral cones, *circa* 1902), provides a clue:

8.1.0.2.1 Lemma. *Semidefinite Farkas' lemma.*[8.2]
Given an arbitrary set $\{A_i \in \mathbb{S}^N,\ i=1\ldots m\}$ and a vector $b\in\mathbb{R}^m$, define the affine set

$$\mathcal{A} \triangleq \{X\in\mathbb{S}^N \mid \langle A_i\,, X\rangle = b_i\,,\ i=1\ldots m\} \tag{797}$$

Then $\mathcal{A}\cap\mathbb{S}_+^N$ is nonempty if and only if, for each and every $\|y\|=1$,

$$\sum_{i=1}^m y_iA_i \succeq 0 \;\Rightarrow\; y^Tb \geq 0 \tag{798}$$

◇

8.1.0.3 PSD cone intersection

Semidefinite Farkas' lemma follows directly from a membership relation (§2.8.2.0.1) and the convex cones from Example 2.8.2.4.1. It provides the conditions required for a set of hyperplanes to share a common intersection with the positive semidefinite cone. To apply the lemma to a semidefinite completion problem, one simply substitutes members of the standard orthonormal basis[8.3] in isomorphic $\mathbb{R}^{N(N+1)/2}$ (38) for the A_i corresponding to known entries b_i . Mere existence of any particular $y=y_p$, failing to fulfill implication (798), is a certificate attesting: no positive semidefinite completion exists.

[8.2] While the lemma as stated is correct, Ye [4, §1.3.8] points out that a positive definite version of this lemma is required for semidefinite programming because a feasible point in $\mathcal{A}\cap\operatorname{int}\mathbb{S}_+^N$ is required by *Slater's condition* [1, §5.2.3] to achieve 0 duality gap. In our circumstance, assuming a nonempty intersection, a positive definite lemma is required to insure a point of intersection closest to the origin is not at infinity; *e.g.*, Figure **2.14**. A positive definite Farkas' lemma can easily be constructed from a membership relation (187).

[8.3] When $m=N(N+1)/2$ and $\{A_i\}$ constitutes the standard orthonormal basis for $\mathbb{S}^N$ (38), then *semidefinite Farkas' lemma* reduces to a theorem of Fejér (200).

8.1.0.4 EDM cone intersection

We know any EDM is a member of a pointed closed convex cone $\mathbb{EDM}^N$. (§5) If one or more entries of a particular EDM are fixed, then the geometric interpretation of the feasible set of completions is like the semidefinite completion problem; it is the intersection of the EDM cone in isomorphic $\mathbb{R}^{N(N-1)/2}$ with as many hyperplanes as there are fixed symmetric entries. Unless the common intersection is a point (assuming it is nonempty) then the number of completions is generally infinite, and those corresponding to particular affine dimension $r < N-1$ belong to some non-convex subset of that intersection (*confer* §3.2.0.0.1).

Depicted in Figure **8.1**(a) is an intersection of the EDM cone $\mathbb{EDM}^{\mathbf{3}}$ with a hyperplane representing the set of all EDMs having one fixed symmetric entry. In this dimension, it is impossible to represent a unique nonzero completion corresponding to affine dimension 1, for example, using a single hyperplane because any hyperplane supporting the relative boundary at a particular point Γ contains an entire ray $\{\zeta\Gamma \mid \zeta \geq 0\}$ belonging to $\operatorname{rel}\partial\mathbb{EDM}^{\mathbf{3}}$ by *lemma* 2.6.3.0.1. Yet it is easy to realize a unique intersection of two hyperplanes with the relative boundary at Γ.[8.4]

The sheer number of possible completions may be minimized, of course, by introducing more constraints or by optimizing some objective function over the feasible set which is the intersection $\mathcal{A} \cap \mathbb{S}^N_+$.

Non-uniqueness of a completed EDM translates to non-uniqueness of an isometric reconstruction;[8.5] in other words, a multiplicity of completions correspond to incongruent realizations.

[8.4] Because any affine transformation of a hyperplane remains affine (§2.1.0.10.2), we may instead realize the intersection with the associated positive semidefinite cone $\mathbb{S}^{\mathbf{2}}_+ = -V_{\mathcal{N}}^T \,\mathbb{EDM}^{\mathbf{3}} V_{\mathcal{N}}$ (614) for a rank-one solution. Barvinok (§2.6.6.4.1) provides a least upper bound on the affine dimension ($\operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}}$) in which there can exist a corresponding (not necessarily unique) completion given a number m of fixed symmetric entries; this bound increases as $\sqrt{m}$. When the feasible set of completions consists of a single point, then Barvinok's bound becomes the greatest upper bound; in this case $m=2$, the bound equals affine dimension 1.

[8.5] Isometric reconstruction from an EDM means building a list X correct to within a rotation, reflection, and translation. (§4.5.3)

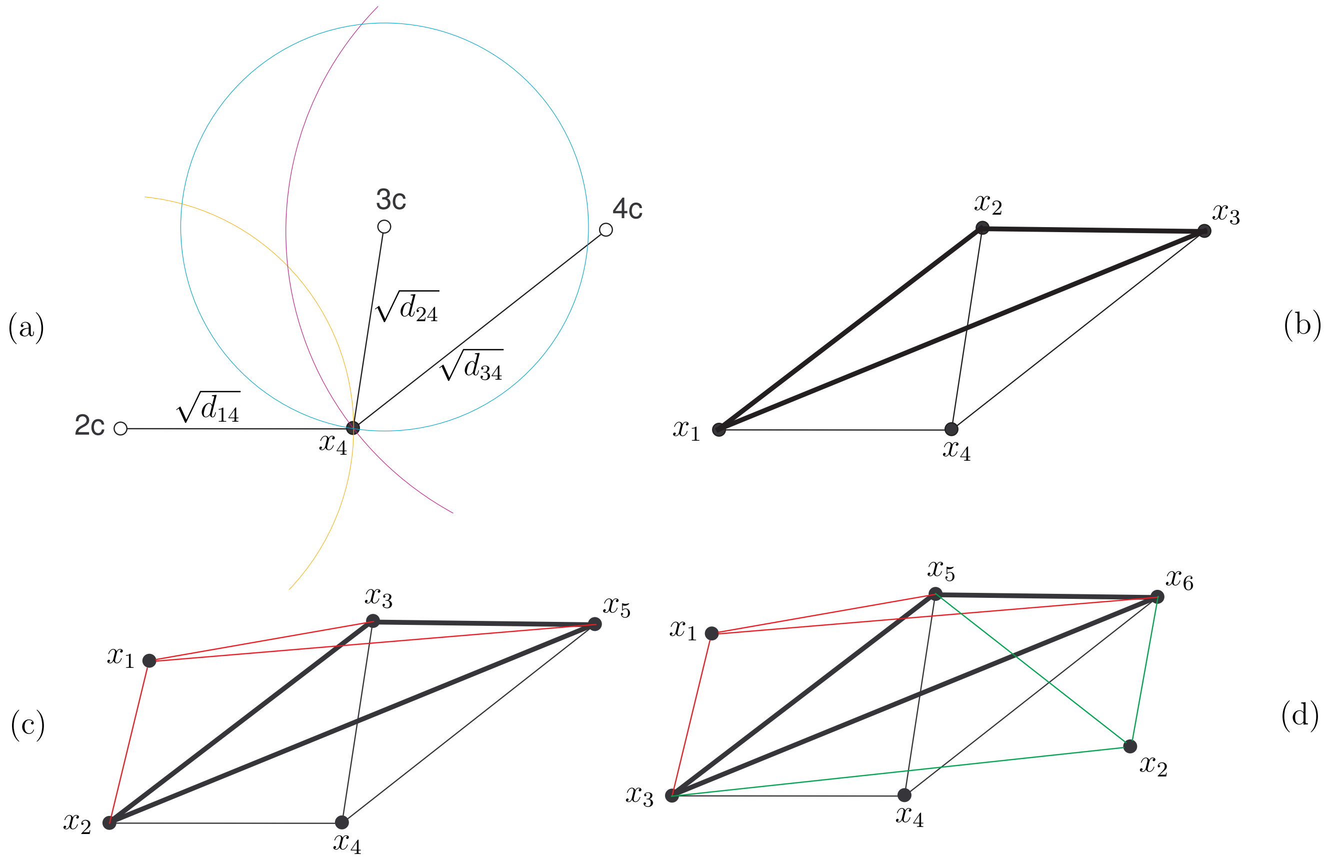


Figure 8.2: **(a)** Given three distances indicated with absolute point positions x_1, x_2, x_3 known and not collinear, then absolute position of x_4 can be precisely and uniquely determined in $\mathbb{R}^2$ by trilateration. If list is realizable in $\mathbb{R}^2$, then realization is unique. Ignoring x_3 for example, position of x_4 acquires ambiguity. Yet four-point list must always be embeddable in subspace having affine dimension $\operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}}$ not exceeding 3. EDM graphs **(b)** **(c)** and **(d)** represent EDMs in various states of completion. Line segments represent known distances, and may cross without vertex at intersection. **(b)** Now only relative position of non-collinear x_1, x_2, x_3 is known; indicated by heavy reference triangle. Knowing all distance information, relative point position x_4 can be precisely and uniquely determined. If list is realizable in $\mathbb{R}^2$, then isometric realization is unique. **(c)** When fifth point is introduced, only distances to x_1, x_2, x_3 are required to unambiguously determine relative position of x_5 in $\mathbb{R}^2$ with respect to reference triangle. Graph represents first instance of missing distance information; $\sqrt{d_{45}}$. **(d)** For six points in $\mathbb{R}^2$, there are three distances absent from complete set of inter-point distances; $\sqrt{d_{45}}$, $\sqrt{d_{46}}$, $\sqrt{d_{56}}$. Yet unique isometric reconstruction is certain.

8.2 Requirements for unique completion

8.2.1 Conservative requirements in $\mathbb{R}^2$

The well-known geometric technique *trilateration* requires only three non-collinear absolute point-positions x_1, x_2, x_3 in $\mathbb{R}^2$ to uniquely determine absolute position of a fourth point x_4 from distance information $\sqrt{d_{14}}$, $\sqrt{d_{24}}$, $\sqrt{d_{34}}$. (Figure **8.2**(a)) The classical calculation finds the common intersection of three circles respectively centered at x_1, x_2, and x_3 having radii $\sqrt{d_{14}}$, $\sqrt{d_{24}}$, and $\sqrt{d_{34}}$. This technique is used by GPS receivers (global positioning system, §4.11.3.0.1).

If only isometric reconstruction is desired, then we need have only relative position of the three non-collinear points; and then trilateration is no longer possible. To determine relative position of x_1, x_2, x_3, the triangle inequality axiom of the Euclidean metric is necessary and sufficient. (§4.12.1) Combining with $\sqrt{d_{14}}$, $\sqrt{d_{24}}$, $\sqrt{d_{34}}$ the new distances between unknown x_1, x_2, x_3 represented by the heavy *reference triangle* in Figure **8.2**(b), then we have a complete EDM for four points;

$$\begin{bmatrix} 0 & \mathbf{d_{12}} & \mathbf{d_{13}} & d_{14} \\ \mathbf{d_{12}} & 0 & \mathbf{d_{23}} & d_{24} \\ \mathbf{d_{13}} & \mathbf{d_{23}} & 0 & d_{34} \\ d_{14} & d_{24} & d_{34} & 0 \end{bmatrix} \tag{799}$$

(The bold entries represent the reference triangle in a principal 3×3 submatrix; all entries here are known.) If a realization exists in $\mathbb{R}^2$, then their isometric reconstruction is unique by injectivity of $\mathbf{D}$; (§4.6) meaning, if the EDM describing the four-point list is unique, then so will be its corresponding isometric realization.

Now consider augmentation of our four-point list with a fifth point x_5 illustrated in Figure **8.2**(c). To unambiguously describe the relative position of x_5 in $\mathbb{R}^2$, we need only the reference triangle and $\sqrt{d_{15}}$, $\sqrt{d_{25}}$, $\sqrt{d_{35}}$. If a realization exists in $\mathbb{R}^2$, then it exists in the plane of the reference triangle. This means the two isometric realizations thus far $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{x}_4$ and $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{x}_5$ coexist in $\mathbb{R}^2$. Since each realization is unique with respect to the reference triangle, then the combined realization is unambiguous in $\mathbb{R}^2$. Relative position of five points in $\mathbb{R}^2$ is therefore specified uniquely by only $5(5-1)/2-1$ distances;

$$\begin{bmatrix} 0 & \mathbf{d_{12}} & \mathbf{d_{13}} & d_{14} & d_{15} \\ \mathbf{d_{12}} & 0 & \mathbf{d_{23}} & d_{24} & d_{25} \\ \mathbf{d_{13}} & \mathbf{d_{23}} & 0 & d_{34} & d_{35} \\ d_{14} & d_{24} & d_{34} & 0 & ? \\ d_{15} & d_{25} & d_{35} & ? & 0 \end{bmatrix} \tag{800}$$

one distance-square shy of the total amount of information $N(N-1)/2$ for an EDM in $\mathbb{EDM}^N$.

Augmenting now with a sixth point in $\mathbb{R}^2$, we count $6(6-1)/2-3$ required distances illustrated in Figure **8.2**(d). The emergent pattern becomes clear and we find for $N>3$, only

$$N(N-1)/2-(N-3)(N-4)/2 \;=\; 3N-6 \tag{801}$$

distances need be known for unique isometric reconstruction in $\mathbb{R}^2$. In terms of the noiseless EDM $D\in\mathbb{EDM}^N$, assuming the reference triangle has nonempty interior[8.6] and vertices corresponding to the first three elements from a corresponding list X, the known distances-square need constitute only the first three rows of D;

$$\begin{bmatrix} 0 & \mathbf{d_{12}} & \mathbf{d_{13}} & d_{14} & d_{15} & d_{16} \\ \mathbf{d_{12}} & 0 & \mathbf{d_{23}} & d_{24} & d_{25} & d_{26} \\ \mathbf{d_{13}} & \mathbf{d_{23}} & 0 & d_{34} & d_{35} & d_{36} \\ d_{14} & d_{24} & d_{34} & 0 & ? & ? \\ d_{15} & d_{25} & d_{35} & ? & 0 & ? \\ d_{16} & d_{26} & d_{36} & ? & ? & 0 \end{bmatrix} \tag{802}$$

8.2.1.1 Other EDM completion patterns

The tie between a planar reference triangle and particular rows of D is unnecessary. We may justifiably assert without loss of generality: If a list is realizable in $\mathbb{R}^2$, then its unique isometric reconstruction is certain given at least any three complete rows of the corresponding noiseless EDM that contain a representation of a reference triangle (having nonempty interior) in a 3×3 principal submatrix. [Caetano...]

[8.6] non-degenerate; planar; the vertices are non-collinear.

8.2.2 Unique completion in any dimension r

Extension to affine dimension r greater than 2 is now clear. Continuing any inductive proof by beginning with unique absolute reconstruction of five points in $\mathbb{R}^{\mathbf{3}}$ via trilateration using four spheres, we jump to the logical conclusion:

- Given a *reference simplex* in $\mathbb{R}^r$ (§2.7.3) whose vertices correspond to any complete principal submatrix $D_i \in \mathbb{EDM}^{r+1}$ of an incomplete noiseless EDM D in $\mathbb{EDM}^N$, if a list is realizable in $\mathbb{R}^r$ then its unique isometric reconstruction in $\mathbb{R}^r$ is certain knowing at least any $r+1$ complete rows containing submatrix D_i.

That lower bound on the total number of entries dispels any notion of distance data proliferation in low affine dimension. For unique isometric reconstruction in subspace $\mathbb{R}^r$, the lower bound on the total number of known distances is $O(N)$ when affine dimension r is less than $N-2$; *id est*, for $N > r+1$ [*sic*],[8.7] [140]

$$\frac{1}{2}N(N-1) - \frac{1}{2}(N-(r+1))(N-(r+2)) \;=\; (r+1)N - \frac{(r+1)(r+2)}{2} \tag{803}$$

is a sufficient number of known distances for unique isometric reconstruction. When affine dimension r reaches $N-2$, then all distances-square in the EDM must be known for unique isometric reconstruction in $\mathbb{R}^r$. Going the other way, when $r=1$ then bound (803) is equivalent to the constraint that the EDM graph be connected. [141, §2.2]

8.2.2.1 Connecting instead to other simplices

Assuming the existence of multiple $r+1$-tuples of points from a list, each comprising vertices of a simplex in $\mathbb{R}^r$, then some freedom is gained in construction of a corresponding EDM having a minimal number of known entries. Assembly of an EDM graph is equally simple as Figure **8.2**:

1. Vertices of a simplex are chosen and assigned the smallest indices as before. All inter-point distances between vertices $\{x_1\,,\, x_2 \ldots x_{r+1}\}$ of this initial simplex are assumed known.

[8.7]The strict inequality follows from trilateration and eliminates local ambiguity due to reflective isometry.

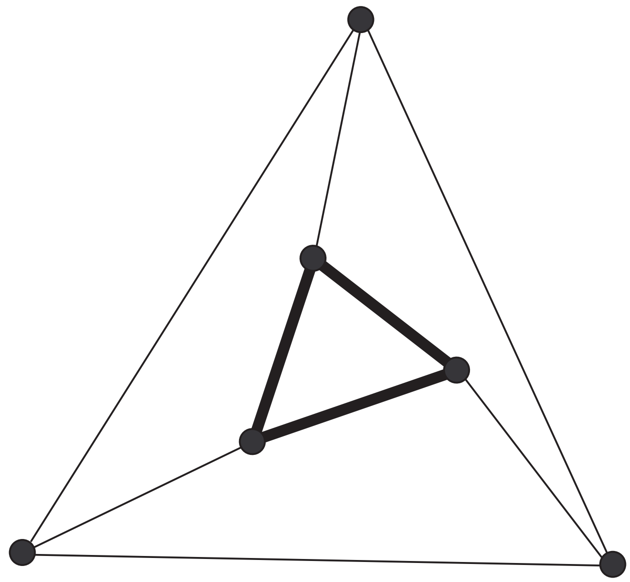


Figure 8.3: EDM graphs having $2N-3$ known distances. **(a)** Redrawing of Figure **4.2** to emphasize obscured segments $\overline{x_2x_4}$, $\overline{x_4x_3}$, and $\overline{x_2x_3}$. Five distances are specified, while the reference simplex is the triangle. The EDM so represented is incomplete, missing d_{14} as in (326), yet the isometric reconstruction is unique as shown in §4.9.3 and §4.12.4.1. **(b)** The corresponding incomplete EDM has a unique isometric reconstruction.

2. Each successive point chosen is labelled ordinally (beginning x_{r+2}), and then connected to any set of $r+1$ points of lower index whose convex hull would make a simplex. (Inter-vertex distances of this simplex need not necessarily be known.)

3. Step 2 is repeated until the last point is connected.[8.8]

This means we may redistribute the (803) known distances-square in an incomplete EDM so that each column beyond the $r+1^{\text{th}}$ contains at least $r+1$ known and noiseless entries above the main diagonal. [Caetano...] There are, for example, forty matrices like (802) for unique isometric reconstruction in

[8.8]Proof of this procedure is left pending.

$\mathbb{R}^2$ having only three entries per column above the main diagonal in columns 4, 5, and 6; here is one:

$$\begin{bmatrix} 0 & \mathbf{d_{12}} & \mathbf{d_{13}} & d_{14} & ? & ? \\ \mathbf{d_{12}} & 0 & \mathbf{d_{23}} & d_{24} & d_{25} & ? \\ \mathbf{d_{13}} & \mathbf{d_{23}} & 0 & d_{34} & d_{35} & d_{36} \\ d_{14} & d_{24} & d_{34} & 0 & d_{45} & d_{46} \\ ? & d_{25} & d_{35} & d_{45} & 0 & d_{56} \\ ? & ? & d_{36} & d_{46} & d_{56} & 0 \end{bmatrix} \tag{804}$$

8.2.2.2 Greatest lower bound

The lower bound on the number of known distances for unique isometric reconstruction in low affine dimension remains $O\big((r+1)N\big)$ as in bound (803). Yet as claimed by Huang, Liang, & Pardalos in [54, §4.2], bound (803) is the greatest lower bound; in that light, we may regard it as a conservative but reliable estimate of the minimum number of entries required in an incomplete EDM for unique isometric reconstruction. Further reduction in the number of distances required for unique isometric reconstruction is achievable under certain conditions on connectivity and arrangement of points; namely, $O(2N)$ independent of affine dimension r; *e.g.*, Figure **8.3**(b). Figure **8.3**(a), originally presented on page 133 from *small completion problem* Example 4.3.0.0.2, is an example of such a reduction in $\mathbb{R}^2$ with $N = 4$ points and only $2N - 3 = 5$ known symmetric entries. The incomplete four-point EDM that Figure **8.3**(a) represents corresponds to a unique realization, although the complete four-point example in Figure **8.4**(b) will not yield a unique realization when any one of the distances is left unspecified. Figure **8.4**(c) and (d) represent further reduction with respect to bound (803) corresponding to the already incomplete EDMs represented in Figure **8.2**(c) and (d).

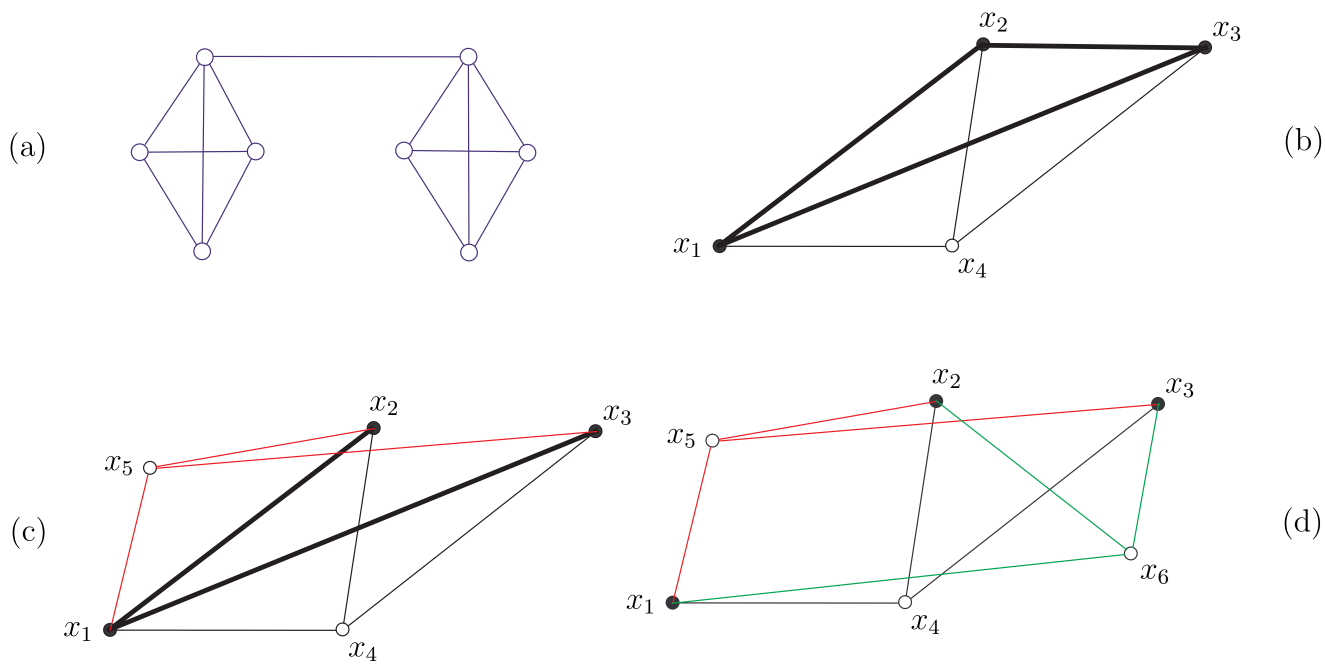


Figure 8.4: EDM graphs. **(a)** Minimum connectivity per vertex **(**say, 3 per vertex ($3N$) in $\mathbb{R}^{\mathbf{2}}$**)** is an insufficient rule for unique isometric reconstruction; illustrated by the dangling diamonds. Yet **(b)** **(c)** and **(d)** each produce a unique isometric reconstruction.

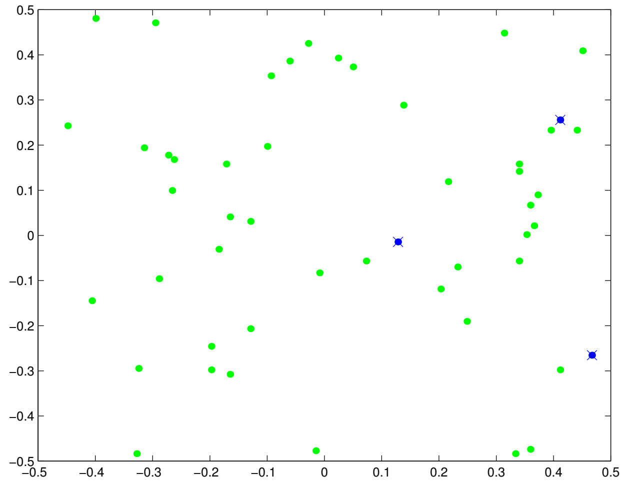


Figure 8.5: Actual positions of fifty sensors in $\mathbb{R}^{\mathbf{2}}$, only three of which (the anchors) have position $\times$ known precisely.

8.3 Completion problems

8.3.1 Cattle problem

The following scenario is motivated by the ancient problem of determining the whereabouts of livestock. Each cow is outfitted with a low-power transceiver from which distance information can be determined to all the others to within a specified accuracy. Because of the requirement for very low power consumption and operation over long periods measured in years, each transmitter is necessarily limited in its effective range and its accuracy is modest.

A large number of sensors correspond to N points in $\mathbb{R}^{\mathbf{2}}$. We are given absolute position with high precision of each point in a small subset of *anchors* $\{x_\ell \in \mathbb{R}^{\mathbf{2}},\ \ell = 1 \ldots M\}$ where without loss of generality we make $x_1 \triangleq \mathbf{0}$ and $0 \leq M \leq N$. For each point pair, known and unknown, is given an upper and lower bound on their squared separation; respectively, $\overline{d_{ij}}$ and $\underline{d_{ij}}$, $i \neq j$. If one sensor is in radio-range ϱ of another, then the actual distance $\sqrt{d_{ij}}$ between them can be determined only to within a constant factor η of the measured distance $\sqrt{\hat{d}_{ij}}$;

$$\underline{d_{ij}} = \hat{d}_{ij}(1-\eta)^2 \;\leq\; d_{ij} \;\leq\; \hat{d}_{ij}(1+\eta)^2 = \overline{d_{ij}} \;, \quad i \neq j \tag{805}$$

id est, all actual distances $\sqrt{d_{ij}}$ are unknown except those between the anchors. If one sensor is out of radio-range of another, then

$$\varrho^2 \leq d_{ij} < \infty \ , \quad i \neq j \tag{806}$$

is all that is known. From this information we must determine absolute position of the remaining $N-M$ sensors.

8.3.1.1 Problem insight

From the parameters of this problem, it is apparent that a low-dimensional solution exists because the origin of the data is earthly terrain. Even with the uncertainty caused by the accuracy tolerance η, we know *a priori* that within the bounds (805) there must lie a two- or at most three-dimensional solution. We therefore design the problem statement to have this low dimensionality built-in.

For convenience, we normalize all quantities; *id est*, distance is unitless.

8.3.1.1.1 Example. *Radio-wave sensor network localization...* [142, §5] [143] We are given N sensors and M anchors (as already explained), and incomplete noisy distance information in $\mathbb{R}^2$. This problem can be posed in terms of the Gram matrix (378) having $(M-1)M/2$ affine equality constraints on it

$$G = X^TX = \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^TDV_{\mathcal{N}} \end{bmatrix}, \qquad x_1 = \mathbf{0} \tag{807}$$

accounting for the M known sensor positions. We substitute the convex rank envelope $\operatorname{tr}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}})$ (§7.2.2) for affine dimension:

$$\begin{array}{cl} \underset{D}{\text{minimize}} & \operatorname{tr}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \\ \text{subject to} & \operatorname{tr}\big(-V_{\mathcal{N}}^TDV_{\mathcal{N}}E_{i-1,j-1}\big) = b_{ij}\;, \quad 2 \leq i \leq j = 2 \ldots M \\ & \underline{D} \leq D \leq \overline{D} \\ & D \in \mathbb{EDM}^N \end{array} \tag{808}$$

where

$$\operatorname{cenv}\operatorname{rank}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \;\propto\; \operatorname{tr}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}) \tag{809}$$

where $E_{ij} \in \mathbb{S}^{N-1}$ is a member of the standard orthonormal basis for $\mathbb{S}^{N-1}$ (38), where $b_{ii} = G_{ii}$ and $b_{ij} = \sqrt{2}G_{ij}\,,\ i \neq j\,,$ and where $\overline{D} = \big[\,\overline{d_{ij}}\,\big]$ and $\underline{D} = \big[\underline{d_{ij}}\big]$. Using this approach, there is no guarantee that affine dimension of the reconstruction is 2.

Figure **8.5** shows $N = 50$ sensors. Only $M = 3$ sensor positions are known. $\overline{D}$ and $\underline{D}$ are known and respectively within ±10% of actual distance-square. Solving (808), we find

$$\lambda(-V_{\mathcal{N}}^TDV_{\mathcal{N}}) = \{11.72\,,\ 3.397\,,\ 0.06208\,,\ 0.01160\,,\ 0.00005193\ldots\} \tag{810}$$

meaning, the list reconstructed from D thus found does not have affine dimension 2 in the Platonic sense. Calculating the Cholesky factorization of $-V_{\mathcal{N}}^TDV_{\mathcal{N}}$ (§4.10.1), we find the list depicted by $\circ$ in Figure **8.6** by projecting the result on the $\mathbb{R}^2$ plane.[8.9]

There is significant energy in the higher-dimensional coordinates of the factorization (not illustrated) that can account for the discrepancy between

[8.9] Projecting instead $-V_{\mathcal{N}}^TDV_{\mathcal{N}}$ on the positive semidefinite cone produces no better result.

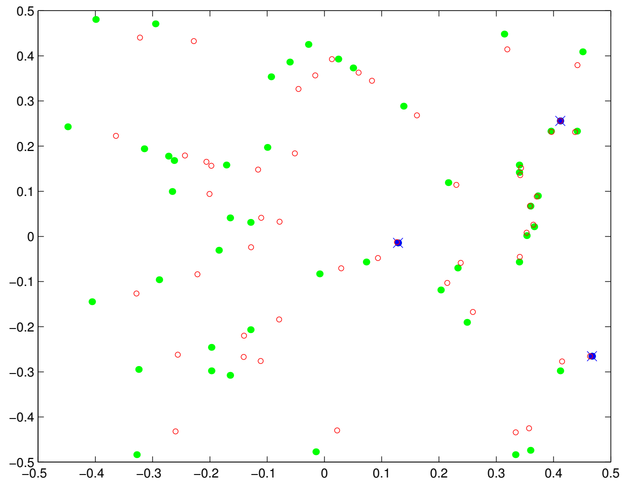


Figure 8.6: Solution **o** to problem (808) having Figure **8.5** input overlaid. Solution data required translation and rotation compensation (§C.2).

actual and estimated position; meaning, our only choice is to seek another algorithm that produces a result having affine dimension equal to 2. We will return to this example. □

8.3.2 Chemistry problem

One of the most successful applications of Euclidean distance geometry appears to be in computational chemistry. [49, in cit.] In [144] [127], for example, Trosset applies distance geometry to an important problem called *molecular conformation* [22] where H represents measurements of interatomic distance, each with specified tolerance.

8.3.2.0.2 Example. *Molecular conformation.*
Here we reproduce the work of.... □

8.3.2.0.3 notes...

inequality constraints only; no fixed data... Of special interest is the case when there are no equality constraints; in effect, we are asked to synthesize the entire EDM based only upon the known upper and lower bounds...

solution of completion problem by alternating projection; *e.g.*, appendix...

applications in [86, in cit.]...

physical barrier problem...

Other researchers [47] [94] have formulated this completion problem in a non-convex way... We will utilize convexity of $-V_{\mathcal{N}}^T\mathbf{D}(X)V_{\mathcal{N}}$ (§4.4.1) to reconstruct the list.

Objective is real (not matrix-valued) when you use the equivalent formulation (329). z becomes another variable, though.

Minimize affine dimension §7.2.2... this works (see comp.sdp and Trosset's example)

$$\begin{array}{cl}\underset{D}{\text{minimize}} & -\operatorname{tr}(V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}})\\ \text{subject to} & \langle E_{ij}\,,\,D\rangle = h_{ij}\,,\quad i\,,j=1\ldots M\\ & \text{or } D\circ\Phi = H\\ & D\in\mathbb{EDM}^N\end{array}\tag{811}$$

Use the vector form (330) in a sum of d_{ij} that is trace, to express the problem in X.

Chapter 9

Piano tuning

Appendix A

Linear algebra

A.1 Main diagonal δ operator, trace, vec

When linear function δ operates on a square matrix $A \in \mathbb{R}^{N\times N}$, $\delta(A)$ returns a vector composed of all the entries from the main diagonal in the natural order;

$$\delta(A) \in \mathbb{R}^N \qquad (42)$$

Operating on a vector, δ naturally returns a diagonal matrix. Operating recursively on a diagonal matrix $\Lambda \in \mathbb{R}^{N\times N}$, $\delta\big(\delta(\Lambda)\big)$ returns Λ itself;

$$\delta^2(\Lambda) \triangleq \delta\big(\delta(\Lambda)\big) \triangleq \Lambda \in \mathbb{R}^{N\times N} \tag{812}$$

Defined in this manner, linear operator δ is *self-adjoint* [38, §3.10, §9.5-1];[A.1] *videlicet*, for $y \in \mathbb{R}^N$, (§2.1.1)

$$\delta(A)^T y \;=\; \langle \delta(A)\,,\, y\rangle \;=\; \langle A\,, \delta(y)\rangle \;=\; \operatorname{tr}\big(A^T\delta(y)\big) \tag{813}$$

This δ notation is efficient and unambiguous as illustrated in the following examples where $A \circ B$ denotes the Hadamard product [28] [44, §1.1.4] of

[A.1] Linear operator $T : \mathbb{R}^{m\times n} \to \mathbb{R}^{M\times N}$ is self-adjoint when, for each and every $X_1\,,\, X_2 \in \mathbb{R}^{m\times n}$,

$$\langle T(X_1)\,,\, X_2\rangle = \langle X_1\,,\, T(X_2)\rangle$$

matrices of like size, σ denotes a vector of non-increasingly ordered singular values, and λ denotes a vector of non-increasingly ordered eigenvalues: for $A\,, B \in \mathbb{R}^{N\times N}$,

1. $\delta(A) = \delta(A^T)$

2. $\operatorname{tr}(A) = \operatorname{tr}(A^T) = \delta(A)^T\mathbf{1}$

3. $\langle I\,, A\rangle = \operatorname{tr} A$

4. $\delta(cA) = c\,\delta(A)\,,\quad c\in\mathbb{R}$

5. $\operatorname{tr}(c\sqrt{A^TA}\,) = c\,\operatorname{tr}\sqrt{A^TA} = c\mathbf{1}^T\sigma(A)\,,\quad c\in\mathbb{R}$

6. $\operatorname{tr}(cA) = c\,\operatorname{tr}(A) = c\mathbf{1}^T\lambda(A)\,,\quad c\in\mathbb{R}$

7. $\delta(A+B) = \delta(A) + \delta(B)$

8. $\operatorname{tr}(A+B) = \operatorname{tr}(A) + \operatorname{tr}(B)$

9. $\delta(AB) = (A\circ B^T)\mathbf{1} = (B^T\circ A)\mathbf{1}$

10. $\delta(AB)^T = \mathbf{1}^T(A^T\circ B) = \mathbf{1}^T(B\circ A^T)$

11. $\delta(uv^T) = \begin{bmatrix} u_1v_1 \\ \vdots \\ u_N v_N \end{bmatrix} = u\circ v\,,\quad u,v\in\mathbb{R}^N$

12. $\operatorname{tr}(A^TB) = \operatorname{tr}(AB^T) = \operatorname{tr}(BA^T) = \operatorname{tr}(B^TA)$
$= \mathbf{1}^T(A\circ B)\mathbf{1} = \mathbf{1}^T\delta(AB^T) = \delta(A^TB)^T\mathbf{1} = \delta(BA^T)^T\mathbf{1} = \delta(B^TA)^T\mathbf{1}$

13. $y^TB\,\delta(A) = \operatorname{tr}\big(B\,\delta(A)y^T\big) = \operatorname{tr}\big(\delta(B^Ty)A\big) = \operatorname{tr}\big(A\,\delta(B^Ty)\big)$
$= \delta(A)^TB^Ty = \operatorname{tr}\big(y\,\delta(A)^TB^T\big) = \operatorname{tr}\big(A^T\delta(B^Ty)\big) = \operatorname{tr}\big(\delta(B^Ty)A^T\big)$

14. $\delta^2(A^TA) = \sum_i e_ie_i^TA^TAe_ie_i^T$

15. $\delta\big(\delta(A)\mathbf{1}^T\big) = \delta\big(\mathbf{1}\,\delta(A)^T\big) = \delta(A)$

16. $\operatorname{vec}(AXB) = (B^T\otimes A)\operatorname{vec} X$

17. $\operatorname{vec}(BXA) = (A^T\otimes B)\operatorname{vec} X$

18. $\operatorname{tr}(AXBX^T) \;=\; \operatorname{vec}(X)^T \operatorname{vec}(AXB) \;=\; \operatorname{vec}(X)^T (B^T \otimes A) \operatorname{vec} X$ [40]

19. $\operatorname{tr}(AX^TBX) \;=\; \operatorname{vec}(X)^T \operatorname{vec}(BXA) \;=\; \operatorname{vec}(X)^T (A^T \otimes B) \operatorname{vec} X$

20. For $\zeta = [\zeta_i] \in \mathbb{R}^k$ and $x = [x_i] \in \mathbb{R}^k$, $\sum\limits_i \zeta_i / x_i \;=\; \zeta^T \delta(x)^{-1} \mathbf{1}$.

21. Let $\lambda(A) \in \mathbb{C}^N$ denote the eigenvalues of $A \in \mathbb{R}^{N \times N}$. Then

$$\delta(A) = \lambda(I \circ A) \tag{814}$$

22. For any permutation matrix Ξ and dimensionally compatible vector y or matrix A,

$$\delta(\Xi\, y) \;=\; \Xi\, \delta(y)\, \Xi^T \tag{815}$$
$$\delta(\Xi\, A\, \Xi^T) = \Xi\, \delta(A) \tag{816}$$

So given any permutation matrix Ξ and any compatible matrix B, for example,

$$\delta^2(B) = \;\Xi\, \delta^2(\Xi^T B\, \Xi)\Xi^T \tag{817}$$

23. **Theorem (Schur).** *Majorization.* [45, §7.4] [28, §4.3] [25, §5.5]
Let $\lambda \in \mathbb{R}^N$ denote a vector of eigenvalues, and let $\delta \in \mathbb{R}^N$ denote a vector of main diagonal entries, both arranged in nonincreasing order. Then

$$\exists\, A \in \mathbb{S}^N \;\ni\; \lambda(A) = \lambda \;\text{ and }\; \delta(A) = \delta \quad \Leftarrow \quad \lambda - \delta \in \mathcal{K}_{\lambda\delta}^* \tag{818}$$

and conversely

$$A \in \mathbb{S}^N \;\Rightarrow\; \lambda(A) - \delta(A) \in \mathcal{K}_{\lambda\delta}^* \tag{819}$$

the pointed empty-interior polyhedral cone of majorization (*confer* (178))

$$\mathcal{K}_{\lambda\delta}^* \triangleq \mathcal{K}_{\mathcal{M}+}^* \cap \{\zeta \mathbf{1} \mid \zeta \in \mathbb{R}\}^* \tag{820}$$

where $\mathcal{K}_{\mathcal{M}+}^*$ is the dual monotone nonnegative cone (250), and where the dual of the line is a hyperplane; $\partial\mathcal{H} = \{\zeta\mathbf{1} \mid \zeta \in \mathbb{R}\}^* = \mathbf{1}^\perp$. $\diamond$

In the particular circumstance $\delta(A) = \mathbf{0}$, we get:

Corollary. *Symmetric hollow majorization.*
Let $\lambda \in \mathbb{R}^N$ denote a vector of eigenvalues arranged in nonincreasing order. Then

$$\exists\, A \in \mathbb{S}_{\mathbf{0}}^N \ni \lambda(A) = \lambda \quad \Leftarrow \quad \lambda \in \mathcal{K}_{\lambda\delta}^* \tag{821}$$

and conversely

$$A \in \mathbb{S}_{\mathbf{0}}^N \;\Rightarrow\; \lambda(A) \in \mathcal{K}_{\lambda\delta}^* \tag{822}$$

where $\mathcal{K}_{\lambda\delta}^*$ is defined in (820). $\diamond$

The majorization cone $\mathcal{K}_{\lambda\delta}^*$ is a natural consequence of the traditional definition of majorization; *id est*, vector $y \in \mathbb{R}^N$ majorizes vector x if and only if

$$\sum_{i=1}^k x_i \leq \sum_{i=1}^k y_i \quad \forall\, 1 \leq k \leq N \tag{823}$$

and

$$\mathbf{1}^T x = \mathbf{1}^T y \tag{824}$$

Under these circumstances, rather, vector x is majorized by vector y.

A.2 Semidefiniteness: domain of test

The most fundamental necessary, sufficient, and definitive test for positive semidefiniteness of matrix $A \in \mathbb{R}^{n\times n}$ is: [25, §1]

$$x^T\!A\, x \geq 0 \;\text{ for each and every } x \in \mathbb{R}^n \text{ such that } \|x\| = 1. \tag{825}$$

Traditionally, authors demand evaluation over broader domain; namely, over all $x \in \mathbb{R}^n$ which is sufficient but unnecessary. Indeed, that standard textbook requirement is far over-reaching because if $x^T\!Ax$ is nonnegative for particular $x = x_p$, then it is nonnegative for any αx_p where $\alpha \in \mathbb{R}$. Thus, only normalized x in $\mathbb{R}^n$ need be evaluated.

Many authors add the further requirement that the domain be complex; the broadest domain. By so doing, only *Hermitian matrices* $(A^H = A$ where superscript ^{H} denotes conjugate transpose$)$[A.2] are admitted to the set of positive semidefinite matrices (829); an unnecessary prohibitive constraint.

[A.2] Hermitian symmetry is the complex analogue; the real part of a Hermitian matrix is symmetric while its imaginary part is antisymmetric. A Hermitian matrix has real eigenvalues and real main diagonal.

A.2.1 Symmetry *versus* semidefiniteness

We call (825) *the most fundamental test* of positive semidefiniteness. Yet some authors instead say, for real A and complex domain ($x \in \mathbb{C}^n$), the complex test $x^HAx \geq 0$ is most fundamental. That complex broadening of the domain of test causes nonsymmetric real matrices to be excluded from the set of positive semidefinite matrices. Yet admitting nonsymmetric real matrices or not is a matter of preference[A.3] unless that complex test is adopted, as we shall now explain.

Any real square matrix A has a representation in terms of its symmetric and antisymmetric parts; *id est*,

$$A = \frac{(A+A^T)}{2} + \frac{(A-A^T)}{2} \tag{826}$$

Because, for all real A, the antisymmetric part vanishes under real test,

$$x^T \frac{(A-A^T)}{2}\, x = 0 \tag{827}$$

only the symmetric part of A, $(A+A^T)/2$, has a role determining positive semidefiniteness. Hence the oft-made presumption that only symmetric matrices may be positive semidefinite is, of course, erroneous under (825). Because eigenvalue-signs of a symmetric matrix translate unequivocally to its semidefiniteness, the eigenvalues that determine semidefiniteness are always those of the *symmetrized* matrix. (§A.3) For that reason, and because symmetric (or Hermitian) matrices must have real eigenvalues, the convention adopted in the literature is that semidefinite matrices are synonymous with symmetric semidefinite matrices. Certainly misleading under (825), that presumption is typically bolstered with compelling examples from the physical sciences where symmetric matrices occur within the mathematical exposition of natural phenomena.[A.4] [145, §52]

Perhaps a better explanation of this pervasive presumption of symmetry comes from Horn & Johnson [28, §7.1] whose perspective[A.5] is the complex matrix, thus necessitating the complex domain of test throughout their treatise. They explain, if $A \in \mathbb{C}^{n\times n}$

[A.3] Golub & Van Loan [44, §4.2.2], for example, admit nonsymmetric real matrices.

[A.4] Symmetric matrices are certainly pervasive in the our chosen subject as well.

[A.5] A totally complex perspective is not necessarily more advantageous. The positive semidefinite cone, for example, is not self-dual (§2.8.2.4) in the ambient space of Hermitian matrices. [58, §II]

> *... and if $x^H A x$ is real for all $x \in \mathbb{C}^n$, then A is Hermitian. Thus, the assumption that A is Hermitian is not necessary in the definition of positive definiteness. It is customary, however.*

Their comment is best explained by noting, the real part of $x^H A x$ comes from the Hermitian part $(A + A^H)/2$ of A;

$$\operatorname{Re}(x^H A x) = x^H \frac{A + A^H}{2}\, x \tag{828}$$

rather,

$$x^H A x \in \mathbb{R} \;\Leftrightarrow\; A^H = A \tag{829}$$

because the imaginary part of $x^H A x$ comes from the anti-Hermitian part $(A - A^H)/2$;

$$\operatorname{Im}(x^H A x) = x^H \frac{A - A^H}{2}\, x \tag{830}$$

that vanishes for nonzero x if and only if $A = A^H$. So the Hermitian symmetry assumption is unnecessary, according to Horn & Johnson, not because non-Hermitian matrices could be regarded positive semidefinite, rather because non-Hermitian (includes nonsymmetric real) matrices are not comparable on the real line under $x^H A x$. Yet that complex edifice is dismantled in the test of real matrices (825) because the domain of test is no longer necessarily complex; meaning, $x^T A x$ will certainly always be real, regardless of symmetry, and so real A will always be comparable.

In summary, if we limit the domain of test to x in $\mathbb{R}^n$ as in (825), then nonsymmetric real matrices are admitted to the realm of semidefinite matrices because they become comparable on the real line. One important exception occurs for rank-one matrices $\Psi = uv^T$ where u and v are real vectors: Ψ is positive semidefinite if and only if $\Psi = uu^T$. (§A.3.1.0.7)

We might choose to expand the domain of test to x in $\mathbb{C}^n$ so that only symmetric matrices would be comparable. The alternative to expanding the domain of test is to exclusively assume all matrices of interest to be symmetric; that is commonly done, hence the synonymous relationship with semidefinite matrices.

A.2.1.0.1 Example. *Nonsymmetric positive definite product.* Horn & Johnson assert and Zhang agrees:

> *If $A,B\in\mathbb{C}^{n\times n}$ are positive definite, then we know that the product AB is positive definite if and only if AB is Hermitian.* [28, §7.6, prob.10] [45, §6.2, §3.2]

Implicitly in their statement, A and B are assumed individually Hermitian and the domain of test is assumed complex.

We prove that assertion to be false for real matrices under (825) that adopts a real domain of test.

$$A^T = A = \begin{bmatrix} 3 & 0 & -1 & 0 \\ 0 & 5 & 1 & 0 \\ -1 & 1 & 4 & 1 \\ 0 & 0 & 1 & 4 \end{bmatrix}, \qquad \lambda(A) = \begin{bmatrix} 5.9 \\ 4.5 \\ 3.4 \\ 2.0 \end{bmatrix} \tag{831}$$

$$B^T = B = \begin{bmatrix} 4 & 4 & -1 & -1 \\ 4 & 5 & 0 & 0 \\ -1 & 0 & 5 & 1 \\ -1 & 0 & 1 & 4 \end{bmatrix}, \qquad \lambda(B) = \begin{bmatrix} 8.8 \\ 5.5 \\ 3.3 \\ 0.24 \end{bmatrix} \tag{832}$$

$$(AB)^T \neq AB = \begin{bmatrix} 13 & 12 & -8 & -4 \\ 19 & 25 & 5 & 1 \\ -5 & 1 & 22 & 9 \\ -5 & 0 & 9 & 17 \end{bmatrix}, \qquad \lambda(AB) = \begin{bmatrix} 36. \\ 29. \\ 10. \\ 0.72 \end{bmatrix} \tag{833}$$

$$\tfrac{1}{2}(AB + (AB)^T) = \begin{bmatrix} 13 & 15.5 & -6.5 & -4.5 \\ 15.5 & 25 & 3 & 0.5 \\ -6.5 & 3 & 22 & 9 \\ -4.5 & 0.5 & 9 & 17 \end{bmatrix}, \quad \lambda\big(\tfrac{1}{2}(AB + (AB)^T)\big) = \begin{bmatrix} 36. \\ 30. \\ 10. \\ 0.014 \end{bmatrix} \tag{834}$$

Whenever $A\in\mathbb{S}_+^n$ and $B\in\mathbb{S}_+^n$, then $\lambda(AB)=\lambda(A^{1/2}BA^{1/2})$ will always be a nonnegative vector by (852) and Corollary A.3.1.0.5. Yet positive definiteness of the product AB is certified instead by the nonnegative eigenvalues

$\lambda\big(\frac{1}{2}(AB+(AB)^T)\big)$ in (834) (§A.3.1.0.1) despite the fact AB is not symmetric.[A.6] Horn & Johnson and Zhang resolve the anomaly by choosing to exclude nonsymmetric matrices and products; they do so by expanding the domain of test to $\mathbb{C}^n$. $\square$

A.3 Proper statements of positive semidefiniteness

Unlike Horn & Johnson and Zhang, we never adopt the complex domain of test in regard to real matrices. So motivated is our consideration of proper statements of positive semidefiniteness under real domain of test. This restriction, ironically, complicates the facts when compared to the corresponding statements for the complex case (found elsewhere, [28] [45]).

We state several fundamental facts regarding positive semidefiniteness of real matrix A and the product AB and sum $A+B$ of real matrices under fundamental real test (825); a few require proof as they depart from the standard texts, while those remaining are well established or obvious.

A.3.0.0.1 Theorem. *Positive (semi)definite matrix.*
$A\in\mathbb{S}^M$ is positive semidefinite if and only if for each and every real vector x of unit norm, $\|x\|=1$,[A.7] we have $x^TAx\geq 0$ (825);

$$A\succeq 0 \;\Leftrightarrow\; \operatorname{tr}(xx^TA) \,=\, x^TAx \,\geq\, 0 \tag{835}$$

Matrix $A\in\mathbb{S}^M$ is positive definite if and only if for each and every $\|x\|=1$ we have $x^TAx>0$;

$$A\succ 0 \;\Leftrightarrow\; \operatorname{tr}(xx^TA) \,=\, x^TAx \,>\, 0 \tag{836}$$

$\diamond$

[A.6] It is a little more difficult to find a counter-example in $\mathbb{R}^{2\times2}$ or $\mathbb{R}^{3\times3}$; which may have served to advance any confusion.

[A.7] The traditional condition requiring all $x\in\mathbb{R}^M$ for defining positive (semi)definiteness is actually far more than what is necessary. The restriction to norm-1 vectors is necessary and sufficient; actually, any particular norm and any nonzero norm-constant will work.

Proof. Statements (835) and (836) are each a particular instance of generalized inequality (§2.8.2) with respect to the positive semidefinite cone; *videlicet*,

$$\begin{array}{l} A \succeq 0 \;\Leftrightarrow\; \langle xx^T, A\rangle \geq 0 \;\; \forall\, xx^T(\succeq 0) \\ A \succ 0 \;\Leftrightarrow\; \langle xx^T, A\rangle > 0 \;\; \forall\, xx^T(\succeq 0)\,,\;\; xx^T \neq \mathbf{0} \end{array} \tag{837}$$

Relations (835) and (836) remain true when xx^T is replaced with "for each and every" $X \in \mathbb{S}_+^M$ [1, §2.6.1] (§2.8.2.4) of unit norm $\|X\| = 1$ as in

$$\begin{array}{l} A \succeq 0 \;\Leftrightarrow\; \operatorname{tr}(XA) \geq 0 \;\; \forall\, X \in \mathbb{S}_+^M \\ A \succ 0 \;\Leftrightarrow\; \operatorname{tr}(XA) > 0 \;\; \forall\, X \in \operatorname{int} \mathbb{S}_+^M \end{array} \tag{838}$$

but this condition is far far more than what is necessary. By the *discrete membership theorem* in §2.8.2.1.3, the extreme directions xx^T of the positive semidefinite cone constitute the minimal set of generators required for necessary and sufficient discretization of the generalized inequality (838) certifying membership to that cone. ♦

A.3.1 Eigenvalues, semidefiniteness, nonsymmetric

When $A \in \mathbb{R}^{n\times n}$, let $\lambda\big(\frac{1}{2}(A + A^T)\big) \in \mathbb{R}^n$ denote eigenvalues of the symmetrized matrix[A.8] arranged in nonincreasing order.

- By positive semidefiniteness of $A \in \mathbb{R}^{n\times n}$ we mean,[A.9] [146, §1.3.1] (*confer* §A.3.1.0.1)

$$x^T A\, x \geq 0 \;\; \forall\, x \in \mathbb{R}^n \;\Leftrightarrow\; A + A^T \succeq 0 \;\Leftrightarrow\; \lambda(A + A^T) \succeq 0 \tag{839}$$

- (§2.6.6.1)

$$A \succeq 0 \;\Rightarrow\; A^T = A \tag{840}$$

$$A \succeq B \;\Leftrightarrow\; A - B \succeq 0 \;\not\Rightarrow\; A \succeq 0 \;\text{ or }\; B \succeq 0 \tag{841}$$

$$x^T A\, x \geq 0 \;\; \forall\, x \;\not\Rightarrow\; A^T = A \tag{842}$$

[A.8] The symmetrization of A is $(A + A^T)/2$. $\lambda\big(\frac{1}{2}(A + A^T)\big) = \lambda(A + A^T)/2$.

[A.9] Strang agrees [26, p.334] it is not $\lambda(A)$ that requires observation. Yet he is mistaken by proposing the Hermitian part alone $x^H(A + A^H)x$ be tested, because the anti-Hermitian part does not vanish under complex test unless A is Hermitian. (830)

- Matrix symmetry is not intrinsic to positive semidefiniteness;

$$A^T = A\,, \quad \lambda(A) \succeq 0 \;\Rightarrow\; x^T\! A\, x \geq 0 \;\; \forall\, x \tag{843}$$

$$\lambda(A) \succeq 0 \;\Leftarrow\; A^T = A\,, \quad x^T\! A\, x \geq 0 \;\; \forall\, x \tag{844}$$

- If $A^T = A$ then

$$\lambda(A) \succeq 0 \;\Leftrightarrow\; A \succeq 0 \tag{845}$$

meaning, matrix A belongs to the positive semidefinite cone in the subspace of symmetric matrices if and only if its eigenvalues belong to the nonnegative orthant.

- For A diagonalizable,

$$\operatorname{rank} A = \operatorname{rank} \delta(\lambda(A)) \tag{846}$$

meaning, the rank is the same as the number of nonzero eigenvalues by the 0 *eigenvalues theorem* (§A.7.2.0.1).

- [28, §2.5.4] (*confer* (25))

$$A \text{ is normal} \;\Leftrightarrow\; \|A\|_{\mathrm{F}}^2 = \lambda(A)^T \lambda(A) \tag{847}$$

- For $A \in \mathbb{R}^{m\times n}$,

$$A^TA \succeq 0\,, \qquad AA^T \succeq 0 \tag{848}$$

because, for dimensionally compatible vector x, $\quad x^TA^TAx = \|Ax\|_2^2$, $x^TAA^Tx = \|A^Tx\|_2^2$.

- For $A \in \mathbb{R}^{n\times n}$ and $c \in \mathbb{R}$,

$$\operatorname{tr}(cA) \;=\; c\operatorname{tr}(A) \;=\; c\,\mathbf{1}^T\lambda(A) \qquad\qquad (\text{§A.1 no.6})$$

$\det A = \prod\limits_i \lambda(A)_i$

- For $\mu \in \mathbb{R}$, all $A \in \mathbb{R}^{n\times n}$, and vector $\lambda(A) \in \mathbb{C}^n$ holding the ordered eigenvalues of A,

$$\lambda(I + \mu A) = \mathbf{1} + \lambda(\mu A) \tag{849}$$

Proof: $A = MJM^{-1}$ and $I + \mu A = M(I + \mu J)M^{-1}$ where J is the Jordan form for A; [26, §5.6] *id est*, $\delta(J) = \lambda(A)$, so $\lambda(I + \mu A) = \delta(I + \mu J)$ because $I + \mu J$ is also a Jordan form. ♦

Similarly, $\lambda(\mu I + A) = \mu\mathbf{1} + \lambda(A)$. For $\sigma(A)$ holding the singular values of any matrix A, $\sigma(I + \mu A^T A) = \Xi\,|\mathbf{1} + \mu\sigma(A^T A)|$ and $\sigma(\mu I + A^T A) = \Xi\,|\mu\mathbf{1} + \sigma(A^T A)|$ where Ξ is a permutation matrix sorting $|\cdot|$ into nonincreasing order.

- For $A, B \in \mathbb{S}^n$ [39, §1.2] (Fan) (*confer* (1059))

$$\operatorname{tr}(AB) \le \lambda(A)^T \lambda(B) \tag{850}$$

with equality (Theobald) when A and B are simultaneously diagonalizable with the same ordering of eigenvalues.

- For $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{n\times m}$,

$$\operatorname{tr}(AB) = \operatorname{tr}(BA) \tag{851}$$

and the nonzero eigenvalues of the product and commuted product are identical, including their multiplicity; [45, §2.5] [28, §1.3.20]

$$\lambda_{1:\eta}(AB) = \lambda_{1:\eta}(BA)\,, \qquad \eta \overset{\Delta}{=} \min\{m, n\} \tag{852}$$

By the 0 *eigenvalues theorem* (§A.7.2.0.1),

$$\operatorname{rank}(AB) = \operatorname{rank}(BA)\,, \quad AB \text{ and } BA \text{ diagonalizable} \tag{853}$$

- For $A \in \mathbb{S}^n$ and any nonsingular matrix Y,

$$\operatorname{inertia}(A) = \operatorname{inertia}(YAY^T) \tag{854}$$

Known as *Sylvester's law of inertia.* (891) [50, §2.4.3]

- For $A, B \in \mathbb{R}^{n\times n}$ square,

$$\det(AB) = \det(BA) \tag{855}$$

- For $A, B \in \mathbb{S}^n$, product AB is symmetric if and only if AB is commutative;

$$(AB)^T = AB \;\Leftrightarrow\; AB = BA \tag{856}$$

Proof. ($\Longrightarrow$) Suppose $AB = (AB)^T$. $(AB)^T = B^TA^T = BA$. $AB = (AB)^T \Rightarrow AB = BA$.
($\Longleftarrow$) Suppose $AB = BA$. $BA = B^TA^T = (AB)^T$. $AB = BA \Rightarrow AB = (AB)^T$. ♦

Commutativity alone is insufficient for symmetry of the product. [26, p.26] Diagonalizable matrices $A, B \in \mathbb{R}^{n\times n}$ commute if and only if they are simultaneously diagonalizable. [28, §1.3.12]

- For $A, B \in \mathbb{R}^{n\times n}$ and $AB = BA$,

$$x^TA\,x \geq 0,\; x^TB\,x \geq 0\;\; \forall\, x \;\Rightarrow\; \lambda(A+A^T)_i\, \lambda(B+B^T)_i \geq 0\;\; \forall\, i \;\;\not\Leftrightarrow\;\; x^TAB\,x \geq 0\;\; \forall\, x \tag{857}$$

the negative result arising because of the schism between the product of eigenvalues $\lambda(A+A^T)_i\, \lambda(B+B^T)_i$ and the eigenvalues of the symmetrized matrix product $\lambda\big(AB+(AB)^T\big)_i$. For example, X^2 is generally not positive semidefinite unless matrix X is symmetric; then (848) applies. Simply substituting symmetric matrices changes the outcome:

- For $A, B \in \mathbb{S}^n$ and $AB = BA$,

$$A \succeq 0\,,\ B \succeq 0 \ \Rightarrow\ \lambda(AB)_i = \lambda(A)_i\, \lambda(B)_i \geq 0 \ \ \forall\, i \ \Leftrightarrow\ AB \succeq 0 \tag{858}$$

Positive semidefiniteness of A and B is sufficient but not a necessary condition for positive semidefiniteness of the product AB.

Proof. Because all symmetric matrices are diagonalizable, [26, §5.6] we have $A = S\Lambda S^T$ and $B = T\Delta T^T$, where Λ and Δ are real diagonal matrices while S and T are orthogonal matrices. Because $(AB)^T = AB$, then T must equal S, [28, §1.3] and the eigenvalues of A are ordered identically to those of B; *id est*, $\lambda(A)_i = \delta(\Lambda)_i$ and $\lambda(B)_i = \delta(\Delta)_i$ correspond to the same eigenvector.
($\Longrightarrow$) Assume $\lambda(A)_i\, \lambda(B)_i \geq 0$ for $i = 1 \ldots n$. $AB = S\Lambda\Delta S^T$ is symmetric and has nonnegative eigenvalues contained in diagonal matrix $\Lambda\Delta$ by assumption; hence positive semidefinite by (839). Now assume $A, B \succeq 0$. That, of course, implies $\lambda(A)_i\, \lambda(B)_i \geq 0$ for all i because all the individual eigenvalues are nonnegative.
($\Longleftarrow$) Suppose $AB = S\Lambda\Delta S^T \succeq 0$. Then $\Lambda\Delta \succeq 0$ by (839), and so all products $\lambda(A)_i\, \lambda(B)_i$ must be nonnegative; meaning, $\operatorname{sgn}(\lambda(A)) = \operatorname{sgn}(\lambda(B))$. We may, therefore, conclude nothing about the semidefiniteness of A and B. ♦

- For $A, B \in \mathbb{S}^n$ and $A \succeq 0\,,\ B \succeq 0\,,$ (Example A.2.1.0.1)

$$AB = BA \ \Rightarrow\ \lambda(AB)_i = \lambda(A)_i\, \lambda(B)_i \geq 0 \ \ \forall\, i \ \Rightarrow\ AB \succeq 0 \tag{859}$$

$$AB = BA \ \Rightarrow\ \lambda(AB)_i \geq 0\,,\ \lambda(A)_i\, \lambda(B)_i \geq 0 \ \forall\, i \ \Leftrightarrow\ AB \succeq 0 \tag{860}$$

- For $A, B \in \mathbb{S}^n$, [45, §6.2]

$$A \succeq 0 \ \Rightarrow\ \operatorname{tr} A \geq 0 \tag{861}$$

$$A \succeq 0\,,\ B \succeq 0 \ \Rightarrow\ \operatorname{tr} A \operatorname{tr} B \ \geq\ \operatorname{tr}(AB) \geq 0 \tag{862}$$

We have $\operatorname{tr}(AB) \geq 0$ because $A \succeq 0\,,\ B \succeq 0 \ \Rightarrow\ \lambda(AB) = \lambda(A^{1/2} B A^{1/2}) \succeq 0$ by (852) and Corollary A.3.1.0.5.

$$A \succeq 0 \ \Leftrightarrow\ \operatorname{tr}(AB) \geq 0\,,\ \forall\, B \succeq 0 \tag{200}$$

- For $A, B, C \in \mathbb{S}^n$ (Löwner)

$$A \preceq B\,, \quad B \preceq C \;\Rightarrow\; A \preceq C \tag{863}$$

$$A \preceq B \;\Leftrightarrow\; A + C \preceq B + C \tag{864}$$

$$A \preceq B\,, \quad A \succeq B \;\Rightarrow\; A = B \tag{865}$$

- For $A, B \in \mathbb{R}^{n \times n}$

$$x^T\! A\, x \geq x^T\! B\, x \;\;\forall x \;\;\Rightarrow\;\; \operatorname{tr} A \geq \operatorname{tr} B \tag{866}$$

Proof. $x^T\! A\, x \geq x^T\! B\, x \;\forall x \Leftrightarrow \lambda\big((A - B) + (A - B)^T\big)/2 \succeq 0 \Rightarrow \operatorname{tr}\big(A + A^T - (B + B^T)\big)/2 = \operatorname{tr}(A - B) \geq 0$. There is no converse.

♦

- For $A, B \in \mathbb{S}^n$ [45, §6.2, prob.1]

$$A \succeq B \;\Rightarrow\;\; \operatorname{tr} A \geq \operatorname{tr} B \tag{867}$$

There is no converse. From [45, §6.2],

$$A \succeq B \succeq 0 \;\Rightarrow\;\; \operatorname{rank} A \geq \operatorname{rank} B \tag{868}$$

$$A \succeq B \succeq 0 \;\Rightarrow\;\; \det A \geq \det B \geq 0 \tag{869}$$

- For $A, B \in \operatorname{int} \mathbb{S}^n_+$ [7, §4.2] [28, §7.7.4],

$$A \succeq B \;\Leftrightarrow\; A^{-1} \preceq B^{-1} \tag{870}$$

- For $A, B \in \mathbb{S}^n$ [45, §6.2]

$$A \succeq B \succeq 0 \;\Rightarrow\; A^{1/2} \succeq B^{1/2} \tag{871}$$

- For $A, B \in \mathbb{S}^n$ and $AB = BA$ [45, §6.2, prob.3]

$$A \succeq B \succeq 0 \;\Rightarrow\; A^k \succeq B^k\,, \quad k = 1, 2, \ldots \tag{872}$$

A.3.1.0.1 Theorem. *Positive semidefinite ordering of eigenvalues.*
For $A\,,B\in\mathbb{R}^{M\times M}$, place the eigenvalues of each symmetrized matrix into the respective vectors $\lambda\big(\frac{1}{2}(A+A^T)\big)\,,\,\lambda\big(\frac{1}{2}(B+B^T)\big)\in\mathbb{R}^M$. Then, [26, §6]

$$x^TA\,x\geq 0\;\;\forall\,x\;\;\Leftrightarrow\;\;\lambda\big(A+A^T\big)\succeq 0 \tag{873}$$

$$x^TA\,x> 0\;\;\forall\,x\;\;\Leftrightarrow\;\;\lambda\big(A+A^T\big)\succ 0 \tag{874}$$

because $x^T(A-A^T)x=0$. (827) Now arrange the entries of $\lambda\big(\frac{1}{2}(A+A^T)\big)$ and $\lambda\big(\frac{1}{2}(B+B^T)\big)$ in nonincreasing order so $\lambda\big(\frac{1}{2}(A+A^T)\big)_{\mathbf{1}}$ holds the largest eigenvalue of symmetrized A while $\lambda\big(\frac{1}{2}(B+B^T)\big)_{\mathbf{1}}$ holds the largest eigenvalue of symmetrized B, and so on. Then [28, §7.7, prob.1, prob.9] for $\kappa\in\mathbb{R}$,

$$\begin{aligned} x^TA\,x\geq x^TB\,x\;\;\forall\,x &\;\;\Rightarrow\;\; \lambda\big(A+A^T\big)\succeq\lambda\big(B+B^T\big)\\ x^TA\,x\geq x^TI\,x\,\kappa\;\;\forall\,x &\;\;\Leftrightarrow\;\; \lambda\big(\tfrac{1}{2}(A+A^T)\big)\succeq\kappa\mathbf{1}\end{aligned} \tag{875}$$

Now let $A\,,B\in\mathbb{S}^M$ have diagonalizations $A=Q\Lambda Q^T$ and $B=U\Upsilon U^T$ with $\lambda(A)=\delta(\Lambda)$ and $\lambda(B)=\delta(\Upsilon)$ arranged in nonincreasing order. Then

$$A\succeq B\;\Leftrightarrow\;\lambda(A-B)\succeq 0 \tag{876}$$

$$A\succeq B\;\Rightarrow\;\lambda(A)\succeq\lambda(B) \tag{877}$$

$$A\succeq B\;\not\Leftarrow\;\lambda(A)\succeq\lambda(B) \tag{878}$$

$$S^TAS\succeq B\;\Leftarrow\;\lambda(A)\succeq\lambda(B) \tag{879}$$

where $S=QU^T$. [45, §7.5] ◇

A.3.1.0.2 Theorem (Weyl). *Eigenvalues of sum.* [28, §4.3]
For $A\,,B\in\mathbb{R}^{M\times M}$, place the eigenvalues of each symmetrized matrix into the respective vectors $\lambda\big(\frac{1}{2}(A+A^T)\big)\,,\,\lambda\big(\frac{1}{2}(B+B^T)\big)\in\mathbb{R}^M$ in nonincreasing order so $\lambda\big(\frac{1}{2}(A+A^T)\big)_{\mathbf{1}}$ holds the largest eigenvalue of symmetrized A while $\lambda\big(\frac{1}{2}(B+B^T)\big)_{\mathbf{1}}$ holds the largest eigenvalue of symmetrized B, and so on. Then, for any $k\in\{1\ldots M\}$,

$$\lambda\big(A+A^T\big)_k+\,\lambda\big(B+B^T\big)_M\;\leq\;\lambda\big((A+A^T)+(B+B^T)\big)_k\;\leq\;\lambda\big(A+A^T\big)_k+\,\lambda\big(B+B^T\big)_{\mathbf{1}} \tag{880}$$

◇

Weyl's theorem establishes positive semidefiniteness of a sum of positive semidefinite matrices. In fact because $\mathbb{S}_+^M$ is a convex cone, then by (111)

$$A\,,B\succeq 0\;\Rightarrow\;\zeta A+\xi B\succeq 0\;\text{ for all }\zeta\,,\xi\geq 0 \tag{881}$$

A.3.1.0.3 Corollary. *Eigenvalues of sum and difference.* [28, §4.3]
For $A\in\mathbb{S}^M$ and $B\in\mathbb{S}_+^M$, place the eigenvalues of each matrix into the respective vectors $\lambda(A), \lambda(B)\in\mathbb{R}^M$ in nonincreasing order so $\lambda(A)_{\mathbf{1}}$ holds the largest eigenvalue of A while $\lambda(B)_{\mathbf{1}}$ holds the largest eigenvalue of B, and so on. Then, for any $k\in\{1\ldots M\}$,

$$\lambda(A-B)_k \;\leq\; \lambda(A)_k \;\leq\; \lambda(A+B)_k \tag{882}$$

⋄

When B is rank-one positive semidefinite, the eigenvalues interlace; *id est*, for $B=qq^T$,

$$\lambda(A)_{k-1} \;\leq\; \lambda(A-qq^T)_k \;\leq\; \lambda(A)_k \;\leq\; \lambda(A+qq^T)_k \;\leq\; \lambda(A)_{k+1} \tag{883}$$

A.3.1.0.4 Theorem. *Positive (semi)definite principal submatrices.*[A.10]

- $A\in\mathbb{S}^M$ is positive definite if and only if any one principal submatrix of dimension $M-1$ is positive definite and $\det A$ is positive.

- $A\in\mathbb{S}^M$ is positive semidefinite if and only if all M principal submatrices of dimension $M-1$ are positive semidefinite and $\det A$ is nonnegative.

- $A\in\mathbb{S}^M$ is positive semidefinite if and only if each and every principal submatrix is positive semidefinite. [45, §6.1]

⋄

Regardless of symmetry, if $A\in\mathbb{R}^{M\times M}$ is positive (semi)definite, then the determinant of each and every principal submatrix is (nonnegative) positive. [146, §1.3.1]

[A.10] A recursive condition for positive (semi)definiteness, this theorem is a synthesis of facts from [28, §7.2] [26, §6.3] (*confer* [146, §1.3.1]). Principal submatrices are formed by discarding any subset of rows and columns having the same indices. There are $M!/(1!(M-1)!)$ principal 1×1 submatrices, $M!/(2!(M-2)!)$ principal 2×2 submatrices, and so on, totaling 2^M-1 principal submatrices including A itself. By loading y in y^TAy with various patterns of ones and zeros, it follows that any principal submatrix must be positive (semi)definite whenever A is.

A.3.1.0.5 Corollary. *Positive (semi)definite symmetric products.*

- If $A \in \mathbb{S}^M$ is positive definite and any particular dimensionally compatible matrix Z has no nullspace, then $Z^T\!AZ$ is positive definite.
- If matrix $A \in \mathbb{S}^M$ is positive (semi)definite then, for any matrix Z of compatible dimension, $Z^T\!AZ$ is positive semidefinite.
- $A \in \mathbb{S}^M$ is positive (semi)definite if and only if there exists a nonsingular Z such that $Z^T\!AZ$ is positive (semi)definite. [28, p.399]
- If $A \in \mathbb{S}^M$ is positive semidefinite and singular it remains possible, for some $Z \in \mathbb{R}^{M\times N}$ with $N < M$, that $Z^T\!AZ$ becomes positive definite. [28, p.399][A.11]

$\diamond$

Given nonsingular matrix Z, it is easy to deduce from these: $A \in \mathbb{S}^M$ is positive (semi)definite if and only if $\begin{bmatrix} Z^T \\ Y^T \end{bmatrix} A \,[\,Z \quad Y\,]$ is positive semidefinite for any particular compatible Y.

Products such as $Z^\dagger Z$ and $ZZ^\dagger$ are symmetric and positive semidefinite although, given $A \succeq 0$, $Z^\dagger AZ$ and $ZAZ^\dagger$ are neither necessarily symmetric or positive semidefinite.

A.3.1.0.6 Theorem. *Symmetric projector semidefinite.* [62, §III] [55, §6] [147, p.55] For symmetric idempotent matrices P and R,

$$\begin{gathered} P, R \succeq 0 \\ P \succeq R \;\Leftrightarrow\; \mathcal{R}(P) \supseteq \mathcal{R}(R) \;\Leftrightarrow\; \mathcal{N}(P) \subseteq \mathcal{N}(R) \end{gathered} \tag{884}$$

Projector P is never positive definite [27, §6.5, prob.20] unless it is the identity matrix. $\diamond$

A.11 Using the interpretation in §E.6.4.2.1, this means that the coefficients of orthogonal projection of vectorized A on a subset of extreme directions from $\mathbb{S}_+^M$ determined by Z can be positive.

A.3.1.0.7 Theorem. *Symmetric positive semidefinite.*
Given real matrix Ψ with $\operatorname{rank}\Psi = 1$,

$$\Psi \succeq 0 \;\Leftrightarrow\; \Psi = uu^T \tag{885}$$

$\diamond$

Proof. Any rank-one matrix must have the form $\Psi = uv^T$. (§B.1) Suppose Ψ is symmetric; *id est*, $v = u$. For all $y \in \mathbb{R}^M$, $y^T u\, u^T y \geq 0$. Conversely, suppose uv^T is positive semidefinite. We know that can hold if and only if $uv^T + vu^T \succeq 0 \;\Leftrightarrow\;$ for all normalized $y \in \mathbb{R}^M$, $2\, y^T u\, v^T y \geq 0$; but that is possible only if $v = u$. ♦

The same does not hold true for matrices of higher rank, as the Example in §A.2.1.0.1 shows.

A.4 Schur complement

Consider the block matrix G: Given $A^T = A$ and $C^T = C$, then [3]

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \succeq 0 \\ \Leftrightarrow\; A \succeq 0,\;\; B^T(I - AA^\dagger) = \mathbf{0},\;\; C - B^T A^\dagger B \succeq 0 \\ \Leftrightarrow\; C \succeq 0,\;\; B(I - CC^\dagger) = \mathbf{0},\;\; A - BC^\dagger B^T \succeq 0 \end{aligned} \tag{886}$$

where $A^\dagger$ denotes the Moore-Penrose (pseudo)inverse (§E). In the first instance, $I - AA^\dagger$ is a symmetric projection matrix orthogonally projecting on $\mathcal{N}(A^T)$. (1202) It is apparently required that

$$\mathcal{R}(B) \perp \mathcal{N}(A^T) \tag{887}$$

which precludes $A = \mathbf{0}$ when B is any nonzero matrix. Note that $A \succ 0 \Rightarrow A^\dagger = A^{-1}$; thereby, the projection matrix vanishes. Likewise, in the second instance, $I - CC^\dagger$ projects orthogonally on $\mathcal{N}(C^T)$. It is required that

$$\mathcal{R}(B^T) \perp \mathcal{N}(C^T) \tag{888}$$

which precludes $C = \mathbf{0}$ for B nonzero. Again, $C \succ 0 \Rightarrow C^\dagger = C^{-1}$. So we get, for A and C nonsingular,

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \succeq 0 \\ \Leftrightarrow\; A \succ 0,\;\; C - B^T A^{-1} B \succeq 0 \\ \Leftrightarrow\; C \succ 0,\;\; A - BC^{-1} B^T \succeq 0 \end{aligned} \tag{889}$$

When A is full-rank then, for all B of compatible dimension, $\mathcal{R}(B)$ is in $\mathcal{R}(A)$. Likewise, when C is full-rank, $\mathcal{R}(B^T)$ is in $\mathcal{R}(C)$. Thus the variation,

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \succ 0 \\ \Leftrightarrow\; A \succ 0,\;\; C - B^T A^{-1} B \succ 0 \\ \Leftrightarrow\; C \succ 0,\;\; A - BC^{-1} B^T \succ 0 \end{aligned} \tag{890}$$

where $C - B^T A^{-1} B$ is called the *Schur complement of A in G*, while the *Schur complement of C in G* is $A - BC^{-1}B^T$. [148, §4.8]

The origin of the term *Schur complement* is from complementary inertia: [50, §2.4.4] Define

$$\text{inertia}\big(G\in\mathbb{S}^M\big) \triangleq \{p\,,z\,,n\} \tag{891}$$

where $p\,,z\,,n$ respectively represent the number of positive, zero, and negative eigenvalues of G; *id est*,

$$M = p+z+n \tag{892}$$

Then, when C is invertible,

$$\text{inertia}(G) = \text{inertia}(C) + \text{inertia}(A - BC^{-1}B^T) \tag{893}$$

and when A is invertible,

$$\text{inertia}(G) = \text{inertia}(A) + \text{inertia}(C - B^TA^{-1}B) \tag{894}$$

When $A = C = \mathbf{0}$, denoting by $\sigma(B)\in\mathbb{R}^m$ the non-increasingly ordered singular values of matrix $B\in\mathbb{R}^{m\times m}$, then we have the eigenvalues [39, §1.2, prob.17]

$$\lambda(G) \;=\; \lambda\left(\begin{bmatrix}\mathbf{0} & B\\ B^T & \mathbf{0}\end{bmatrix}\right) \;=\; \begin{bmatrix}\sigma(B)\\ -\Xi\,\sigma(B)\end{bmatrix} \tag{895}$$

where Ξ is the order-reversing permutation matrix defined in (1046), and we have

$$\text{inertia}(G) = \text{inertia}(B^TB) + \text{inertia}(-B^TB) \tag{896}$$

A.4.0.0.1 Example. *Rank of partitioned matrices.* [28, §0.4.6(c), §7.7.6] When symmetric matrix A is invertible and C is symmetric,

$$\begin{gathered}\text{rank}\begin{bmatrix}A & B\\ B^T & C\end{bmatrix} = \text{rank}\begin{bmatrix}A & \mathbf{0}\\ \mathbf{0}^T & C-B^TA^{-1}B\end{bmatrix}\\ \Leftrightarrow\\ \exists\text{ nonsingular } X,Y \;\ni\; X\begin{bmatrix}A & B\\ B^T & C\end{bmatrix}Y = \begin{bmatrix}A & \mathbf{0}\\ \mathbf{0}^T & C-B^TA^{-1}B\end{bmatrix}\end{gathered} \tag{897}$$

Proof. Let

$$Y \;=\; X^T = \begin{bmatrix}I & -A^{-1}B\\ \mathbf{0}^T & I\end{bmatrix} \qquad \blacklozenge \tag{898}$$

Similarly, when symmetric matrix C is invertible and A is symmetric,

$$\operatorname{rank}\begin{bmatrix} A & B \\ B^T & C \end{bmatrix} = \operatorname{rank}\begin{bmatrix} A - BC^{-1}B^T & \mathbf{0} \\ \mathbf{0}^T & C \end{bmatrix} \tag{899}$$

Setting matrix A to the identity simplifies the Schur conditions; one consequence relates the definiteness of three quantities:

$$\begin{bmatrix} I & \mathbf{0} \\ \mathbf{0}^T & C-B^TB \end{bmatrix} \succeq 0 \quad\Leftrightarrow\quad C - B^TB \succeq 0 \quad\Leftrightarrow\quad \begin{bmatrix} I & B \\ B^T & C \end{bmatrix} \succeq 0 \tag{900}$$

$\square$

A.4.1 Semidefinite program via Schur

The Schur complement (886) can be used to convert a projection problem to an optimization problem in *epigraph form.* Suppose, for example, we are presented with the constrained projection problem studied by Wells in [97] (who gives an analytical solution): Given $A \in \mathbb{R}^{M\times M}$ and some full-rank nonzero matrix $S\in\mathbb{R}^{M\times L}$ with $L<M$,

$$\begin{array}{cl} \underset{X\in\mathbb{S}^M}{\text{minimize}} & \|A-X\|_{\mathrm{F}}^2 \\ \text{subject to} & S^TXS \succeq 0 \end{array} \tag{901}$$

Variable X is constrained to be positive semidefinite, but only on a subspace determined by S. First we write the epigraph form (§3.1.1.2):

$$\begin{array}{cl} \underset{X\in\mathbb{S}^M,\, t\in\mathbb{R}}{\text{minimize}} & t \\ \text{subject to} & \|A-X\|_{\mathrm{F}} \leq t \\ & S^TXS \succeq 0 \end{array} \tag{902}$$

Next we use the Schur complement [6, §6.4.3] [149] and matrix vectorization (§2.1.1):

$$\begin{array}{cl} \underset{X\in\mathbb{S}^M,\, t\in\mathbb{R}}{\text{minimize}} & t \\ \text{subject to} & \begin{bmatrix} tI & \operatorname{vec}(A-X) \\ \operatorname{vec}^T(A-X) & t \end{bmatrix} \succeq 0 \\ & S^TXS \succeq 0 \end{array} \tag{903}$$

This semidefinite program is an epigraph form in disguise, equivalent to (901).

A.4.2 Determinant

$$G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \tag{904}$$

We consider again a matrix G partitioned similarly to (886), but not necessarily positive (semi)definite, where $A\,, C \in \mathbb{S}^M$.

- When A is invertible,

$$\det G \;=\; \det A \;\; \det(C - B^T A^{-1} B) \tag{905}$$

When C is invertible,

$$\det G \;=\; \det C \;\; \det(A - B C^{-1} B^T) \tag{906}$$

- When B is full-rank and skinny, $C = \mathbf{0}$, and $A \succeq 0$, then [1, §10.1.1]

$$\det G \neq 0 \;\Leftrightarrow\; A + BB^T \succ 0 \tag{907}$$

When B is a (column) vector, then for all $C \in \mathbb{R}$ and all A of dimension compatible with G,

$$\det G \;=\; \det(A)C - B^T A_{cof}^T B \tag{908}$$

while for $C \neq 0$,

$$\det G \;=\; C \det(A - \frac{1}{C} BB^T) \tag{909}$$

- When B is full-rank and fat, $A = \mathbf{0}$, and $C \succeq 0$, then

$$\det G \neq 0 \;\Leftrightarrow\; C + B^T B \succ 0 \tag{910}$$

When B is a row vector, then for $A \neq 0$ and all C of dimension compatible with G,

$$\det G \;=\; A \det(C - \frac{1}{A} B^T B) \tag{911}$$

while for all $A \in \mathbb{R}$,

$$\det G \;=\; \det(C)A - B\,C_{cof}^T B^T \tag{912}$$

where A_{cof} and C_{cof} are matrices of cofactors [26, §4] (the *adjugates*) respectively corresponding to A and C.

A.5 Eigen-decomposition

When a matrix $X \in \mathbb{R}^{m\times m}$ is *diagonalizable*, [26, §5.6] then

$$X \;=\; S\Lambda S^{-1} \;=\; [\, s_1 \cdots s_m \,]\; \Lambda \begin{bmatrix} w_1^T \\ \vdots \\ w_m^T \end{bmatrix} \;=\; \sum_{i=1}^{m} \lambda_i \, s_i w_i^T \tag{913}$$

where $s_i \in \mathbb{C}^m$ are linearly independent (right-)eigenvectors constituting the columns of $S \in \mathbb{C}^{m\times m}$ defined by

$$XS = S\Lambda \tag{914}$$

$w_i^T \in \mathbb{C}^m$ are linearly independent *left-eigenvectors* of X constituting the rows of S^{-1} defined by [28]

$$S^{-1}X = \Lambda S^{-1} \tag{915}$$

and where $\lambda_i \in \mathbb{C}$ are eigenvalues (in diagonal matrix $\Lambda \in \mathbb{C}^{m\times m}$) corresponding to both left and right eigenvectors.

There is no connection between diagonalizability and invertibility of X. [26, §5.2] Diagonalizability is guaranteed by a full set of linearly independent eigenvectors, whereas invertibility is guaranteed by all nonzero eigenvalues.

$$\begin{array}{c} \text{distinct eigenvalues} \Rightarrow \text{diagonalizable} \\ \text{not diagonalizable} \Rightarrow \text{repeated eigenvalue} \end{array} \tag{916}$$

A.5.0.0.1 Theorem. *Real eigenvector.* Eigenvectors of a real matrix corresponding to real eigenvalues must be real.

Proof. $Ax = \lambda x$. Given $\lambda = \lambda^*$, $x^HAx = \lambda x^Hx = \lambda\|x\|^2 = x^TAx^* \Rightarrow x = x^*$, where $x^H = x^{*T}$. The converse is equally simple. ♦

A.5.0.1 Uniqueness

From the *fundamental theorem of algebra* it follows: Eigenvalues, including their multiplicity, for a given matrix are unique.

When eigenvectors are unique, we mean their directions are unique to within a linear real scaling. Eigenvectors corresponding to a repeated eigenvalue of a diagonalizable matrix are not unique. [99]

$$\text{diagonalizable, repeated eigenvalue} \Rightarrow \text{eigenvectors not unique} \tag{917}$$

The proof follows from the observation that any linear combination of distinct eigenvectors, corresponding to a particular eigenvalue, produces another eigenvector.

A.5.1 Eigenmatrix

The (right-)eigenvectors $\{s_i\}$ are naturally orthogonal to the left-eigenvectors $\{w_i\}$ except, for $i=1 \ldots m$, $w_i^T s_i = 1$; called a biorthogonality condition [43, §2.2.4] [28] because neither set of left or right eigenvectors is necessarily an orthogonal set. Consequently, each dyad from a diagonalization is an independent (§B.1.1) nonorthogonal projector because

$$s_i w_i^T s_i w_i^T = s_i w_i^T \tag{918}$$

(whereas the dyads of singular value decomposition are not inherently projectors (*confer* (922))).

The dyads of eigen-decomposition can be termed *eigenmatrices* because

$$X\, s_i w_i^T = \lambda_i\, s_i w_i^T \tag{919}$$

A.5.2 Symmetric diagonalization

The set of *normal matrices* is, precisely, that set of all real matrices having a complete orthonormal set of eigenvectors; [45, §8.1] [27, prob.10.2.31] *e.g.*, orthogonal and circulant matrices [81]. All normal matrices are diagonalizable. A symmetric matrix is a special normal matrix, whose eigenvalues must be real and whose eigenvectors can be chosen to make a real orthonormal set; *id est*, for $X \in \mathbb{S}^m$,

$$X = S\Lambda S^T = [\, s_1 \cdots s_m \,]\, \Lambda \begin{bmatrix} s_1^T \\ \vdots \\ s_m^T \end{bmatrix} = \sum_{i=1}^m \lambda_i\, s_i s_i^T \tag{920}$$

where $\delta^2(\Lambda) = \Lambda \in \mathbb{R}^{m\times m}$ (§A.1) and $S^{-1} = S^T \in \mathbb{R}^{m\times m}$ (§B.5). Because the arrangement of eigenvectors and their corresponding eigenvalues is arbitrary, we almost always arrange the eigenvalues in nonincreasing order as is the convention for singular value decomposition.

When $X \in \mathbb{S}_+^m$, its unique matrix square root is defined

$$\sqrt{X} \triangleq S\sqrt{\Lambda}\, S^T \in \mathbb{S}_+^m \tag{921}$$

where the square root of the nonnegative diagonal matrix $\sqrt{\Lambda}$ is taken entry-wise. Then $X=\sqrt{X}\sqrt{X}$.

A.6 Singular value decomposition, SVD

A.6.1 Compact SVD

For any $A\in\mathbb{R}^{m\times n}$,

$$A \;=\; U\Sigma Q^T \;=\; [\,u_1 \cdots\, u_\eta\,]\;\Sigma \begin{bmatrix} q_1^T \\ \vdots \\ q_\eta^T \end{bmatrix} \;=\; \sum_{i=1}^{\eta}\sigma_i\, u_i q_i^T \qquad U\in\mathbb{R}^{m\times\eta},\quad \Sigma\in\mathbb{R}^{\eta\times\eta},\quad Q\in\mathbb{R}^{n\times\eta} \tag{922}$$

where U and Q are always skinny-or-square each having orthonormal columns, and where

$$\eta \triangleq \min\{m,n\} \tag{923}$$

Square matrix Σ is diagonal (§A.1)

$$\delta^2(\Sigma) = \Sigma\in\mathbb{R}^{\eta\times\eta} \tag{924}$$

holding the singular values σ_i of A which are always arranged in nonincreasing order by convention and are related to eigenvalues by[A.12]

$$\sigma(A)_i = \begin{cases} \sqrt{\lambda(A^TA)_i} \;=\; \sqrt{\lambda(AA^T)_i} \;=\; \lambda\Big(\sqrt{A^TA}\Big)_i \;=\; \lambda\Big(\sqrt{AA^T}\Big)_i >\; 0\,, & i=1\ldots\rho \\ 0\,, & i=\rho+1\ldots\eta \end{cases} \tag{925}$$

of which the last $\eta-\rho$ are 0,[A.13] where

$$\rho \triangleq \operatorname{rank} A \;=\; \operatorname{rank}\Sigma \tag{926}$$

A point sometimes lost is that any real matrix may be decomposed in terms of its real singular values $\sigma(A)\in\mathbb{R}^\eta$ and real matrices U and Q as in (922), where [44, §2.5.3]

[A.12] When A is normal, $\sigma(A)=|\lambda(A)|$. [45, §8.1]

[A.13] For $\eta=n$, $\sigma(A)=\sqrt{\lambda(A^TA)}=\lambda\Big(\sqrt{A^TA}\Big)$ where λ denotes eigenvalues. For $\eta=m$, $\sigma(A)=\sqrt{\lambda(AA^T)}=\lambda\Big(\sqrt{AA^T}\Big)$.

$$\begin{array}{l}\mathcal{R}\{u_i \mid \sigma_i \neq 0\} = \mathcal{R}(A)\\ \mathcal{R}\{u_i \mid \sigma_i = 0\} \subseteq \mathcal{N}(A^T)\\ \mathcal{R}\{q_i \mid \sigma_i \neq 0\} = \mathcal{R}(A^T)\\ \mathcal{R}\{q_i \mid \sigma_i = 0\} \subseteq \mathcal{N}(A)\end{array} \tag{927}$$

A.6.2 Subcompact SVD

Some authors allow only nonzero singular values. In that case the compact decomposition can be made smaller; it can be redimensioned in terms of rank ρ because, for any $A \in \mathbb{R}^{m\times n}$,

$$\rho \;=\; \operatorname{rank} A \;=\; \operatorname{rank} \Sigma \;=\; \max\{i \in \{1 \ldots \eta\} \mid \sigma_i \neq 0\} \;\leq\; \eta \tag{928}$$

rank is equivalent to the number of nonzero singular values, as is well known. Now

$$\begin{array}{c} A \;=\; U\Sigma Q^T \;=\; [\, u_1 \cdots u_\rho \,]\; \Sigma \begin{bmatrix} q_1^T \\ \vdots \\ q_\rho^T \end{bmatrix} \;=\; \sum_{i=1}^{\rho} \sigma_i\, u_i q_i^T \\ U \in \mathbb{R}^{m\times\rho}, \quad \Sigma \in \mathbb{R}^{\rho\times\rho}, \quad Q \in \mathbb{R}^{n\times\rho} \end{array} \tag{929}$$

where the main diagonal of diagonal matrix Σ has no 0 entries, and

$$\begin{array}{l}\mathcal{R}\{u_i\} = \mathcal{R}(A)\\ \mathcal{R}\{q_i\} = \mathcal{R}(A^T)\end{array} \tag{930}$$

A.6.3 Full SVD

Another common and useful expression of the SVD makes U and Q square; making the decomposition larger than compact SVD. Completing the null-space bases in U and Q from (927) provides what is called the *full singular value decomposition* of $A \in \mathbb{R}^{m\times n}$ [26, App.A]. Orthonormal matrices U and Q become orthogonal matrices (§B.5):

$$\begin{array}{l}\mathcal{R}\{u_i \mid \sigma_i \neq 0\} = \mathcal{R}(A)\\ \mathcal{R}\{u_i \mid \sigma_i = 0\} = \mathcal{N}(A^T)\\ \mathcal{R}\{q_i \mid \sigma_i \neq 0\} = \mathcal{R}(A^T)\\ \mathcal{R}\{q_i \mid \sigma_i = 0\} = \mathcal{N}(A)\end{array} \tag{931}$$

For any matrix A with rank ρ $(=\operatorname{rank}\Sigma)$,

$$\begin{aligned}
A &= U\Sigma Q^T = [\,u_1 \cdots u_m\,]\;\Sigma \begin{bmatrix} q_1^T \\ \vdots \\ q_n^T \end{bmatrix} = \sum_{i=1}^{\eta} \sigma_i\, u_i q_i^T \\
&= \big[\, m\times\rho \ \text{ basis}\,\mathcal{R}(A) \;\big|\; m\times m-\rho \ \text{ basis}\,\mathcal{N}(A^T)\,\big] \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \ddots \\ & & \end{bmatrix} \left[\begin{array}{c} \big(n\times\rho \ \text{ basis}\,\mathcal{R}(A^T)\big)^T \\ \hline (n\times n-\rho \ \text{ basis}\,\mathcal{N}(A))^T \end{array}\right] \\
& \qquad U\in\mathbb{R}^{m\times m}, \quad \Sigma\in\mathbb{R}^{m\times n}, \quad Q\in\mathbb{R}^{n\times n}
\end{aligned} \tag{932}$$

where the upper limit of summation η is defined in (923). Matrix Σ is no longer necessarily square, now padded with respect to (924) by $m-\eta$ zero rows or $n-\eta$ zero columns; the nonincreasingly ordered (possibly 0) singular values appear along its main diagonal as for compact SVD (925).

A.6.4 SVD of symmetric matrices

Definition. *Step function.* Define the signum-like entry-wise vector-valued function $\psi:\mathbb{R}^n\to\mathbb{R}^n$ that takes the value 1 corresponding to given argument entry 0. For $a\in\mathbb{R}$,

$$\psi(a) \triangleq \lim_{x\to a}\frac{x}{|x|} = \begin{cases} \;\;1\,, & a\geq 0 \\ -1\,, & a<0 \end{cases} \tag{933}$$

Were argument a instead a vector, then $|x|$ denotes absolute value of each individual entry while the division is also entry-wise. △

Signs of the real eigenvalues of a symmetric matrix, for example, can be absorbed into either real U or Q from the SVD; [150, p.34]

$$A = U|\Lambda|\,\delta(\psi(\delta(\Lambda)))U^T = Q\,\delta(\psi(\delta(\Lambda)))\,|\Lambda|Q^T \in \mathbb{S}^n \tag{934}$$

where $|\Lambda|$ denotes entry-wise absolute value of diagonal matrix Λ. A symmetric but complex SVD of a (real) symmetric matrix is given in §C.2.1.2.1.

A.6.5 Pseudoinverse by SVD

The matrix pseudoinverse (§E) is nearly synonymous with singular value decomposition because of the elegant expression,

$$A^\dagger = Q\Sigma^{\dagger T}U^T \in \mathbb{R}^{n\times m} \tag{935}$$

where $\Sigma^\dagger$ simply inverts the nonzero entries of matrix Σ.

Given symmetric matrix A and its diagonalization, then its pseudoinverse simply inverts the nonzero eigenvalues; for $A\in\mathbb{S}^n$,

$$A = Q\Lambda Q^T\ , \qquad A^\dagger = Q\Lambda^\dagger Q^T \tag{936}$$

A.7 Zeros

A.7.1 0 entry

If a positive semidefinite matrix $A=[A_{ij}]\in\mathbb{R}^{n\times n}$ has a 0 entry A_{ii} on its main diagonal, then $A_{ij}+A_{ji}=0\ \ \forall\, j$. [146, §1.3.1]

Any symmetric positive semidefinite matrix having a 0 entry on its main diagonal must be 0 along the entire row and column to which that 0 entry belongs. [44, §4.2.8] [28, §7.1, prob.2]

A.7.2 *0 eigenvalues theorem*

A.7.2.0.1 Theorem. *Number of* 0 *eigenvalues.*

For any matrix $A\in\mathbb{R}^{m\times n}$,

$$\operatorname{rank}(A) + \dim\mathcal{N}(A) = n \tag{937}$$

by conservation of dimension. [28, §0.4.4]

For any square matrix $A\in\mathbb{R}^{m\times m}$, the number of 0 eigenvalues is at least equal to $\dim\mathcal{N}(A)$,

$$\dim\mathcal{N}(A) \;\leq\; \text{number of } 0 \text{ eigenvalues} \;\leq\; m \tag{938}$$

while the eigenvectors corresponding to those 0 eigenvalues belong to $\mathcal{N}(A)$. [26, §5.1][A.14]

[A.14] We take as given the well-known fact that the number of 0 eigenvalues cannot be less

For diagonalizable matrix A (§A.5), the number of 0 eigenvalues is precisely $\dim\mathcal{N}(A)$ while the corresponding eigenvectors span $\mathcal{N}(A)$. The real and imaginary parts of the eigenvectors remaining span $\mathcal{R}(A)$.

TRANSPOSE.

Likewise, for any matrix $A\in\mathbb{R}^{m\times n}$,

$$\operatorname{rank}(A^T) + \dim\mathcal{N}(A^T) = m \tag{939}$$

For any square $A\in\mathbb{R}^{m\times m}$, the number of 0 eigenvalues is at least equal to $\dim\mathcal{N}(A^T) = \dim\mathcal{N}(A)$ while the left-eigenvectors (eigenvectors of A^T) corresponding to those 0 eigenvalues belong to $\mathcal{N}(A^T)$.

For diagonalizable A, the number of 0 eigenvalues is precisely $\dim\mathcal{N}(A^T)$ while the corresponding left-eigenvectors span $\mathcal{N}(A^T)$. The real and imaginary parts of the left-eigenvectors remaining span $\mathcal{R}(A^T)$.

$\diamond$

Proof. First we show, for a diagonalizable matrix, the number of 0 eigenvalues is precisely the dimension of its nullspace while the eigenvectors corresponding to those 0 eigenvalues span the nullspace:

Any diagonalizable matrix $A\in\mathbb{R}^{m\times m}$ must possess a complete set of linearly independent eigenvectors. If A is full-rank (invertible), then all $m = \operatorname{rank}(A)$ eigenvalues are nonzero. [26, §5.1]

Suppose $\operatorname{rank}(A) < m$. Then $\dim\mathcal{N}(A) = m - \operatorname{rank}(A)$. Thus there is a set of $m - \operatorname{rank}(A)$ linearly independent vectors spanning $\mathcal{N}(A)$. Each of those can be an eigenvector associated with a 0 eigenvalue because A is diagonalizable $\Leftrightarrow \exists\, m$ linearly independent eigenvectors. [26, §5.2] Eigenvectors of a real matrix corresponding to 0 eigenvalues must be real.[A.15] Thus A has at least $m - \operatorname{rank}(A)$ eigenvalues equal to 0.

---

than the dimension of the nullspace. We offer an example of the converse:

$$A = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$\dim\mathcal{N}(A) = 2$, $\lambda(A) = [\,0\ 0\ 0\ 1\,]^T$; three eigenvectors in the nullspace but only two are independent. The right-hand side of (938) is tight for nonzero matrices; *e.g.*, (§B.1) dyad $uv^T\in\mathbb{R}^{m\times m}$ has m 0-eigenvalues when $u\in v^\perp$.

[A.15] Let $*$ denote complex conjugation. Suppose $A = A^*$ and $As_i = \mathbf{0}$. Then $s_i = s_i^* \Rightarrow As_i = As_i^* \Rightarrow As_i^* = \mathbf{0}$. Conversely, $As_i^* = \mathbf{0} \Rightarrow As_i = As_i^* \Rightarrow s_i = s_i^*$.

Now suppose A has more than $m-\text{rank}(A)$ eigenvalues equal to 0. Then there are more than $m-\text{rank}(A)$ linearly independent eigenvectors associated with 0 eigenvalues, and each of those eigenvectors must be in $\mathcal{N}(A)$. Thus there are more than $m-\text{rank}(A)$ linearly independent vectors in $\mathcal{N}(A)$; a contradiction.

Therefore diagonalizable A has $\text{rank}(A)$ nonzero eigenvalues and exactly $m-\text{rank}(A)$ eigenvalues equal to 0 whose corresponding eigenvectors span $\mathcal{N}(A)$.

By similar argument, the left-eigenvectors corresponding to 0 eigenvalues span $\mathcal{N}(A^T)$.

Next we show when A is diagonalizable, the real and imaginary parts of its eigenvectors (corresponding to nonzero eigenvalues) span $\mathcal{R}(A)$:

The right-eigenvectors of a diagonalizable matrix $A\in\mathbb{R}^{m\times m}$ are linearly independent if and only if the left-eigenvectors are. So, matrix A has a representation in terms of its right and left-eigenvectors; from the diagonalization (913), assuming 0 eigenvalues are ordered last,

$$A = \sum_{i=1}^{m} \lambda_i\, s_i w_i^T = \sum_{\substack{i=1\\ \lambda_i\neq 0}}^{k\,\leq\, m} \lambda_i\, s_i w_i^T \tag{940}$$

From the *linearly independent dyads theorem* (§B.1.1.0.1), the dyads $\{s_i w_i^T\}$ must be independent because each set of eigenvectors are; hence $\text{rank}\, A = k$, the number of nonzero eigenvalues. Complex eigenvectors and eigenvalues are common for real matrices, and must come in complex conjugate pairs for the summation to remain real. Assume that conjugate pairs of eigenvalues appear in sequence. Given any particular conjugate pair from (940), we get the partial summation

$$\begin{aligned}\lambda_i\, s_i w_i^T + \lambda_i^*\, s_i^* w_i^{*T} &= 2\,\text{Re}(\lambda_i\, s_i w_i^T)\\ &= 2\big(\text{Re}\, s_i\ \text{Re}(\lambda_i\, w_i^T) - \text{Im}\, s_i\ \text{Im}(\lambda_i\, w_i^T)\big)\end{aligned} \tag{941}$$

where[A.16] $\lambda_i^* \triangleq \lambda_{i+1}$, $s_i^* \triangleq s_{i+1}$, and $w_i^* \triangleq w_{i+1}$. Then (940) is equivalently written

$$A = 2\sum_{\substack{i\\ \lambda\in\mathbb{C}\\ \lambda_i\neq 0}} \text{Re}\, s_{2i}\ \text{Re}(\lambda_{2i}\, w_{2i}^T) - \text{Im}\, s_{2i}\ \text{Im}(\lambda_{2i}\, w_{2i}^T) + \sum_{\substack{j\\ \lambda\in\mathbb{R}\\ \lambda_j\neq 0}} \lambda_j\, s_j w_j^T \tag{942}$$

[A.16] The complex conjugate of w is denoted w^*, while its conjugate transpose is denoted by $w^H = w^{*T}$.

The summation (942) shows that A is a linear combination of real and imaginary parts of its right-eigenvectors corresponding to nonzero eigenvalues. Therefore, the k vectors $\{\operatorname{Re} s_i\,, \operatorname{Im} s_i \mid \lambda_i \neq 0,\ i \in \{1 \ldots m\}\}$ must span the range of diagonalizable matrix A.

The argument is similar regarding the span of the left-eigenvectors. ♦

A.7.3 0 trace and product

For $X, A \in \mathbb{S}_+^M$ [7, §2.6.1, exer.2.8] [69, §3.1],

$$\operatorname{tr}(XA) = 0 \;\Leftrightarrow\; XA = AX = \mathbf{0} \tag{943}$$

Symmetric matrices A and X are *simultaneously diagonalizable* because they commute; (856) [28, p.50] *id est*, they share a complete set of eigenvectors.

Proof. ($\Longleftarrow$) Suppose $XA = AX = \mathbf{0}$. Then $\operatorname{tr}(XA) = 0$ is obvious. ($\Longrightarrow$) Suppose $\operatorname{tr}(XA) = 0$. $\operatorname{tr}(XA) = \operatorname{tr}(A^{1/2}XA^{1/2})$ whose argument is positive semidefinite by Corollary A.3.1.0.5. Trace of any square matrix is equivalent to the sum of its eigenvalues. Eigenvalues of a positive semidefinite matrix can total 0 if and only if each and every nonnegative eigenvalue is 0. The only feasible positive semidefinite matrix, having all 0 eigenvalues, resides at the origin; *id est*,

$$A^{1/2}XA^{1/2} = \left(X^{1/2}A^{1/2}\right)^T X^{1/2}A^{1/2} = \mathbf{0} \tag{944}$$

which in turn implies $XA = \mathbf{0}$. A similar argument shows $AX = \mathbf{0}$. ♦

A.7.4 Zero definite

The domain over which an arbitrary real matrix A is zero definite can exceed its left and right nullspaces. The positive semidefinite matrix

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \tag{945}$$

for example, has no nullspace. Yet

$$\{x \mid x^T A x = 0\} \;=\; \{x \mid \mathbf{1}^T x = 0\} \subset \mathbb{R}^{\mathbf{2}} \tag{946}$$

which is the nullspace of the symmetrized matrix. Symmetric matrices are not spared from the excess; *videlicet*,

$$B = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \tag{947}$$

has eigenvalues $\{-1, 3\}$, no nullspace, but is zero definite on[A.17]

$$\mathcal{X} = \{x \in \mathbb{R}^{\mathbf{2}} \mid x_2 = (-2 \pm \sqrt{3})x_1\} \tag{948}$$

For any positive semidefinite matrix $A \in \mathbb{R}^{M\times M}$, in particular,

$$\{x \mid x^TAx = 0\,,\ A + A^T \succeq 0\} \;=\; \mathcal{N}(A + A^T) \tag{949}$$

because $\exists\, R \ \ni\ A+A^T = R^TR\,,\ \|Rx\| = 0 \Leftrightarrow Rx = 0$, and $\mathcal{N}(A+A^T) = \mathcal{N}(R)$. For a positive definite matrix A,

$$\{x \mid x^TAx = 0\,,\ A + A^T \succ 0\} \;=\; \mathbf{0} \tag{950}$$

Further, [45, §3.2, prob.5]

$$\{x \mid x^TAx = 0\} = \mathbb{R}^M \;\Leftrightarrow\; A^T = -A \tag{951}$$

while

$$\{x \mid x^HAx = 0\} = \mathbb{C}^M \;\Leftrightarrow\; A = \mathbf{0} \tag{952}$$

A.7.4.0.1 Lemma. *Dyad-decompositions...* [151]
Given symmetric matrix $A \in \mathbb{S}^M$, let $X \in \mathbb{S}^M_+$ be a symmetric positive semidefinite matrix having rank ρ such that $\langle A\,, X\rangle = 0$. Then there is a dyad-decomposition of X

$$X = \sum_{j=1}^{\rho} x_j x_j^T \tag{953}$$

satisfying

$$\langle A\,, x_j x_j^T\rangle = \langle A\,, X\rangle = 0 \quad \text{for all } j \tag{954}$$

Proof... ♦

[A.17] These two lines represent the limit in the union of two generally distinct hyperbolae; *id est*,

$$\lim_{\varepsilon\downarrow 0}\{x \in \mathbb{R}^{\mathbf{2}} \mid x^TBx = \varepsilon\} \;=\; \mathcal{X}$$

A.7.4.0.2 Example. *Dyad.*
The dyad $uv^T \in \mathbb{R}^{M\times M}$ (§B.1) is zero definite on all x for which either $x^Tu=0$ or $x^Tv=0$;

$$\{x \mid x^Tuv^Tx = 0\} \;=\; \{x \mid x^Tu=0\} \cup \{x \mid v^Tx=0\} \tag{955}$$

id est, on $u^\perp \cup v^\perp$. Symmetrizing the dyad does not change the outcome:

$$\{x \mid x^T(uv^T + vu^T)x/2 = 0\} \;=\; \{x \mid x^Tu=0\} \cup \{x \mid v^Tx=0\} \tag{956}$$

$\square$

Appendix B

Simple matrices

Mathematicians also attempted to develop algebra of vectors but there was no natural definition of the product of two vectors that held in arbitrary dimensions. The first vector algebra that involved a noncommutative vector product (that is, v×w *need not equal* w×v*) was proposed by Hermann Grassmann in his book* Ausdehnungslehre *(1844). Grassmann's text also introduced the product of a column matrix and a row matrix, which resulted in what is now called a simple or a rank-one matrix. In the late 19th century the American mathematical physicist Willard Gibbs published his famous treatise on vector analysis. In that treatise Gibbs represented general matrices, which he called* dyadics, *as sums of simple matrices, which Gibbs called* dyads. *Later the physicist P. A. M. Dirac introduced the term "bra-ket" for what we now call the scalar product of a "bra" (row) vector times a "ket" (column) vector and the term "ket-bra" for the product of a ket times a bra, resulting in what we now call a simple matrix, as above. Our convention of identifying column matrices and vectors was introduced by physicists in the 20th century.*

−Marie A. Vitulli, [130]

B.1 Rank-one matrix (dyad)

Any matrix formed from the unsigned outer product of two vectors,

$$\Psi = uv^T \in \mathbb{R}^{M\times N} \tag{957}$$

where $u\in\mathbb{R}^M$ and $v\in\mathbb{R}^N$, is rank-one and called a *dyad*. Conversely, any rank-one matrix must have the form Ψ. [28, prob.1.4.1] The product $-uv^T$ is a *negative dyad*. For matrix products AB^T, in general, we have

$$\mathcal{R}(AB^T) \subseteq \mathcal{R}(A)\,, \qquad \mathcal{N}(AB^T) \supseteq \mathcal{N}(B^T) \tag{958}$$

with equality when $B = A$ [26, §3.3, §3.6][B.1] or respectively when B is invertible and $\mathcal{N}(A)=\mathbf{0}$. Yet for all nonzero dyads we have

$$\mathcal{R}(uv^T) = \mathcal{R}(u)\,, \qquad \mathcal{N}(uv^T) = \mathcal{N}(v^T) \equiv v^\perp \tag{959}$$

where $\dim v^\perp = N-1$.

It is obvious a dyad can be $\mathbf{0}$ only when u or v is $\mathbf{0}$;

$$\Psi = uv^T = \mathbf{0} \;\Leftrightarrow\; u = \mathbf{0} \;\text{ or }\; v = \mathbf{0} \tag{960}$$

The matrix 2-norm for Ψ is equivalent to the Frobenius norm;

$$\|\Psi\| \;=\; \|uv^T\|_{\mathrm F} \;=\; \|uv^T\|_2 \;=\; \|u\|\,\|v\| \tag{961}$$

When u and v are normalized, the pseudoinverse is the transposed dyad. Otherwise,

$$\Psi^\dagger \;=\; (uv^T)^\dagger \;=\; \frac{vu^T}{\|u\|^2\,\|v\|^2} \tag{962}$$

When dyad $uv^T\in\mathbb{R}^{N\times N}$ is square, uv^T has at least $N-1$ 0-eigenvalues and corresponding eigenvectors spanning $v^\perp$. The remaining eigenvector u spans the range of uv^T with corresponding eigenvalue

$$\lambda \;=\; v^Tu \;=\; \mathrm{tr}(uv^T) \in \mathbb{R} \tag{963}$$

[B.1] **Proof.** $\mathcal{R}(AA^T) \subseteq \mathcal{R}(A)$ is obvious.

$$\begin{aligned}\mathcal{R}(AA^T) \;&=\; \{AA^Ty \mid y\in\mathbb{R}^m\}\\ &\supseteq\; \{AA^Ty \mid A^Ty\in\mathcal{R}(A^T)\} = \mathcal{R}(A) \;\text{ by (90).}\end{aligned}$$

◆

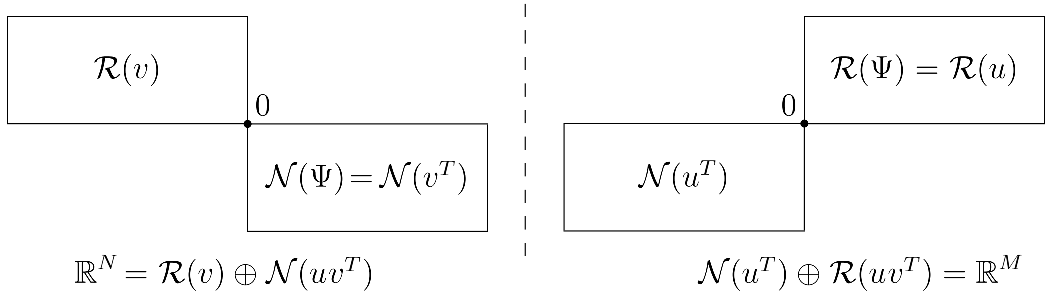


Figure B.1: The four fundamental subspaces [27, §3.6] of any dyad $\Psi = uv^T \in \mathbb{R}^{M\times N}$. $\Psi(x) = uv^T x$ is a linear mapping from $\mathbb{R}^N$ to $\mathbb{R}^M$. The map from $\mathcal{R}(v)$ to $\mathcal{R}(u)$ is one-to-one and onto (bijective). [26, §3.1]

The determinant is the product of the eigenvalues; so, it is always true that

$$\det \Psi \;=\; \det(uv^T) \;=\; 0 \tag{964}$$

When $\lambda = 1$, the square dyad is a nonorthogonal projector on its range ($\Psi^2 = \Psi$, §E.1). It is quite possible that $u \in v^\perp$ making the remaining eigenvalue instead 0 ;[B.2] $\lambda = 0$ together with the first $N-1$ 0-eigenvalues; *id est*, it is possible uv^T were nonzero while all its eigenvalues are 0. The matrix

$$\begin{bmatrix} 1 \\ -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} \tag{965}$$

for example, has two 0-eigenvalues. In other words, the value of eigenvector u may simultaneously be a member of the nullspace and range of the dyad. The explanation is, simply, because u and v share the same dimension, $\dim u = M = \dim v = N$:

Figure **B.1** shows the four fundamental subspaces for the dyad. Linear operator $\Psi(x) : \mathbb{R}^N \to \mathbb{R}^M$ is a mapping between vector spaces that remain distinct when $M = N$;

$$\begin{gathered} u \in \mathcal{R}(uv^T) \\ u \in \mathcal{N}(uv^T) \;\Leftrightarrow\; v^T u = 0 \\ \mathcal{R}(uv^T) \cap \mathcal{N}(uv^T) = \emptyset \end{gathered} \tag{966}$$

♦

[B.2] The dyad is not always diagonalizable (§A.5) because the eigenvectors are not necessarily independent.

B.1.0.1 rank-one modification

If A is any nonsingular compatible matrix and $1 + v^T A^{-1} u \neq 0$, then [152, App.6] [45, §2.3, prob.16] [148, §4.11.2] (Sherman-Morrison)

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1} uv^T A^{-1}}{1 + v^T A^{-1} u} \tag{967}$$

B.1.0.2 dyad symmetry

In the specific circumstance that $v = u$, then $uu^T \in \mathbb{R}^{N\times N}$ is symmetric, rank-one, and positive semidefinite having exactly $N-1$ 0-eigenvalues. In fact, (§A.3.1.0.7)

$$uv^T \succeq 0 \;\Leftrightarrow\; v = u \tag{968}$$

and the remaining eigenvalue is almost always positive;

$$\lambda \;=\; u^T u \;=\; \operatorname{tr}(uu^T) \;>\; 0 \;\text{ unless }\; u = \mathbf{0} \tag{969}$$

The matrix

$$\begin{bmatrix} \Psi & u \\ u^T & 1 \end{bmatrix} \tag{970}$$

for example, is rank 1 positive semidefinite if and only if $\Psi = uu^T$.

B.1.1 Dyad independence

Now we consider a sum of dyads like (957) as encountered in diagonalization and singular value decomposition:

$$\mathcal{R}\left(\sum_{i=1}^{k} s_i w_i^T\right) \;=\; \sum_{i=1}^{k} \mathcal{R}\big(s_i w_i^T\big) \;=\; \sum_{i=1}^{k} \mathcal{R}(s_i) \;\Leftarrow\; w_i \;\forall\, i \;\text{ are l.i.} \tag{971}$$

range of the summation is the vector sum of ranges.[B.3] (Theorem B.1.1.1.1) Under the assumption the dyads are linearly independent (l.i.), then the vector sums are unique (p.447): $\forall\, i$, w_i l.i. and s_i l.i.,

$$\mathcal{R}\left(\sum_{i=1}^{k} s_i w_i^T\right) = \mathcal{R}\big(s_1 w_1^T\big) \oplus \ldots \oplus \mathcal{R}\big(s_k w_k^T\big) \;=\; \mathcal{R}(s_1) \oplus \ldots \oplus \mathcal{R}(s_k) \tag{972}$$

[B.3] Movement of range $\mathcal{R}$ inside the summation depends on linear independence of $\{w_i\}$.

B.1.1.0.1 Definition. *Linearly independent dyads.* [153, p.29, thm.11] [154, p.2] The set of k dyads

$$\left\{ s_i w_i^T \mid i=1 \ldots k \right\} \tag{973}$$

where $s_i \in \mathbb{C}^M$ and $w_i \in \mathbb{C}^N$, is said to be linearly independent iff

$$\operatorname{rank}\left(SW^T \triangleq \sum_{i=1}^{k} s_i w_i^T \right) = k \tag{974}$$

where $S \triangleq [s_1 \cdots s_k] \in \mathbb{C}^{M\times k}$ and $W \triangleq [w_1 \cdots w_k] \in \mathbb{C}^{N\times k}$. $\triangle$

As defined, dyad independence does not preclude existence of a nullspace $\mathcal{N}(SW^T)$, nor does it imply SW^T is full-rank. In the absence of an assumption of independence, generally, $\operatorname{rank} SW^T \leq k$. Conversely, any rank-$k$ matrix can be written in the form SW^T by singular value decomposition. (§A.6)

Theorem. *Linearly independent dyads.* The vectors $\left\{ s_i \in \mathbb{C}^M,\ i=1 \ldots k \right\}$ are linearly independent and the vectors $\left\{ w_i \in \mathbb{C}^N,\ i=1 \ldots k \right\}$ are linearly independent if and only if the dyads $\left\{ s_i w_i^T,\ i=1 \ldots k \right\}$ are linearly independent. $\diamond$

Proof. Linear independence of k dyads is identical to definition (974).
($\Longrightarrow$) Suppose $\{s_i\}$ and $\{w_i\}$ are each linearly independent sets. Invoking Sylvester's rank inequality, [28, §0.4] [45, §2.4]

$$\operatorname{rank} S + \operatorname{rank} W - k \;\leq\; \operatorname{rank}(SW^T) \;\leq\; \min\{\operatorname{rank} S\,,\ \operatorname{rank} W\} \;\;(\leq\, k) \tag{975}$$

Then $k \leq \operatorname{rank}(SW^T) \leq k$ that implies the dyads are independent.
($\Longleftarrow$) Conversely, suppose $\operatorname{rank}(SW^T) = k$. Then

$$k \leq \min\{\operatorname{rank} S\,,\ \operatorname{rank} W\} \leq k \tag{976}$$

implying the vector sets are each independent. $\blacklozenge$

B.1.1.1 Biorthogonality condition, Range, Nullspace

Dyads characterized by a biorthogonality condition $W^T S = I$ are independent; *id est*, for $S \in \mathbb{C}^{M\times k}$ and $W \in \mathbb{C}^{N\times k}$, if $W^T S = I$ then $\operatorname{rank}(SW^T) = k$

by the *linearly independent dyads theorem* because (*e.g.*, §E.1.1)

$$W^T S = I \quad\Leftrightarrow\quad \operatorname{rank} S = \operatorname{rank} W = k \leq M = N \tag{977}$$

To see that, we need only show: $\mathcal{N}(S) = \mathbf{0} \;\Leftrightarrow\; \exists\, B \;\ni\; BS = I$.[B.4]
($\Longleftarrow$) Assume $BS = I$. Then $\mathcal{N}(BS) = \mathbf{0} = \{x \mid BSx = \mathbf{0}\} \supseteq \mathcal{N}(S)$. (958)
($\Longrightarrow$) If $\mathcal{N}(S) = \mathbf{0}$ then S must be full-rank skinny-or-square.
$\therefore\; \exists\, A, B, C \;\ni\; \begin{bmatrix} B \\ C \end{bmatrix} [\, S\;\; A\,] = I$ (*id est*, $[\, S\;\; A\,]$ is invertible) $\Rightarrow\; BS = I$.
Left inverse B is given as W^T here. Because of reciprocity with S, it immediately follows: $\mathcal{N}(W) = \mathbf{0} \;\Leftrightarrow\; \exists\, S \;\ni\; S^T W = I$. ♦

Dyads produced by diagonalization, for example, are independent because of their inherent biorthogonality. (§A.5.1) The converse is generally false; *id est*, linearly independent dyads are not necessarily biorthogonal.

B.1.1.1.1 Theorem. *Nullspace and range of dyad sum.*
Given a sum of dyads represented by SW^T where $S \in \mathbb{C}^{M\times k}$ and $W \in \mathbb{C}^{N\times k}$,

$$\begin{aligned} \mathcal{N}(SW^T) = \mathcal{N}(W^T) &\quad\Leftarrow\quad \exists\, B \;\ni\; BS = I \\ \mathcal{R}(SW^T) = \mathcal{R}(S) &\quad\Leftarrow\quad \exists\, Z \;\ni\; W^T Z = I \end{aligned} \tag{978}$$

◇

Proof. ($\Longrightarrow$) $\mathcal{N}(SW^T) \supseteq \mathcal{N}(W^T)$ and $\mathcal{R}(SW^T) \subseteq \mathcal{R}(S)$ are obvious.
($\Longleftarrow$) Assume the existence of a left inverse $B \in \mathbb{R}^{k\times N}$ and a right inverse $Z \in \mathbb{R}^{N\times k}$.[B.5]

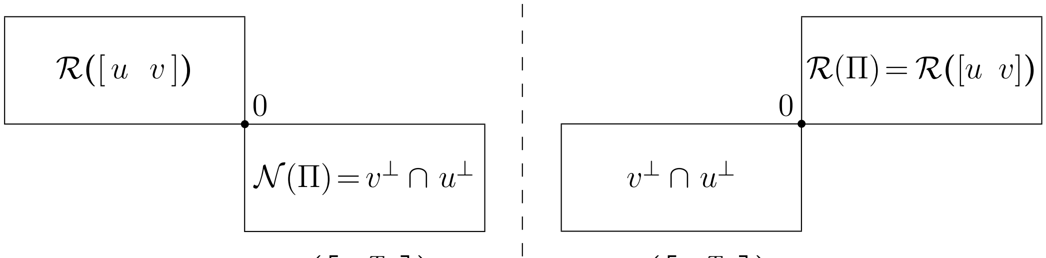
$$\mathcal{N}(SW^T) \;=\; \{x \mid SW^T x = \mathbf{0}\} \;\subseteq\; \{x \mid BSW^T x = \mathbf{0}\} \;=\; \mathcal{N}(W^T) \tag{979}$$

$$\mathcal{R}(SW^T) \;=\; \{SW^T x \mid x \in \mathbb{R}^N\} \;\supseteq\; \{SW^T Z y \mid Zy \in \mathbb{R}^N\} \;=\; \mathcal{R}(S) \tag{980}$$

♦

Under the biorthogonality condition $W^T S = I$ of diagonalization, for example, nullspace $\mathcal{N}(SW^T)$ must be equivalent to $\mathcal{N}(W^T)$ and $\mathcal{R}(SW^T) \equiv \mathcal{R}(S)$.

[B.4] Left inverse is not unique, in general.
[B.5] By counter example, the converse cannot be true; *e.g.*, $S = W = [\,\mathbf{1}\;\; \mathbf{0}\,]$.



$$\mathbb{R}^N = \mathcal{R}([u\ \ v]) \oplus \mathcal{N}\left(\begin{bmatrix} v^T \\ u^T \end{bmatrix}\right) \qquad\qquad \mathcal{N}\left(\begin{bmatrix} v^T \\ u^T \end{bmatrix}\right) \oplus \mathcal{R}([u\ \ v]) = \mathbb{R}^N$$

Figure B.2: Four fundamental subspaces [27, §3.6] of a doublet $\Pi = uv^T + vu^T \in \mathbb{S}^N$. $\Pi(x) = (uv^T + vu^T)x$ is a linear bijective mapping from $\mathcal{R}([u\ \ v])$ to $\mathcal{R}([u\ \ v])$.

B.2 Doublet

Consider a sum of two linearly independent square dyads, one a transposition of the other:

$$\Pi = uv^T + vu^T = [\,u\ \ v\,] \begin{bmatrix} v^T \\ u^T \end{bmatrix} = SW^T \in \mathbb{S}^N \tag{981}$$

where $u\,, v \in \mathbb{R}^N$. Like the dyad, a doublet can be $\mathbf{0}$ only when u or v is $\mathbf{0}$;

$$\Pi = uv^T + vu^T = \mathbf{0} \;\Leftrightarrow\; u = \mathbf{0} \;\text{ or }\; v = \mathbf{0} \tag{982}$$

By assumption of independence, a nonzero doublet has two nonzero eigenvalues

$$\lambda_1 \triangleq u^T v + \|uv^T\|\,, \qquad \lambda_2 \triangleq u^T v - \|uv^T\| \tag{983}$$

where $\lambda_1 > 0 > \lambda_2$, with corresponding eigenvectors

$$x_1 \triangleq \frac{u}{\|u\|} + \frac{v}{\|v\|}\,, \qquad x_2 \triangleq \frac{u}{\|u\|} - \frac{v}{\|v\|} \tag{984}$$

spanning the doublet range. Eigenvalue λ_1 cannot be 0 unless u and v have opposing directions, but that is antithetical since then the dyads would no longer be independent. Eigenvalue λ_2 is 0 if and only if u and v share the same direction, again antithetical. Generally we have $\lambda_1 > 0$ and $\lambda_2 < 0$, so Π is indefinite.

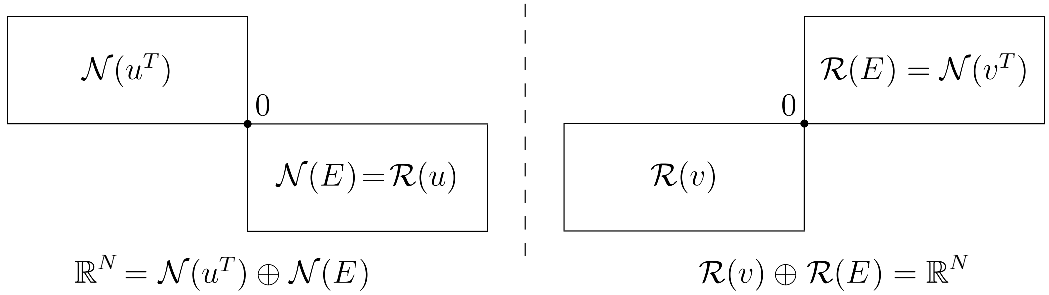


Figure B.3: $v^Tu = 1/\zeta$. The four fundamental subspaces [27, §3.6] of elementary matrix E as a linear mapping $E(x) = \left(I - \dfrac{uv^T}{v^Tu}\right)x$.

By the *nullspace and range of dyad sum theorem*, doublet Π has $N-2$ 0-eigenvalues remaining and corresponding eigenvectors spanning $\mathcal{N}\left(\begin{bmatrix} v^T \\ u^T \end{bmatrix}\right)$. We therefore have

$$\mathcal{R}(\Pi) = \mathcal{R}([\,u \;\; v\,])\,, \qquad \mathcal{N}(\Pi) = v^\perp \cap u^\perp \tag{985}$$

of respective dimension 2 and $N-2$.

B.3 Elementary matrix

A matrix of the form

$$E = I - \zeta uv^T \in \mathbb{R}^{N\times N} \tag{986}$$

where $\zeta \in \mathbb{R}$ is finite and $u,v \in \mathbb{R}^N$, is called an *elementary matrix* or a *rank-one modification of the identity.* [155] Any elementary matrix in $\mathbb{R}^{N\times N}$ has $N-1$ eigenvalues equal to 1 corresponding to real eigenvectors that span $v^\perp$. The remaining eigenvalue

$$\lambda = 1 - \zeta v^Tu \tag{987}$$

corresponds to eigenvector u .[B.6] From [152, App.7.A.26] the determinant:

$$\det E \;=\; 1 - \operatorname{tr}\big(\zeta uv^T\big) \;=\; \lambda \tag{988}$$

[B.6] Elementary matrix E is not always diagonalizable because eigenvector u need not be independent of the others; *id est*, $u \in v^\perp$ is possible.

If $\lambda \neq 0$ then E is invertible; [148]

$$E^{-1} = I + \frac{\zeta}{\lambda} u v^T \tag{989}$$

Eigenvectors corresponding to 0 eigenvalues belong to $\mathcal{N}(E)$, and the number of 0 eigenvalues must be at least $\dim \mathcal{N}(E)$ that, here, can be at most one. (§A.7.2.0.1) The nullspace exists, therefore, when $\lambda = 0$; *id est*, when $v^T u = 1/\zeta$, rather, whenever u belongs to the hyperplane $\{z \in \mathbb{R}^N \mid v^T z = 1/\zeta\}$. Then (when $\lambda = 0$) elementary matrix E is a nonorthogonal projector on its range ($E^2 = E$, §E.1) and $\mathcal{N}(E) = \mathcal{R}(u)$; eigenvector u spans the nullspace when it exists. By conservation of dimension, $\dim \mathcal{R}(E) = N - \dim \mathcal{N}(E)$. It is apparent from (986) that $v^\perp \subseteq \mathcal{R}(E)$, but $\dim v^\perp = N - 1$. Hence $\mathcal{R}(E) \equiv v^\perp$ when the nullspace exists, and the remaining eigenvectors span it.

In summary, when a nontrivial nullspace of E exists,

$$\mathcal{R}(E) = \mathcal{N}(v^T), \qquad \mathcal{N}(E) = \mathcal{R}(u), \qquad v^T u = 1/\zeta \tag{990}$$

illustrated in Figure **B.3**, which is opposite to the assignment of subspaces for a dyad (Figure **B.1**). Otherwise, $\mathcal{R}(E) = \mathbb{R}^N$.

When $E = E^T$, the spectral norm is

$$\|E\|_2 = \max\{1\,, |\lambda|\} \tag{991}$$

B.3.1 Householder matrix

An elementary matrix E is called a Householder matrix H when, for nonzero vector u, E has the defining form [44, §5.1.2] [148, §4.10.1] [26, §7.3] [28, §2.2]

$$H = I - 2\frac{uu^T}{u^T u} \in \mathbb{S}^N \tag{992}$$

which is a symmetric orthogonal (reflection) matrix $(H^{-1} = H^T = H$ (§B.5)$)$. Vector u is normal to an $N-1$-dimensional subspace $u^\perp$ through which this particular H effects point-wise reflection; *e.g.*, $Hu^\perp = u^\perp$ while $Hu = -u$.

Matrix H has $N-1$ orthonormal eigenvectors spanning that reflecting subspace $u^\perp$, with corresponding eigenvalues equal to 1. The remaining eigenvector u has corresponding eigenvalue -1. Due to symmetry of H, the matrix 2-norm (the spectral norm) is equal to the largest eigenvalue-magnitude. A Householder matrix is thus characterized,

$$H^T = H\,, \qquad H^{-1} = H^T\,, \qquad \|H\|_2 = 1\,, \qquad H \nsucceq 0 \tag{993}$$

For example, the permutation matrix

$$\Xi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{994}$$

is a Householder matrix having $u = [\,0 \quad 1 \quad -1\,]^T/\sqrt{2}$. Not all permutation matrices are Householder matrices, although all permutation matrices are orthogonal matrices. [26, §3.4] Neither are all symmetric permutation matrices Householder matrices; *e.g.*,

$$\Xi = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \tag{995}$$

is not a Householder matrix.

B.4 Auxiliary V-matrices

B.4.1 Auxiliary matrix V

It is convenient to define a matrix V that arises naturally as a consequence of translating the geometric center α_g (§4.5.1.0.1) of some list X to the origin. In place of $X - \alpha_g \mathbf{1}^T$ we may write XV as in (391) where

$$V \;\triangleq\; I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^N \tag{996}$$

is an elementary matrix called the *geometric centering matrix.*

Any elementary matrix in $\mathbb{R}^{N\times N}$ has $N-1$ eigenvalues equal to 1. For the particular elementary matrix V , the N^{th} eigenvalue equals 0. The number of 0 eigenvalues must equal $\dim\mathcal{N}(V)=1$, by the 0 *eigenvalues theorem* (§A.7.2.0.1), because $V=V^T$ is diagonalizable. Because

$$V\mathbf{1} = \mathbf{0} \tag{997}$$

the nullspace $\mathcal{N}(V)=\mathcal{R}(\mathbf{1})$ is spanned by the eigenvector $\mathbf{1}$. The remaining eigenvectors span $\mathcal{R}(V) \equiv \mathbf{1}^{\perp} = \mathcal{N}(\mathbf{1}^T)$.

Because

$$V^2 = V \tag{998}$$

and $V^T = V$, the elementary matrix V is also a projection matrix (§E.3) projecting orthogonally on its range $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$ that has dimension $N-1$.

$$V = I - \mathbf{1}(\mathbf{1}^T\mathbf{1})^{-1}\mathbf{1}^T \tag{999}$$

The $\{0,1\}$ eigenvalues also indicate that diagonalizable V is a projection matrix. [45, §4.1, thm.4.1] The symmetry of V denotes orthogonal projection; [48] hence, (1207)

$$V^T = V\,, \qquad V^{\dagger} = V\,, \qquad \|V\|_2 = 1\,, \qquad V \succeq 0 \tag{1000}$$

Matrix V is also circulant. (§B.6) [81] Circulant matrices form a subspace, symmetric circulant matrices form another. Yet the set of all (symmetric) *circulant projection matrices* cannot be convex because the eigenvalues of some convex combination of such matrices will not remain 0 or 1.

- Let $H \in \mathbb{S}^N$ be a Householder matrix (992) defined by

$$u = \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 1+\sqrt{N} \end{bmatrix} \in \mathbb{R}^N \tag{1001}$$

Then we have [136, §2]

$$V = H \begin{bmatrix} I & \mathbf{0} \\ \mathbf{0}^T & 0 \end{bmatrix} H \tag{1002}$$

Let $D \in \mathbb{S}^N_{\mathbf{0}}$ and define

$$-HDH \triangleq -\begin{bmatrix} A & b \\ b^T & c \end{bmatrix} \tag{1003}$$

where b is a vector. Then because H is nonsingular (§A.3.1.0.5) [97, §3]

$$-VDV = -H \begin{bmatrix} A & \mathbf{0} \\ \mathbf{0}^T & 0 \end{bmatrix} H \succeq 0 \;\Leftrightarrow\; -A \succeq 0 \tag{1004}$$

and affine dimension is $r = \operatorname{rank} A$ when D is an EDM.

B.4.2 Schoenberg auxiliary matrix $V_{\mathcal{N}}$

1. $V_{\mathcal{N}} = \frac{1}{\sqrt{2}}\begin{bmatrix} -\mathbf{1}^T \\ I \end{bmatrix} \in \mathbb{R}^{N\times N-1}$

2. $V_{\mathcal{N}}^T\mathbf{1} = \mathbf{0}$

3. $I - e_1\mathbf{1}^T = \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix}$

4. $\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} V_{\mathcal{N}} = V_{\mathcal{N}}$

5. $\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix}\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix}$

6. $V_{\mathcal{N}}^\dagger = \sqrt{2}\left[-\frac{1}{N}\mathbf{1} \quad I - \frac{1}{N}\mathbf{1}\mathbf{1}^T\right] \in \mathbb{R}^{N-1\times N}, \qquad \left(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^{N-1}\right)$

7. $V_{\mathcal{N}}^\dagger\mathbf{1} = \mathbf{0}$

8. $V_{\mathcal{N}}^\dagger V_{\mathcal{N}} = I$

9. $\left[\, V_{\mathcal{N}} \quad \frac{1}{\sqrt{2}}\mathbf{1}\,\right]^{-1} = \begin{bmatrix} V_{\mathcal{N}}^\dagger \\ \frac{\sqrt{2}}{N}\mathbf{1}^T \end{bmatrix}$

10. $V^T = V = V_{\mathcal{N}}V_{\mathcal{N}}^\dagger = I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^N$

11. $D = [d_{ij}] \in \mathbb{S}_{\mathbf{0}}^N$

    $\operatorname{tr}(-VDV) = \operatorname{tr}(-VD) = \operatorname{tr}(-V_{\mathcal{N}}^\dagger DV_{\mathcal{N}}) = \frac{1}{N}\mathbf{1}^T D\,\mathbf{1} = \frac{1}{N}\operatorname{tr}(\mathbf{1}\mathbf{1}^T D) = \frac{1}{N}\sum_{i,j} d_{ij}$

    Any elementary matrix $E \in \mathbb{S}^N$ of the particular form

    $$E = k_1 I - k_2\,\mathbf{1}\mathbf{1}^T \tag{1005}$$

    where $k_1, k_2 \in \mathbb{R}$,[B.7] will make $\operatorname{tr}(-ED)$ proportional to $\sum d_{ij}$.

12. $D = [d_{ij}] \in \mathbb{S}^N$

    $\operatorname{tr}(-VDV) = \frac{1}{N}\sum_{\substack{i,j\\ i\neq j}} d_{ij} - \frac{N-1}{N}\sum_i d_{ii}$

[B.7] If k_1 is $1-\rho$ while k_2 equals $-\rho \in \mathbb{R}$, then, for $-1/(N-1) < \rho < 1$, all the eigenvalues of E are guaranteed positive and therefore E is guaranteed positive definite. [156]

13. $D = [d_{ij}] \in \mathbb{S}_{\mathbf{0}}^N$
$\operatorname{tr}(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \sum\limits_j d_{\mathbf{1}j}$

B.4.3 Auxiliary matrix $V_{\mathcal{W}}$

The skinny matrix

$$V_{\mathcal{W}} \triangleq \begin{bmatrix} \frac{-1}{\sqrt{N}} & \frac{-1}{\sqrt{N}} & \cdots & \frac{-1}{\sqrt{N}} \\ 1+\frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & \frac{-1}{N+\sqrt{N}} \\ \frac{-1}{N+\sqrt{N}} & \ddots & \ddots & \frac{-1}{N+\sqrt{N}} \\ \vdots & \ddots & \ddots & \vdots \\ \frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & 1+\frac{-1}{N+\sqrt{N}} \end{bmatrix} \in \mathbb{R}^{N\times N-1} \tag{1006}$$

has $\mathcal{R}(V_{\mathcal{W}}) = \mathcal{N}(\mathbf{1}^T)$ and orthonormal columns. [94] We defined three auxiliary V-matrices: V, $V_{\mathcal{N}}$ (339), and $V_{\mathcal{W}}$ sharing some attributes listed in Table **B.4.4**. For example, V can be expressed

$$V = V_{\mathcal{W}} V_{\mathcal{W}}^T = V_{\mathcal{N}} V_{\mathcal{N}}^\dagger \tag{1007}$$

but $V_{\mathcal{W}}^T V_{\mathcal{W}} = I$ means V is an orthogonal projector (1204) and

$$V_{\mathcal{W}}^\dagger = V_{\mathcal{W}}^T\,, \qquad \|V_{\mathcal{W}}\|_2 = 1\,, \qquad V_{\mathcal{W}}^T \mathbf{1} = \mathbf{0} \tag{1008}$$

B.4.4 Auxiliary V-matrix Table

	$\dim V$	$\operatorname{rank} V$	$\mathcal{R}(V)$	$\mathcal{N}(V^T)$	$V^T V$	$V V^T$	$V V^\dagger$
V	$N\times N$	$N-1$	$\mathcal{N}(\mathbf{1}^T)$	$\mathcal{R}(\mathbf{1})$	V	V	V
$V_{\mathcal{N}}$	$N\times(N-1)$	$N-1$	$\mathcal{N}(\mathbf{1}^T)$	$\mathcal{R}(\mathbf{1})$	$\frac{1}{2}(I+\mathbf{1}\mathbf{1}^T)$	$\frac{1}{2}\begin{bmatrix} N-1 & -\mathbf{1}^T \\ -\mathbf{1} & I \end{bmatrix}$	V
$V_{\mathcal{W}}$	$N\times(N-1)$	$N-1$	$\mathcal{N}(\mathbf{1}^T)$	$\mathcal{R}(\mathbf{1})$	I	V	V

B.4.5 More auxiliary matrices

Mathar shows [115, §2] that any elementary matrix (§B.3) of the form

$$V_{\mathcal{M}} = I - b\,\mathbf{1}^T \in \mathbb{R}^{N\times N} \tag{1009}$$

such that $b^T\mathbf{1} = 1$ (*confer* [84, §2]), is an auxiliary V-matrix having

$$\begin{array}{ll} \mathcal{R}(V_{\mathcal{M}}^T) = \mathcal{N}(b^T)\,, & \mathcal{R}(V_{\mathcal{M}}) = \mathcal{N}(\mathbf{1}^T) \\ \mathcal{N}(V_{\mathcal{M}}) = \mathcal{R}(b)\,, & \mathcal{N}(V_{\mathcal{M}}^T) = \mathcal{R}(\mathbf{1}) \end{array} \tag{1010}$$

Given $X \in \mathbb{R}^{n\times N}$, the choice $b = \frac{1}{N}\mathbf{1}$ minimizes $\|X(I - b\,\mathbf{1}^T)\|_{\mathrm{F}}$. [157, §3.2.1]

B.5 Orthogonal matrix

The property $Q^{-1} = Q^T$ completely defines an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ employed to effect vector rotation; [26, §2.6, §3.4] [27, §6.5] [28, §2.1] for $x \in \mathbb{R}^n$,

$$\|Qx\| = \|x\| \tag{1011}$$

The orthogonal matrix is characterized:

$$Q^{-1} = Q^T\,, \qquad \|Q\|_2 = 1 \tag{1012}$$

Applying characterization (1012) to Q^T we see it too is an orthogonal matrix. Hence the rows and columns of Q respectively form an orthonormal set.

All permutation matrices Ξ, for example, are orthogonal matrices. The largest magnitude entry of any orthogonal matrix is 1; for each and every $j \in 1 \ldots n$,

$$\begin{array}{l} \|Q(j\,,:)\|_\infty \leq 1 \\ \|Q(:\,,j)\|_\infty \leq 1 \end{array} \tag{1013}$$

Each and every eigenvalue of an orthogonal matrix has magnitude 1,

$$\lambda(Q) \in \mathbb{C}^n\,, \qquad |\lambda(Q)| = \mathbf{1} \tag{1014}$$

while only the identity matrix can be simultaneously positive definite and orthogonal.

A *unitary matrix* is a complex generalization of the orthogonal matrix. The conjugate transpose defines it: $U^{-1} = U^H$. An orthogonal matrix is simply a real unitary matrix.

B.5.1 Reflection

A matrix for point-wise reflection is defined by imposing symmetry upon the orthogonal matrix; *id est*, a reflection matrix is completely defined by $Q^{-1} = Q^T = Q$. The reflection matrix is an orthogonal matrix, characterized:

$$Q^T = Q\,, \qquad Q^{-1} = Q^T\,, \qquad \|Q\|_2 = 1 \tag{1015}$$

The Householder matrix (§B.3.1) is an example of a symmetric orthogonal (reflection) matrix.

Reflection matrices have eigenvalues equal to ± 1, so it is natural to expect a relationship between reflection and projection matrices because all projection matrices have eigenvalues belonging to $\{0, 1\}$. In fact, any reflection matrix Q is related to some orthogonal projector P by [155, §1, prob.44]

$$Q = I - 2P \tag{1016}$$

Yet P is, generally, neither orthogonal or invertible (1207).

$$\lambda(Q) \in \mathbb{R}^n\,, \qquad |\lambda(Q)| = \mathbf{1} \tag{1017}$$

Reflection is with respect to $\mathcal{R}(P)^{\perp}$. Matrix $2P-I$ represents antireflection.

Every orthogonal matrix can be expressed as the product of a rotation and a reflection. The collection of all orthogonal matrices of particular dimension does not form a convex set.

B.5.2 Matrix rotation

Orthogonal matrices are also employed to rotate or reflect other matrices: [*sic*] [44, §12.4.1] Given orthogonal matrix Q, the product $Q^T A$ will rotate $A \in \mathbb{R}^{n\times n}$ in the vectorization sense in $\mathbb{R}^{n^2}$ because the Frobenius norm is orthogonally invariant (§2.1.1.1);

$$\|Q^T A\|_{\mathrm{F}} = \sqrt{\operatorname{tr}(A^T Q Q^T A)} = \|A\|_{\mathrm{F}} \tag{1018}$$

(likewise for AQ). Were A symmetric, such a rotation would depart from $\mathbb{S}^n$. One remedy is to instead form the product $Q^T A Q$ because

$$\|Q^T A Q\|_{\mathrm{F}} = \sqrt{\operatorname{tr}(Q^T A^T Q Q^T A Q)} = \|A\|_{\mathrm{F}} \tag{1019}$$

This rotation of A in the vectorization sense has an added benefit: the simultaneous rotation/reflection of range and rowspace.[B.8] We see that by recalling, any matrix can be expressed in terms of its singular value decomposition $A = U\Sigma W^T$ (922) where $\delta^2(\Sigma) = \Sigma$, $\mathcal{R}(U) \supseteq \mathcal{R}(A)$, and $\mathcal{R}(W) \supseteq \mathcal{R}(A^T)$.

B.5.2.1 bijection

Any product of orthogonal matrices remains orthogonal. Given a second orthogonal matrix U, the mapping $g(A) = U^T A Q$ is a linear bijection on the domain of orthogonal matrices. [52, §2.1]

B.6 Circulant matrices...

Define circulant and symmetric circulant matrices. Eigenvectors always same. Means *image theorem* may be applied because set of all circulant matrices makes a subspace. Idea is: Interpolating between any two circulant matrices would interpolate the known eigenvalues.

From the *image theorem* in §2.1.0.10.2, it follows that $\langle E_{ij}\,, \mathcal{C}\rangle$ in (1273) is a convex set whenever $\mathcal{C}$ is. The set of all circulant matrices forms a subspace in $\mathbb{R}^{M\times M}$ whose members all have the same eigenvectors; the orthogonal basis from the discrete Fourier transform. So each eigenvalue (1277) of a circulant matrix comes from a convex set of eigenvalues by the image theorem.

Apply this to the previous DFT by making a circulant matrix C from input f.
Justify use of circulant input using applications from DSP.
Because circulant matrices are diagonalizable [81], any circulant matrix C may be represented,

$$C = \frac{1}{n} W \Lambda W^H \tag{1020}$$

where $\Lambda = \delta(W^H f)$.
which is in the final form of (1276),...show this.

[B.8] The product $Q^T A Q$ can be regarded as a coordinate transformation; *e.g.*, given linear map $y = Ax : \mathbb{R}^n \to \mathbb{R}^n$, for orthogonal Q the transformation $Qy = AQx$ is a rotation of the range and rowspace (90) (89) of matrix A.

The set of all circulant matrices forms a subspace. Hence it must follow that any linear combination of circulant matrices remains circulant; for all $\mu, \zeta \in \mathbb{R}$,

$$\mu C_1 + \zeta C_2 = \frac{1}{n} W(\mu\Lambda_1 + \zeta\Lambda_2)W^H \tag{1021}$$

is circulant. We know that each eigenvalue comes from a convex set. The relation (1021) indicates that each convex set of eigenvalues is itself a subspace. The same comments apply to the subspace of symmetric circulant matrices.

Positive definite circulant matrices form a polyhedral (Gallego Circulant.ps paper) cone in the subspace of circulant matrices. -[oldReader,p.35C]

Circulant.ps... set of circulant EDMs is a polyhedral cone.

For C circulant, where the first row is some time sequence $[c_0\,, c_1\,, c_2 \ldots]$, let $X = C^T$. Then (333)

$$\mathbf{D}(C^T) \;=\; k_i\, \mathbf{1}\mathbf{1}^T -\, 2\, CC^T \tag{1022}$$

where $k_i = 2\delta(CC^T)_i$ is any one of the diagonal entries, all identical for circulant matrices. This is classical relationship between autocorrelation and similarity function where CC^T takes on the role of autocorrelation.

Appendix C

Some optimal analytical results

C.1 involving diagonal, trace, eigenvalues

- For $A \in \mathbb{R}^{m\times n}$ and $\sigma(A)$ denoting its singular values, [1, §A.1.6] [133, §1]

$$\sum_i \sigma(A)_i \;=\; \operatorname{tr}\sqrt{A^TA} = \sup_{\|X\|_2\leq 1} \operatorname{tr}(X^TA) \;=\; \begin{array}{ll} \underset{X\in\mathbb{R}^{m\times n}}{\text{maximize}} & \operatorname{tr}(X^TA) \\ \text{subject to} & \begin{bmatrix} I & X \\ X^T & I \end{bmatrix} \succeq 0 \end{array} \tag{1023}$$

- For $X\in\mathbb{S}^m$, $Y\in\mathbb{S}^n$, $A\in\mathcal{C}\subseteq\mathbb{R}^{m\times n}$ for $\mathcal{C}$ convex and $\sigma(A)$ denoting the singular values of A, [133, §3]

$$\begin{array}{ll} \underset{A\in\mathbb{R}^{m\times n}}{\text{minimize}} & \sum\limits_i \sigma(A)_i \\ & A\in\mathcal{C} \end{array} \quad\equiv\quad \begin{array}{ll} \underset{A,\,X,\,Y}{\text{minimize}} & \operatorname{tr}X + \operatorname{tr}Y \\ \text{subject to} & \begin{bmatrix} X & A \\ A^T & Y \end{bmatrix} \succeq 0 \\ & A\in\mathcal{C} \end{array} \tag{1024}$$

- For $A\in\mathbb{S}_+^N$ and $\beta\in\mathbb{R}$,

$$\beta\operatorname{tr}A \;=\; \begin{array}{ll} \underset{X\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}(XA) \\ \text{subject to} & X\preceq\beta I \end{array} \tag{1025}$$

- For $A \in \mathbb{S}^N$ having eigenvalues $\lambda(A) \in \mathbb{R}^N$, [52, §2.1] [158, §I.6.15]

$$\min\{\lambda(A)_i\} = \inf_{\|x\|=1} x^T A x = \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{minimize}} & \operatorname{tr}(XA)\\ \text{subject to} & \operatorname{tr} X = 1\end{array} = \begin{array}{ll}\underset{t\in\mathbb{R}}{\text{maximize}} & t\\ \text{subject to} & A \succeq t\,I\end{array} \tag{1026}$$

$$\max\{\lambda(A)_i\} = \sup_{\|x\|=1} x^T A x = \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{maximize}} & \operatorname{tr}(XA)\\ \text{subject to} & \operatorname{tr} X = 1\end{array} = \begin{array}{ll}\underset{t\in\mathbb{R}}{\text{minimize}} & t\\ \text{subject to} & A \preceq t\,I\end{array} \tag{1027}$$

  The minimum eigenvalue of any symmetric matrix is always a concave function of its entries, while the maximum eigenvalue is always convex. [1, exmp.3.10]

- For $B \in \mathbb{S}^N$ whose eigenvalues $\lambda(B) \in \mathbb{R}^N$ are arranged in nonincreasing order, and for $1 \le k \le N$, [24] [28, §4.3.18] [69, §2] [52, §2.1] (Fan)

$$\begin{aligned}
\sum_{i=N-k+1}^{N} \lambda(B)_i &= \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(U^TBU) = \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{minimize}} & \operatorname{tr}(XB)\\ \text{subject to} & X \preceq I\\ & \operatorname{tr} X = k\end{array} && \text{(a)}\\
\sum_{i=1}^{k} \lambda(B)_i &= \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(U^TBU) = \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{maximize}} & \operatorname{tr}(XB)\\ \text{subject to} & X \preceq I\\ & \operatorname{tr} X = k\end{array} && \text{(b)}\\
&= \begin{array}{ll}\underset{\mu\in\mathbb{R}\,,\,Z\in\mathbb{S}_+^N}{\text{minimize}} & k\mu + \operatorname{tr} Z\\ \text{subject to} & \mu I + Z \succeq B\end{array} && \text{(c)}
\end{aligned} \tag{1028}$$

  Optimal U are respectively $U^\star = W(:\,, N-k+1 : N) \in \mathbb{R}^{N\times k}$ and $U^\star = W(:\,, 1\!:\!k) \in \mathbb{R}^{N\times k}$ where $B = W\Lambda W^T$ is an ordered diagonalization.

- For $B \in \mathbb{S}^N$ whose eigenvalues $\lambda(B) \in \mathbb{R}^N$ are arranged in nonincreasing order, let $\Xi\,\lambda(B)$ be a permutation of $\lambda(B)$ such that $|\Xi\,\lambda(B)|_{\mathbf{1}} \ge |\Xi\,\lambda(B)|_{\mathbf{2}} \ge \cdots \ge |\Xi\,\lambda(B)|_N$. Then, for $1 \le k \le N$,

[51, §6]

$$\sum_{i=1}^{k} |\Xi\,\lambda(B)|_i \;=\; \begin{array}{cl}\underset{z\in\mathbb{R}\,,\,V,W,S,T\in\mathbb{S}_+^N}{\text{minimize}} & kz+\operatorname{tr}(V+W)\\ \text{subject to} & zI+V-W=B\\ & zI+S-T=-B\end{array} \;=\; \begin{array}{cl}\underset{X,Y\in\mathbb{S}_+^N}{\text{maximize}} & \langle B\,,\,X-Y\rangle\\ \text{subject to} & I\succeq X,Y\\ & \operatorname{tr}(X+Y)=k\end{array} \tag{1029}$$

- For $A\,,B\in\mathbb{S}^N$ whose eigenvalues $\lambda(A)\,,\lambda(B)\in\mathbb{R}^N$ are respectively arranged in nonincreasing order, and for non-increasingly ordered diagonalizations $B=W_B\Lambda W_B^T$ and $A=W_A\Upsilon W_A^T$, [159] [52, §2.1]

$$\lambda(A)^T\lambda(B) \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times N}\\ U^TU=I}} \operatorname{tr}(A^TU^TBU) \;\geq\; \operatorname{tr}(A^TB) \tag{1030}$$

(*confer* (1050)) where optimal U is

$$U^\star = W_BW_A^T\in\mathbb{R}^{N\times N} \tag{1031}$$

We push that bound a little higher using a result in §C.2.1.2.1:

$$|\lambda(A)|^T|\lambda(B)| \;=\; \sup_{\substack{U\in\mathbb{C}^{N\times N}\\ U^TU=I}} \operatorname{tr}(A^TU^TBU) \tag{1032}$$

where U^T denotes ordinary transposition (1066). Optimal U becomes

$$U^\star = W_B\sqrt{\delta(\psi(\delta(\Lambda)))}^H\sqrt{\delta(\psi(\delta(\Upsilon)))}\,W_A^T\in\mathbb{C}^{N\times N} \tag{1033}$$

where the step function ψ is defined in (933).

- For $B\in\mathbb{S}^N$ whose eigenvalues $\lambda(B)\in\mathbb{R}^N$ are arranged in nonincreasing order, and for diagonal matrix $\Upsilon\in\mathbb{S}^k$ whose diagonal entries are arranged in nonincreasing order where $1\leq k\leq N$, we utilize the main-diagonal δ operator's property of self-adjointness (813); [160, §4.2]

$$\sum_{i=1}^{k}\Upsilon_{ii}\,\lambda(B)_{N-i+1} \;=\; \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(\Upsilon\,U^TBU) \;=\; \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \delta(\Upsilon)^T\delta(U^TBU) \tag{1034}$$

We speculate,

$$\sum_{i=1}^{k} \Upsilon_{ii}\,\lambda(B)_i \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(\Upsilon\, U^TBU) \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \delta(\Upsilon)^T\delta(U^TBU) \tag{1035}$$

C.2 Orthogonal Procrustes problem

[157] Given matrices $A\,, B\in\mathbb{R}^{n\times N}$, their product having full singular value decomposition (§A.6.3)

$$AB^T \triangleq U\Sigma Q^T \in \mathbb{R}^{n\times n} \tag{1036}$$

then an optimal solution $R^\star$ to the orthogonal Procrustes problem

$$\begin{array}{cl} \underset{R}{\text{minimize}} & \|A - R^TB\|_{\mathrm{F}}^2 \\ \text{subject to} & R^T = R^{-1} \end{array} \tag{1037}$$

maximizes $\operatorname{tr}(A^TR^TB)$ over the non-convex manifold of orthogonal matrices: [28, §7.4.8]

$$R^\star = QU^T \in \mathbb{R}^{n\times n} \tag{1038}$$

The optimal value of the objective is therefore,

$$\begin{aligned} \operatorname{tr}\big(A^TA + B^TB - 2A(B^TR^\star)\big) \;&=\; \operatorname{tr}(A^TA) + \operatorname{tr}(B^TB) - 2\operatorname{tr}(U\Sigma U^T) \\ &=\; \|A\|_{\mathrm{F}}^2 + \|B\|_{\mathrm{F}}^2 - 2\delta(\Sigma)^T\mathbf{1} \end{aligned} \tag{1039}$$

and

$$\sup_{R^T=R^{-1}} \operatorname{tr}(A^TR^TB) \;=\; \operatorname{tr}(A^TR^{\star T}B) \;=\; \delta(\Sigma)^T\mathbf{1} \;\geq\; \operatorname{tr}(A^TB) \tag{1040}$$

This optimization problem is useful for discovering the rotation/reflection of one list A with respect to another list B. (§4.5) The solution is unique if $\operatorname{rank} BV_{\mathcal{N}} = n$. [50, §2.4.1]

C.2.1 Two-sided orthogonal Procrustes problems

Given symmetric $A\,,B\in\mathbb{S}^N$, each having diagonalization

$$A \triangleq Q_A\Lambda_A Q_A^T\;, \qquad B \triangleq Q_B\Lambda_B Q_B^T \tag{1041}$$

where eigenvalues are arranged in their respective diagonal matrix Λ in nonincreasing order, then an optimal solution to the two-sided orthogonal Procrustes problem

$$\begin{array}{cl}\underset{R}{\text{minimize}} & \|A-R^TBR\|_{\mathrm F}\\ \text{subject to} & R^T=R^{-1}\end{array} \;=\; \begin{array}{cl}\underset{R}{\text{minimize}} & \operatorname{tr}\big(A^TA-2A^TR^TBR+B^TB\big)\\ \text{subject to} & R^T=R^{-1}\end{array} \tag{1042}$$

maximizes $\operatorname{tr}(A^TR^TBR)$ over the non-convex manifold of orthogonal matrices: [161]

$$R^\star = Q_B Q_A^T \in \mathbb{R}^{N\times N} \tag{1043}$$

which is an optimal orthogonal matrix. The optimal value of the objective is therefore, (28)

$$\|Q_A\Lambda_A Q_A^T - R^{\star T}Q_B\Lambda_B Q_B^T R^\star\|_{\mathrm F} \;=\; \|Q_A(\Lambda_A-\Lambda_B)Q_A^T\|_{\mathrm F} \;=\; \|\Lambda_A-\Lambda_B\|_{\mathrm F} \tag{1044}$$

and

$$\sup_{R^T=R^{-1}} \operatorname{tr}(A^TR^TBR) \;=\; \operatorname{tr}(A^TR^{\star T}BR^\star) \;=\; \operatorname{tr}(\Lambda_A\Lambda_B) \;\geq\; \operatorname{tr}(A^TB) \tag{1045}$$

Any permutation matrix is an orthogonal matrix. Defining a row and column swapping permutation matrix (B.5.1)

$$\Xi \;=\; \Xi^T \;=\; \begin{bmatrix} \mathbf{0} & & & & 1\\ & & & \cdot & \\ & & \cdot & & \\ & 1 & & & \\ 1 & & & & \mathbf{0}\end{bmatrix} \tag{1046}$$

then an optimal solution to the maximization problem

$$\begin{array}{cl}\underset{R}{\text{maximize}} & \|A-R^TBR\|_{\mathrm F}\\ \text{subject to} & R^T=R^{-1}\end{array} \tag{1047}$$

minimizes $\operatorname{tr}(A^T R^T B R)$: [159] [52, §2.1]

$$R^\star = Q_B \Xi Q_A^T \in \mathbb{R}^{N\times N} \tag{1048}$$

The optimal value of the objective is therefore,

$$\begin{aligned}\|Q_A\Lambda_A Q_A^T - R^{\star T} Q_B \Lambda_B Q_B^T R^\star\|_{\mathrm F} &= \|Q_A\Lambda_A Q_A^T - Q_A \Xi^T \Lambda_B \Xi Q_A^T\|_{\mathrm F} \\ &= \|\Lambda_A - \Xi\Lambda_B\Xi\|_{\mathrm F}\end{aligned} \tag{1049}$$

and

$$\inf_{R^T=R^{-1}} \operatorname{tr}(A^T R^T B R) \;=\; \operatorname{tr}(A^T R^{\star T} B R^\star) \;=\; \operatorname{tr}(\Lambda_A \Xi \Lambda_B \Xi) \tag{1050}$$

C.2.1.1 Procrustes' relation to linear programming

While these two-sided Procrustes problems are non-convex, a connection with *linear programming* was recently found by Anstreicher & Wolkowicz: given $A\,, B \in \mathbb{S}^N$, [160, §3] [52, §2.1]

$$\begin{array}{llcll}\underset{R}{\text{minimize}} & \operatorname{tr}(A^T R^T B R) & = & \underset{S,T\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}(S+T) \\ \text{subject to} & R^T = R^{-1} & & \text{subject to} & A^T\otimes B - I\otimes S - T\otimes I \succeq 0\end{array} \tag{1051}$$

where $\otimes$ signifies the Kronecker product (§D.1.2.1), has solution (1050). These two problems are strong duals (§2.8.1) to each other. Given ordered diagonalizations (1041), make the observation:

$$\inf_R \operatorname{tr}(A^T R^T B R) = \inf_{\hat R} \operatorname{tr}(\Lambda_A \hat R^T \Lambda_B \hat R) \tag{1052}$$

since $\hat R = Q_B^T R Q_A$ is a bijection on the set of orthogonal matrices (which includes the permutation matrices). This means, basically, diagonal eigenvalue matrices Λ_A and Λ_B may be substituted for A and B , so only the main diagonals of S and T come into play;

$$\begin{array}{ll}\underset{S,T\in\mathbb{S}^N}{\text{maximize}} & \mathbf{1}^T\delta(S+T) \\ \text{subject to} & \delta\big(\Lambda_A\otimes(\Xi\Lambda_B\Xi) - I\otimes S - T\otimes I\big) \succeq 0\end{array} \tag{1053}$$

a linear program in $\delta(S)$ and $\delta(T)$ having the same optimal objective value as the semidefinite program.

We relate their results to the Procrustes problem (1042) by manipulating signs (1166) and permuting eigenvalues:

$$\begin{array}{llcll}\underset{R}{\text{maximize}} & \operatorname{tr}(A^TR^TBR) & = & \underset{S,T\in\mathbb{S}^N}{\text{minimize}} & \mathbf{1}^T\delta(S+T)\\ \text{subject to} & R^T=R^{-1} & & \text{subject to} & \delta\big(I\otimes S+T\otimes I-\Lambda_A\otimes\Lambda_B\big)\succeq 0\\ & & = & \underset{S,T\in\mathbb{S}^N}{\text{minimize}} & \operatorname{tr}(S+T)\\ & & & \text{subject to} & I\otimes S+T\otimes I-A^T\otimes B\succeq 0\end{array} \tag{1054}$$

whose solution is (1045).

C.2.1.2 Asymmetric two-sided orthogonal Procrustes

By making the left and right-side orthogonal matrices independent, we can push the upper bound on the optimal trace a little further: Given arbitrary $A\,,B$ each having full singular value decomposition (§A.6.3)

$$A\triangleq U_A\Sigma_A Q_A^T\in\mathbb{R}^{m\times n}\;,\qquad B\triangleq U_B\Sigma_B Q_B^T\in\mathbb{R}^{m\times n} \tag{1055}$$

then the well-known optimal solution to the problem

$$\begin{array}{ll}\underset{R,S}{\text{minimize}} & \|A-SBR\|_{\mathrm F}\\ \text{subject to} & R^H=R^{-1}\\ & S^H=S^{-1}\end{array} \tag{1056}$$

maximizes $\operatorname{Re}\operatorname{tr}(A^TSBR)$: [162] [163] [164] [165]

$$S^\star=U_AU_B^H\in\mathbb{C}^{m\times m}\;,\qquad R^\star=Q_BQ_A^H\in\mathbb{C}^{n\times n} \tag{1057}$$

are optimal unitary matrices (§B.5) which are not necessarily unique [28, §7.4.13] because the feasible set is not convex. The optimal value of the objective is therefore, (28)

$$\|U_A\Sigma_AQ_A^H-S^\star U_B\Sigma_BQ_B^HR^\star\|_{\mathrm F}\;=\;\|U_A(\Sigma_A-\Sigma_B)Q_A^H\|_{\mathrm F}\;=\;\|\Sigma_A-\Sigma_B\|_{\mathrm F} \tag{1058}$$

and, [158, §III.6.12]

$$\sup_{\substack{R^H=R^{-1}\\ S^H=S^{-1}}}|\operatorname{tr}(A^TSBR)|\;=\;\sup_{\substack{R^H=R^{-1}\\ S^H=S^{-1}}}\operatorname{Re}\operatorname{tr}(A^TSBR)\;=\;\operatorname{Re}\operatorname{tr}(A^TS^\star BR^\star)\;=\;\operatorname{tr}(\Sigma_A^T\Sigma_B)\;\geq\;\operatorname{tr}(A^TB) \tag{1059}$$

$$A^T S^\star B R^\star \succeq 0\,, \qquad B R^\star A^T S^\star \succeq 0 \tag{1060}$$

The lower bound on the inner product of singular values in (1059) is due to von Neumann. Equality is achieved if $U_A^H U_B = I$ and $Q_B^H Q_A = I$.

C.2.1.2.1 Symmetric matrices. Suppose $A\,,B$ have diagonalizations (§A.5)

$$A = W_A \Upsilon W_A^T \in \mathbb{S}^n\,, \qquad \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}} \tag{1061}$$

$$B = W_B \Lambda W_B^T \in \mathbb{S}^n\,, \qquad \delta(\Lambda) \in \mathcal{K}_{\mathcal{M}} \tag{1062}$$

with their respective eigenvalues in diagonal matrices $\Upsilon\,,\Lambda \in \mathbb{S}^n$ arranged in nonincreasing order (membership to the monotone cone $\mathcal{K}_{\mathcal{M}}$ (251)). Then we have a symmetric complex singular value decomposition

$$A \triangleq U_A \Sigma_A Q_A^H \in \mathbb{S}^n\;, \qquad B \triangleq U_B \Sigma_B Q_B^H \in \mathbb{S}^n \tag{1063}$$

with $U_A\,, U_B\,, Q_A\,, Q_B \in \mathbb{C}^{n\times n}$ by defining

$$U_A \triangleq W_A \sqrt{\delta(\psi(\delta(\Upsilon)))}\;, \quad Q_A \triangleq W_A \sqrt{\delta(\psi(\delta(\Upsilon)))}^H, \quad \Sigma_A = |\Upsilon| \tag{1064}$$

$$U_B \triangleq W_B \sqrt{\delta(\psi(\delta(\Lambda)))}\;, \quad Q_B \triangleq W_B \sqrt{\delta(\psi(\delta(\Lambda)))}^H, \quad \Sigma_B = |\Lambda| \tag{1065}$$

where step function ψ is defined in (933). In this circumstance,

$$S^\star = \; R^{\star T} \in \mathbb{C}^{n\times n} \tag{1066}$$

the optimal unitary matrices (1057) are related by transposition.

C.2.1.2.2 Diagonal matrices. Now suppose

$$A = \Upsilon = \delta^2(\Upsilon) \in \mathbb{S}^n\,, \quad \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}} \tag{1067}$$

$$B = \Lambda = \delta^2(\Lambda) \in \mathbb{S}^n\,, \quad \delta(\Lambda) \in \mathcal{K}_{\mathcal{M}} \tag{1068}$$

both having their respective entries arranged in nonincreasing order. Then using the step function (933) we have the symmetric complex singular value decomposition (1063) where

$$U_A \triangleq \sqrt{\delta(\psi(\delta(\Upsilon)))}\,, \quad Q_A \triangleq \sqrt{\delta(\psi(\delta(\Upsilon)))}^H, \quad \Sigma_A = |\Upsilon| \tag{1069}$$

$$U_B \triangleq \sqrt{\delta(\psi(\delta(\Lambda)))}\,, \quad Q_B \triangleq \sqrt{\delta(\psi(\delta(\Lambda)))}^H, \quad \Sigma_B = |\Lambda| \tag{1070}$$

The Procrustes solution (1057) again sees $S^\star = R^{\star T} \in \mathbb{C}^{n\times n}$ but both optimal matrices are now themselves diagonal.

Appendix D

Matrix calculus

From too much study, and from extreme passion, cometh madnesse.

−Isaac Newton, [166, §5]

D.1 Directional derivative, Taylor series

D.1.1 Gradients

Traditionally, the gradient of a differentiable real function $f(x):\mathbb{R}^K \to \mathbb{R}$ with respect to its vector domain is defined

$$\nabla f(x) \triangleq \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^K \tag{1071}$$

while the second-order gradient of the twice differentiable real function with respect to its vector domain is traditionally called the *Hessian*;

$$\nabla^2 f(x) \triangleq \begin{bmatrix} \frac{\partial^2 f(x)}{\partial^2 x_1} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_K} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial^2 x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_K \partial x_1} & \frac{\partial^2 f(x)}{\partial x_K \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial^2 x_K} \end{bmatrix} \in \mathbb{S}^K \tag{1072}$$

The gradient of vector-valued function $v(x) : \mathbb{R} \to \mathbb{R}^N$ on real domain is a row-vector

$$\nabla v(x) \triangleq \begin{bmatrix} \frac{\partial v_1(x)}{\partial x} & \frac{\partial v_2(x)}{\partial x} & \cdots & \frac{\partial v_N(x)}{\partial x} \end{bmatrix} \in \mathbb{R}^N \tag{1073}$$

while the second-order gradient is

$$\nabla^2 v(x) \triangleq \begin{bmatrix} \frac{\partial^2 v_1(x)}{\partial x^2} & \frac{\partial^2 v_2(x)}{\partial x^2} & \cdots & \frac{\partial^2 v_N(x)}{\partial x^2} \end{bmatrix} \in \mathbb{R}^N \tag{1074}$$

The gradient of vector function $h(x) : \mathbb{R}^K \to \mathbb{R}^N$ on vector domain is

$$\nabla h(x) \triangleq \begin{bmatrix} \frac{\partial h_1(x)}{\partial x_1} & \frac{\partial h_2(x)}{\partial x_1} & \cdots & \frac{\partial h_N(x)}{\partial x_1} \\ \frac{\partial h_1(x)}{\partial x_2} & \frac{\partial h_2(x)}{\partial x_2} & \cdots & \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \frac{\partial h_1(x)}{\partial x_K} & \frac{\partial h_2(x)}{\partial x_K} & \cdots & \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} = \begin{bmatrix} \nabla h_1(x) & \nabla h_2(x) & \cdots & \nabla h_N(x) \end{bmatrix} \in \mathbb{R}^{K \times N} \tag{1075}$$

while the second-order gradient has a three-dimensional representation dubbed *cubix*;[D.1]

$$\nabla^2 h(x) \triangleq \begin{bmatrix} \nabla \frac{\partial h_1(x)}{\partial x_1} & \nabla \frac{\partial h_2(x)}{\partial x_1} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_1} \\ \nabla \frac{\partial h_1(x)}{\partial x_2} & \nabla \frac{\partial h_2(x)}{\partial x_2} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial h_1(x)}{\partial x_K} & \nabla \frac{\partial h_2(x)}{\partial x_K} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} = \begin{bmatrix} \nabla^2 h_1(x) & \nabla^2 h_2(x) & \cdots & \nabla^2 h_N(x) \end{bmatrix} \in \mathbb{R}^{K \times N \times K} \tag{1076}$$

[D.1] The word *matrix* comes from the Latin for *womb*; related to the prefix *matri-* derived from *mater* meaning *mother*.

where the gradient of each real entry is with respect to vector x as in (1071).

The gradient of real function $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}$ on matrix domain is

$$\nabla g(X) \triangleq \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L}$$
$$= \begin{bmatrix} \nabla_{X(:,1)}\, g(X) & & & \\ & \nabla_{X(:,2)}\, g(X) & & \\ & & \ddots & \\ & & & \nabla_{X(:,L)}\, g(X) \end{bmatrix} \in \mathbb{R}^{K\times 1\times L} \tag{1077}$$

where the gradient $\nabla_{X(:,i)}$ is with respect to the i^{th} column of X. The strange appearance of (1077) in $\mathbb{R}^{K\times 1\times L}$ is meant to suggest a third dimension perpendicular to the page (not a diagonal matrix). The second-order gradient has representation,

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla\frac{\partial g(X)}{\partial X_{11}} & \nabla\frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g(X)}{\partial X_{21}} & \nabla\frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g(X)}{\partial X_{K1}} & \nabla\frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L}$$
$$= \begin{bmatrix} \nabla\nabla_{X(:,1)}\, g(X) & & & \\ & \nabla\nabla_{X(:,2)}\, g(X) & & \\ & & \ddots & \\ & & & \nabla\nabla_{X(:,L)}\, g(X) \end{bmatrix} \in \mathbb{R}^{K\times 1\times L\times K\times L} \tag{1078}$$

where the gradient ∇ is with respect to matrix X.

The gradient of vector function $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}^N$ on matrix domain is a cubix,

$$\nabla g(X) \triangleq \begin{bmatrix} \nabla_{X(:,1)}\, g_1(X) & \nabla_{X(:,1)}\, g_2(X) & \cdots & \nabla_{X(:,1)}\, g_N(X) \\ \nabla_{X(:,2)}\, g_1(X) & \nabla_{X(:,2)}\, g_2(X) & \cdots & \nabla_{X(:,2)}\, g_N(X) \\ \ddots & \ddots & & \ddots \\ \nabla_{X(:,L)}\, g_1(X) & \nabla_{X(:,L)}\, g_2(X) & \cdots & \nabla_{X(:,L)}\, g_N(X) \end{bmatrix} \in \mathbb{R}^{K\times N\times L}$$

$$= [\, \nabla g_1(X) \;\; \nabla g_2(X) \;\; \cdots \;\; \nabla g_N(X)\,] \tag{1079}$$

while the second-order gradient has a five-dimensional representation;

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla\nabla_{X(:,1)}\, g_1(X) & \nabla\nabla_{X(:,1)}\, g_2(X) & \cdots & \nabla\nabla_{X(:,1)}\, g_N(X) \\ \nabla\nabla_{X(:,2)}\, g_1(X) & \nabla\nabla_{X(:,2)}\, g_2(X) & \cdots & \nabla\nabla_{X(:,2)}\, g_N(X) \\ \ddots & \ddots & & \ddots \\ \nabla\nabla_{X(:,L)}\, g_1(X) & \nabla\nabla_{X(:,L)}\, g_2(X) & \cdots & \nabla\nabla_{X(:,L)}\, g_N(X) \end{bmatrix} \in \mathbb{R}^{K\times N\times L\times K\times L}$$

$$= [\, \nabla^2 g_1(X) \;\; \nabla^2 g_2(X) \;\; \cdots \;\; \nabla^2 g_N(X)\,] \tag{1080}$$

The gradient of matrix-valued function $g(X) : \mathbb{R}^{K\times L} \rightarrow \mathbb{R}^{M\times N}$ on matrix domain has a four-dimensional representation called *quartix*,

$$\nabla g(X) \triangleq \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L} \tag{1081}$$

while the second-order gradient has six-dimensional representation

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L\times K\times L} \tag{1082}$$

and so on.

D.1.2 Product rules for matrix-functions

Given compatible matrix-valued functions of matrix variable $f(X)$ and $g(X)$,

$$\nabla_X\big(f(X)^T g(X)\big) = \nabla_X(f)\,g \,+\, \nabla_X(g)\,f \tag{1083}$$

while [100, §8.3] [167]

$$\nabla_X \operatorname{tr}\big(f(X)^T g(X)\big) = \nabla_X\Big(\operatorname{tr}\big(f(X)^T g(Z)\big) \,+\, \operatorname{tr}\big(g(X)\,f(Z)^T\big)\Big)\Big|_{Z\leftarrow X} \tag{1084}$$

These expressions implicitly apply as well to scalar, vector, or matrix functions of scalar, vector, or matrix arguments.

D.1.2.0.1 Example. *Cubix.*
Suppose $f(X) : \mathbb{R}^{\mathbf{2}\times\mathbf{2}} \to \mathbb{R}^{\mathbf{2}} = X^T a$ and $g(X) : \mathbb{R}^{\mathbf{2}\times\mathbf{2}} \to \mathbb{R}^{\mathbf{2}} = Xb$. We wish to find

$$\nabla_X\big(f(X)^T g(X)\big) = \nabla_X\, a^T X^2 b \tag{1085}$$

using the product rule. Formula (1083) calls for

$$\nabla_X\, a^T X^2 b = \nabla_X(X^T a)\, Xb \,+\, \nabla_X(Xb)\, X^T a \tag{1086}$$

Consider the first of the two terms:

$$\begin{aligned}\nabla_X(f)\, g \;&=\; \nabla_X(X^T a)\, Xb\\ &= \big[\, \nabla(X^T a)_1 \;\; \nabla(X^T a)_2 \,\big]\, Xb\end{aligned} \tag{1087}$$

The gradient of $X^T a$ forms a cubix in $\mathbb{R}^{\mathbf{2}\times\mathbf{2}\times\mathbf{2}}$.

$$\nabla_X(X^T a)\, Xb \;=\; \left[\begin{array}{cccc} \frac{\partial(X^Ta)_1}{\partial X_{11}} & & \frac{\partial(X^Ta)_2}{\partial X_{11}} & \\ & \frac{\partial(X^Ta)_1}{\partial X_{12}} & & \frac{\partial(X^Ta)_2}{\partial X_{12}} \\ \frac{\partial(X^Ta)_1}{\partial X_{21}} & & \frac{\partial(X^Ta)_2}{\partial X_{21}} & \\ & \frac{\partial(X^Ta)_1}{\partial X_{22}} & & \frac{\partial(X^Ta)_2}{\partial X_{22}} \end{array}\right] \left[\begin{array}{c} (Xb)_1 \\ \\ (Xb)_2 \end{array}\right] \in \mathbb{R}^{\mathbf{2}\times 1\times\mathbf{2}} \tag{1088}$$

Because the gradient of the product (1085) requires total change with respect to change in each entry of matrix X, the Xb vector must make an inner product with each vector in the second dimension of the cubix (indicated by dotted line segments);

$$\begin{aligned}\nabla_X(X^T a)\, Xb \;&=\; \begin{bmatrix} a_1 & & 0 & \\ & 0 & & a_1 \\ a_2 & & 0 & \\ & 0 & & a_2 \end{bmatrix} \begin{bmatrix} b_1 X_{11} + b_2 X_{12} \\ b_1 X_{21} + b_2 X_{22} \end{bmatrix} \in \mathbb{R}^{\mathbf{2}\times 1\times \mathbf{2}} \\ &=\; \begin{bmatrix} a_1(b_1 X_{11} + b_2 X_{12}) & a_1(b_1 X_{21} + b_2 X_{22}) \\ a_2(b_1 X_{11} + b_2 X_{12}) & a_2(b_1 X_{21} + b_2 X_{22}) \end{bmatrix} \in \mathbb{R}^{\mathbf{2}\times \mathbf{2}} \\ &=\; ab^T X^T \end{aligned} \tag{1089}$$

where the cubix appears as a complete $2\times 2\times 2$ matrix. In like manner for the second term $\nabla_X(g)\, f$,

$$\begin{aligned}\nabla_X(Xb)\, X^T a \;&=\; \begin{bmatrix} b_1 & & 0 & \\ & b_2 & & 0 \\ 0 & & b_1 & \\ & 0 & & b_2 \end{bmatrix} \begin{bmatrix} X_{11} a_1 + X_{21} a_2 \\ X_{12} a_1 + X_{22} a_2 \end{bmatrix} \in \mathbb{R}^{\mathbf{2}\times 1\times \mathbf{2}} \\ &=\; X^T a b^T \in \mathbb{R}^{\mathbf{2}\times \mathbf{2}} \end{aligned} \tag{1090}$$

The solution

$$\nabla_X\, a^T X^2 b = ab^T X^T + X^T a b^T \tag{1091}$$

can be found from Table **D.2.1** or verified using (1084). □

D.1.2.1 Kronecker product

A partial remedy for venturing into *hyper-dimensional* representations, such as the cubix or quartix, is to first vectorize matrices as in (18). This device gives rise to the Kronecker product of matrices $\otimes$; `a.k.a.`, *direct product* or *tensor product.* Its definition is subject to slight variation, [41, §2.1] but in its most conventional form it appears: for $A\in\mathbb{R}^{m\times n}$ and $B\in\mathbb{R}^{p\times q}$,

$$B \otimes A \triangleq \begin{bmatrix} B_{11}A & B_{12}A & \cdots & B_{1q}A \\ B_{21}A & B_{22}A & \cdots & B_{2q}A \\ \vdots & \vdots & & \vdots \\ B_{p1}A & B_{p2}A & \cdots & B_{pq}A \end{bmatrix} \in \mathbb{R}^{pm\times qn} \tag{1092}$$

One advantage is the existence of a traditional two-dimensional matrix representation for the second-order gradient of a scalar function with respect to a vectorized matrix. For example, from §A.1 no.18 (§D.2.1) for square $A, B \in \mathbb{R}^{n\times n}$, [40, §5.2] [160, §3]

$$\nabla^2_{\text{vec}\,X}\operatorname{tr}(AXBX^T) \;=\; \nabla^2_{\text{vec}\,X}\text{vec}^T(X)(B^T\otimes A)\,\text{vec}\,X \;=\; B\otimes A^T + B^T\otimes A \in \mathbb{R}^{n^2\times n^2} \tag{1093}$$

To disadvantage is a large new but known set of algebraic rules, [40] [41] and the fact that its mere use does not generally guarantee two-dimensional representation of gradients.

D.1.3 Chain rules for composite matrix-functions

Given compatible matrix-valued functions of matrix variable $f(X)$ and $g(X)$, [79, §15.7]

$$\nabla_X\, g\big(f(X)^T\big) = \nabla_X f^T\, \nabla_f\, g \tag{1094}$$

$$\nabla^2_X\, g\big(f(X)^T\big) \;=\; \nabla_X\big(\nabla_X f^T\, \nabla_f\, g\big) \;=\; \nabla^2_X f\; \nabla_f\, g \;+\; \nabla_X f^T\, \nabla^2_f g\; \nabla_X f \tag{1095}$$

D.1.3.0.1 Example. *Need better example...*

D.1.3.1 Two arguments

$$\nabla_X\, g\big(f(X)^T,\, h(X)^T\big) = \nabla_X f^T\, \nabla_f\, g \;+\; \nabla_X h^T\, \nabla_h\, g \tag{1096}$$

D.1.3.1.1 Example. *Chain rule for two arguments.* [33, §1.1]

$$g\big(f(x)^T,\, h(x)^T\big) = (f(x) + h(x))^T A\, (f(x) + h(x)) \tag{1097}$$

$$f(x) = \begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix}, \qquad h(x) = \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix} \tag{1098}$$

$$\nabla_x\, g\big(f(x)^T,\, h(x)^T\big) = \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix}(A + A^T)(f + h) + \begin{bmatrix} \varepsilon & 0 \\ 0 & 1 \end{bmatrix}(A + A^T)(f + h) \tag{1099}$$

$$\nabla_x g\big(f(x)^T,\, h(x)^T\big) = \begin{bmatrix} 1+\varepsilon & 0 \\ 0 & 1+\varepsilon \end{bmatrix}(A+A^T)\left(\begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix} + \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix}\right) \tag{1100}$$

$$\lim_{\varepsilon\to 0} \nabla_x g\big(f(x)^T,\, h(x)^T\big) = (A+A^T)x \tag{1101}$$

that can be found in Table **D.2.1**. □

These formulae remain correct when the gradients produce hyper-dimensional representations:

D.1.4 First directional derivative

Assume that a differentiable function $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}^{M\times N}$ has continuous first- and second-order gradients ∇g and $\nabla^2 g$ over $\operatorname{dom} g$ which is an open set. We seek simple expressions for the first and second directional derivatives in direction $Y \in \mathbb{R}^{K\times L}$, $\overset{\to Y}{dg} \in \mathbb{R}^{M\times N}$ and $\overset{\to Y}{dg^2} \in \mathbb{R}^{M\times N}$ respectively.

Assuming that the limit exists, we may state the partial derivative of the mn^{th} entry of g with respect to the kl^{th} entry of X ;

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} = \lim_{\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \tag{1102}$$

where e_k is the k^{th} standard basis vector in $\mathbb{R}^K$ while e_l is the l^{th} standard basis vector in $\mathbb{R}^L$. The total number of partial derivatives equals $KLMN$ while the gradient is defined in their terms; the mn^{th} entry of the gradient is

$$\nabla g_{mn}(X) = \begin{bmatrix} \frac{\partial g_{mn}(X)}{\partial X_{11}} & \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial g_{mn}(X)}{\partial X_{21}} & \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L} \tag{1103}$$

while the gradient is a quartix

$$\nabla g(X) = \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L} \tag{1104}$$

By simply rotating our perspective of the four-dimensional representation of the gradient matrix, we find one of three useful transpositions of this quartix:

$$\nabla g(X)^{T_1} = \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times M\times N} \tag{1105}$$

When the limit for $\Delta t \in \mathbb{R}$ exists, it is easy to show by substitution of variables in (1102)

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} \;=\; \lim_{\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, Y_{kl}\, e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \tag{1106}$$

which may be interpreted as the change in g_{mn} at X when the change in X_{kl} is equal to Y_{kl}, the kl^{th} entry of any $Y \in \mathbb{R}^{K\times L}$. Because the total change in $g_{mn}(X)$ due to Y is the sum of change with respect to each and every X_{kl}, the mn^{th} entry of the directional derivative is the corresponding total differential [79, §15.8]

$$\begin{aligned} dg_{mn}(X)|_{dX\to Y} \;&=\; \sum_{k,l} \frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} \;=\; \operatorname{tr}\big(\nabla g_{mn}(X)^T Y\big) && (1107)\\ &=\; \sum_{k,l} \lim_{\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, Y_{kl}\, e_k e_l^T) - g_{mn}(X)}{\Delta t} && (1108)\\ &=\; \lim_{\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, Y) - g_{mn}(X)}{\Delta t} && (1109)\\ &=\; \frac{d}{dt}\bigg|_{t=0} g_{mn}(X + t\,Y) && (1110) \end{aligned}$$

where $t \in \mathbb{R}$. Assuming finite Y, equation (1109) is called the *Gateaux differential* [65, App.A.5] [29, §D.2.1] [35, §5.28] whose existence is implied by the existence of the *Fréchet differential*, the sum in (1107). [37, §7.2] Each may be understood as the change in g_{mn} at X when the change in X is equal in magnitude and direction to Y.[D.2] Hence the directional derivative,

$$\overset{\rightarrow Y}{dg}(X) \triangleq \left.\begin{bmatrix} dg_{11}(X) & dg_{12}(X) & \cdots & dg_{1N}(X) \\ dg_{21}(X) & dg_{22}(X) & \cdots & dg_{2N}(X) \\ \vdots & \vdots & & \vdots \\ dg_{M1}(X) & dg_{M2}(X) & \cdots & dg_{MN}(X) \end{bmatrix}\right|_{dX\to Y} \in \mathbb{R}^{M\times N}$$

$$= \begin{bmatrix} \operatorname{tr}\big(\nabla g_{11}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{12}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{1N}(X)^T Y\big) \\ \operatorname{tr}\big(\nabla g_{21}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{22}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{2N}(X)^T Y\big) \\ \vdots & \vdots & & \vdots \\ \operatorname{tr}\big(\nabla g_{M1}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{M2}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{MN}(X)^T Y\big) \end{bmatrix}$$

$$= \begin{bmatrix} \sum\limits_{k,l} \frac{\partial g_{11}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{12}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{1N}(X)}{\partial X_{kl}} Y_{kl} \\ \sum\limits_{k,l} \frac{\partial g_{21}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{22}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{2N}(X)}{\partial X_{kl}} Y_{kl} \\ \vdots & \vdots & & \vdots \\ \sum\limits_{k,l} \frac{\partial g_{M1}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{M2}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{MN}(X)}{\partial X_{kl}} Y_{kl} \end{bmatrix} \tag{1111}$$

from which it follows

$$\overset{\rightarrow Y}{dg}(X) = \sum_{k,l} \frac{\partial g(X)}{\partial X_{kl}} Y_{kl} \tag{1112}$$

Yet for all $X \in \operatorname{dom} g$, any $Y \in \mathbb{R}^{K\times L}$, and some open interval of $t \in \mathbb{R}$,

$$g(X + t\,Y) = g(X) \;+\; t\,\overset{\rightarrow Y}{dg}(X) \;+\; o(t^2) \tag{1113}$$

which is the first-order Taylor series expansion about X. [79, §18.4] [66, §2.3.4] Differentiation with respect to t and subsequent t-zeroing isolates the second term of the expansion. Thus differentiating and zeroing $g(X+t\,Y)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X+t\,Y)$ as in (1110). So the directional derivative of $g(X)$ in any direction $Y \in \mathbb{R}^{K\times L}$ evaluated at $X \in \operatorname{dom} g$ becomes

$$\overset{\rightarrow Y}{dg}(X) = \left.\frac{d}{dt}\right|_{t=0} g(X + t\,Y) \;\in \mathbb{R}^{M\times N} \tag{1114}$$

[D.2] Although Y is a matrix, we may regard it as a vector in $\mathbb{R}^{KL}$.

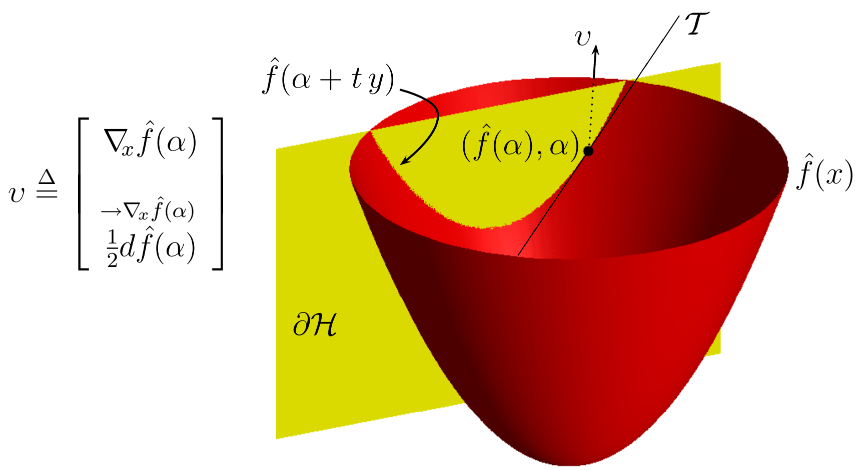


Figure D.1: Drawn is a convex quadratic bowl in $\mathbb{R}^3$; $\hat{f}(x) = x^T x : \mathbb{R}^2 \to \mathbb{R}$ *versus* x on some open disc in $\mathbb{R}^2$. Plane slice $\partial\mathcal{H}$ is perpendicular to domain. Intersection of slice with domain connotes slice direction y in domain. Slope of tangent line $\mathcal{T}$ at point $(\hat{f}(\alpha), \alpha)$ is value of directional derivative at α in slice direction; equivalent to $\nabla_x \hat{f}(\alpha)^T y$ (1141). Recall, the negative gradient is always the direction of steepest descent [168]. [79, §15.6] For this function, the gradient maps to $\mathbb{R}^2$. When vector entry υ_3 is half the directional derivative in direction of the gradient at α, and when $[\,\upsilon_1\ \upsilon_2\,]^T \triangleq \nabla_x \hat{f}(\alpha)$, then $-\upsilon \in \mathbb{R}^3$ points directly toward bottom of bowl.

[6, §2.1, §5.4.5] [7, §6.3.1] which is simplest. The derivative with respect to t makes the directional derivative (1114) resemble ordinary calculus (§D.2); *e.g.*, when $g(X)$ is linear, $\overset{\to Y}{dg}(X) = g(Y)$. [37, §7.2]

D.1.4.1 Interpretation

In the case of a real function $\hat{f}(X) : \mathbb{R}^{K\times L} \to \mathbb{R}$, the directional derivative of $\hat{f}(X)$ at X in any direction Y yields the slope of $\hat{f}$ along the line $X + t\,Y$ through its domain, parametrized by $t \in \mathbb{R}$, evaluated at $t = 0$. Figure **D.1**, for example, shows a plane slice of a real convex bowl-shaped function $\hat{f}(x)$ along a line $\alpha + t\,y$ through its domain. The slice reveals a one-dimensional real function of t; $\hat{f}(\alpha + t\,y)$. The directional derivative at $x = \alpha$ in direction y is the slope of $\hat{f}(\alpha + t\,y)$ with respect to t at $t = 0$.

Notice, unlike the gradient, directional derivative does not expand dimension; directional derivative in (1114) retains the dimensions of g. For higher-dimensional functions, the foregoing slope interpretation can be applied to each entry of the directional derivative by (1111).

In the case of a real function having vector argument $h(X):\mathbb{R}^K\rightarrow\mathbb{R}$, the directional derivative in the normalized direction of the gradient is the magnitude of the gradient. (1141)

Theorem. *Directional derivative condition for optimization.* [37, §7.4] Suppose $\hat{f}(X):\mathbb{R}^{K\times L}\rightarrow\mathbb{R}$ is minimized on convex set $\mathcal{C}\subseteq\mathbb{R}^{p\times k}$ by $X^\star$, and the directional derivative of $\hat{f}$ exists there. Then for all $X\in\mathcal{C}$,

$$\overset{\rightarrow X-X^\star}{d\hat{f}}(X)\geq 0 \tag{1115}$$

$\diamond$

D.1.4.1.1 Example. *Simple bowl.*
Bowl function (Figure **D.1**)

$$\hat{f}(x):\mathbb{R}^K\rightarrow\mathbb{R}\ \triangleq\ (x-a)^T(x-a)-b \tag{1116}$$

has function offset $-b\in\mathbb{R}$, axis of revolution at $x=a$, and positive definite Hessian (1072) everywhere in its domain (an open *hyperdisc* in $\mathbb{R}^K$); *id est*, strictly convex quadratic $\hat{f}(x)$ has global minimum equal to $-b$ at $x=a$. A vector $-\upsilon$ based anywhere in $\operatorname{dom}\hat{f}\times\mathbb{R}$ pointing toward the unique bowl bottom is specified:

$$\upsilon\ \propto\ \begin{bmatrix} x-a \\ \hat{f}(x)+b \end{bmatrix}\in\mathbb{R}^K\times\mathbb{R} \tag{1117}$$

Such a vector is

$$\upsilon\triangleq\begin{bmatrix} \nabla_x\hat{f}(x) \\ \\ \frac{1}{2}\overset{\rightarrow\nabla_x\hat{f}(x)}{d\hat{f}}(x) \end{bmatrix} \tag{1118}$$

since the gradient is

$$\nabla_x\hat{f}(x)=2(x-a) \tag{1119}$$

and the directional derivative in the direction of the gradient is (1141)

$$\overset{\rightarrow\nabla_x\hat{f}(x)}{d\hat{f}}(x)\ =\ \nabla_x\hat{f}(x)^T\nabla_x\hat{f}(x)\ =\ 4(x-a)^T(x-a)\ =\ 4\Big(\hat{f}(x)+b\Big) \tag{1120}$$

$\square$

D.1.5 Second directional derivative

By similar argument, it so happens: the second directional derivative is equally simple. Given $g(X):\mathbb{R}^{K\times L}\to\mathbb{R}^{M\times N}$ on open domain,

$$\nabla\frac{\partial g_{mn}(X)}{\partial X_{kl}} = \frac{\partial\nabla g_{mn}(X)}{\partial X_{kl}} = \begin{bmatrix} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{11}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{12}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{1L}} \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{21}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{22}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{K1}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{K2}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L} \tag{1121}$$

$$\begin{aligned}\nabla^2 g_{mn}(X) &= \begin{bmatrix} \nabla\frac{\partial g_{mn}(X)}{\partial X_{11}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g_{mn}(X)}{\partial X_{21}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g_{mn}(X)}{\partial X_{K1}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L} \\ &= \begin{bmatrix} \frac{\partial\nabla g_{mn}(X)}{\partial X_{11}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial\nabla g_{mn}(X)}{\partial X_{21}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial\nabla g_{mn}(X)}{\partial X_{K1}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{KL}} \end{bmatrix}\end{aligned} \tag{1122}$$

Rotating our perspective, we get several views of the second-order gradient:

$$\nabla^2 g(X) = \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L\times K\times L} \tag{1123}$$

$$\nabla^2 g(X)^{T_1} = \begin{bmatrix} \nabla\frac{\partial g(X)}{\partial X_{11}} & \nabla\frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g(X)}{\partial X_{21}} & \nabla\frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g(X)}{\partial X_{K1}} & \nabla\frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times M\times N\times K\times L} \tag{1124}$$

$$\nabla^2 g(X)^{T_2} = \begin{bmatrix} \frac{\partial \nabla g(X)}{\partial X_{11}} & \frac{\partial \nabla g(X)}{\partial X_{12}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g(X)}{\partial X_{21}} & \frac{\partial \nabla g(X)}{\partial X_{22}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g(X)}{\partial X_{K1}} & \frac{\partial \nabla g(X)}{\partial X_{K2}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L\times M\times N} \tag{1125}$$

Assuming the limits exist, we may state the partial derivative of the mn^{th} entry of g with respect to the kl^{th} and ij^{th} entries of X ;

$$\frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} = \lim_{\Delta\tau,\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, e_k e_l^T + \Delta\tau\, e_i e_j^T) - g_{mn}(X+\Delta t\, e_k e_l^T) - \big(g_{mn}(X+\Delta\tau\, e_i e_j^T) - g_{mn}(X)\big)}{\Delta\tau\,\Delta t} \tag{1126}$$

Differentiating (1106) and then scaling by Y_{ij} ,

$$\begin{aligned} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} &= \lim_{\Delta t\to 0} \frac{\partial g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T) - \partial g_{mn}(X)}{\partial X_{ij}\,\Delta t} Y_{ij} \\ &= \lim_{\Delta\tau,\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T + \Delta\tau\, Y_{ij}\, e_i e_j^T) - g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T) - \big(g_{mn}(X+\Delta\tau\, Y_{ij}\, e_i e_j^T) - g_{mn}(X)\big)}{\Delta\tau\,\Delta t} \end{aligned} \tag{1127}$$

that can be proved by substitution of variables in (1126). The mn^{th} second-order total differential due to any $Y\in\mathbb{R}^{K\times L}$ is

$$d^2 g_{mn}(X)|_{dX\to Y} = \sum_{i,j}\sum_{k,l} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} = \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g_{mn}(X)^T Y\big)^T Y\Big) \tag{1128}$$

$$= \sum_{i,j} \lim_{\Delta t\to 0} \frac{\partial g_{mn}(X+\Delta t\, Y) - \partial g_{mn}(X)}{\partial X_{ij}\,\Delta t} Y_{ij} \tag{1129}$$

$$= \lim_{\Delta t\to 0} \frac{g_{mn}(X+2\Delta t\, Y) - 2g_{mn}(X+\Delta t\, Y) + g_{mn}(X)}{\Delta t^2} \tag{1130}$$

$$= \left.\frac{d^2}{dt^2}\right|_{t=0} g_{mn}(X+t\,Y) \tag{1131}$$

Hence the second directional derivative,

$$\overset{\rightarrow Y}{dg}{}^2(X) \triangleq \left.\begin{bmatrix} d^2g_{11}(X) & d^2g_{12}(X) & \cdots & d^2g_{1N}(X) \\ d^2g_{21}(X) & d^2g_{22}(X) & \cdots & d^2g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ d^2g_{M1}(X) & d^2g_{M2}(X) & \cdots & d^2g_{MN}(X) \end{bmatrix}\right|_{dX\to Y} \in \mathbb{R}^{M\times N}$$

$$= \begin{bmatrix} \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{11}(X)^TY\big)^TY\Big) & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{12}(X)^TY\big)^TY\Big) & \cdots & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{1N}(X)^TY\big)^TY\Big) \\ \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{21}(X)^TY\big)^TY\Big) & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{22}(X)^TY\big)^TY\Big) & \cdots & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{2N}(X)^TY\big)^TY\Big) \\ \vdots & \vdots & & \vdots \\ \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{M1}(X)^TY\big)^TY\Big) & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{M2}(X)^TY\big)^TY\Big) & \cdots & \operatorname{tr}\Big(\nabla\operatorname{tr}\big(\nabla g_{MN}(X)^TY\big)^TY\Big) \end{bmatrix}$$

$$= \begin{bmatrix} \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{11}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{12}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{1N}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} \\ \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{21}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{22}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{2N}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} \\ \vdots & \vdots & & \vdots \\ \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{M1}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{M2}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l}\frac{\partial^2 g_{MN}(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} \end{bmatrix} \tag{1132}$$

from which it follows

$$\overset{\rightarrow Y}{dg}{}^2(X) = \sum_{i,j}\sum_{k,l}\frac{\partial^2 g(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij} = \sum_{i,j}\frac{\partial}{\partial X_{ij}}\overset{\rightarrow Y}{dg}(X)\,Y_{ij} \tag{1133}$$

Yet for all $X\in\operatorname{dom} g$, any $Y\in\mathbb{R}^{K\times L}$, and some open interval of $t\in\mathbb{R}$,

$$g(X+t\,Y) = g(X) \;+\; t\,\overset{\rightarrow Y}{dg}(X) \;+\; \frac{1}{2!}t^2\,\overset{\rightarrow Y}{dg}{}^2(X) \;+\; o(t^3) \tag{1134}$$

which is the second-order Taylor series expansion about X. [79, §18.4] [66, §2.3.4] Differentiating twice with respect to t and subsequent t-zeroing isolates the third term of the expansion. Thus differentiating and zeroing $g(X+t\,Y)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X+t\,Y)$ as in (1131). So the second directional derivative becomes

$$\overset{\rightarrow Y}{dg}{}^2(X) = \left.\frac{d^2}{dt^2}\right|_{t=0} g(X+t\,Y) \in \mathbb{R}^{M\times N} \tag{1135}$$

[6, §2.1, §5.4.5] [7, §6.3.1] which is again simplest. (*confer* (1114))

D.1.6 Taylor series

Series expansions of the differentiable matrix-valued function $g(X)$, of matrix argument, were given earlier in (1113) and (1134). Assuming $g(X)$ has continuous first-, second-, and third-order gradients over the open set $\operatorname{dom} g$, then for $X \in \operatorname{dom} g$ and any $Y \in \mathbb{R}^{K\times L}$ the complete Taylor series on some open interval of $\mu \in \mathbb{R}$ is expressed

$$g(X+\mu Y) = g(X) + \mu \overset{\rightarrow Y}{dg}(X) + \frac{1}{2!}\mu^2 \overset{\rightarrow Y}{dg^2}(X) + \frac{1}{3!}\mu^3 \overset{\rightarrow Y}{dg^3}(X) + o(\mu^4) \tag{1136}$$

or on some open interval of $\|Y\|$

$$g(Y) = g(X) \;+\; \overset{\rightarrow Y-X}{dg}(X) \;+\; \frac{1}{2!}\overset{\rightarrow Y-X}{dg^2}(X) \;+\; \frac{1}{3!}\overset{\rightarrow Y-X}{dg^3}(X) \;+\; o(\|Y\|^4) \tag{1137}$$

which are third-order expansions about X. The *mean value theorem* from calculus is what insures the finite order of the series. [33, §1.1] [65, App.A.5] [29, §0.4] [79]

In the case of a real function $g(X) : \mathbb{R}^{K\times L} \rightarrow \mathbb{R}$, all the directional derivatives are in $\mathbb{R}$:

$$\overset{\rightarrow Y}{dg}(X) = \operatorname{tr}\big(\nabla g(X)^T Y\big) \tag{1138}$$

$$\overset{\rightarrow Y}{dg^2}(X) = \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g(X)^T Y\big)^T Y\Big) = \operatorname{tr}\Big(\nabla_X \overset{\rightarrow Y}{dg}(X)^T Y\Big) \tag{1139}$$

$$\overset{\rightarrow Y}{dg^3}(X) = \operatorname{tr}\bigg(\nabla_X \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g(X)^T Y\big)^T Y\Big)^T Y\bigg) = \operatorname{tr}\bigg(\nabla_X \overset{\rightarrow Y}{dg^2}(X)^T Y\bigg) \tag{1140}$$

In the case $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument, they further simplify:

$$\overset{\rightarrow Y}{dg}(X) = \nabla g(X)^T Y \tag{1141}$$

$$\overset{\rightarrow Y}{dg^2}(X) = Y^T \nabla^2 g(X) Y \tag{1142}$$

$$\overset{\rightarrow Y}{dg^3}(X) = \nabla_X \big(Y^T \nabla^2 g(X) Y\big)^T Y \tag{1143}$$

and so on.

D.1.6.0.1 Example. $\log\det X$. [1, p.644]

We want the first two terms of the Taylor series (1137)...

D.1.7 Correspondence of gradient to derivative

From the foregoing expressions for directional derivative, we derive a relationship between the gradient with respect to matrix X and the derivative with respect to real variable t :

D.1.7.1 first-order

Removing from (1114) the evaluation at $t=0$,[D.3] we find an expression for the directional derivative of $g(X)$ in the direction Y evaluated anywhere along a line $X+tY$ intersecting $\operatorname{dom} g$, parametrized by t ;

$$\overset{\rightarrow Y}{dg}(X+tY) = \frac{d}{dt} g(X+tY) \tag{1144}$$

In the general case $g(X): \mathbb{R}^{K\times L} \rightarrow \mathbb{R}^{M\times N}$, from (1107) and (1110) we find,

$$\operatorname{tr}\left(\nabla_X\, g_{mn}(X+tY)^T Y\right) = \frac{d}{dt} g_{mn}(X+tY) \tag{1145}$$

which is valid at $t=0$, of course, when $X\in\operatorname{dom} g$. In the important case of a real function $g(X): \mathbb{R}^{K\times L} \rightarrow \mathbb{R}$, from (1138) we have simply,

$$\operatorname{tr}\left(\nabla_X\, g(X+tY)^T Y\right) = \frac{d}{dt} g(X+tY) \tag{1146}$$

When, additionally, $g(X): \mathbb{R}^{K} \rightarrow \mathbb{R}$ has vector argument,

$$\nabla_X\, g(X+tY)^T Y = \frac{d}{dt} g(X+tY) \tag{1147}$$

[D.3] Justified by replacing X with $X+tY$ in (1107)-(1109); beginning,

$$dg_{mn}(X+tY)\big|_{dX\rightarrow Y} = \sum_{k,\,l} \frac{\partial g_{mn}(X+tY)}{\partial X_{kl}} Y_{kl}$$

Example. *Gradient.* $g(X) = w^T X^T X w$, $X \in \mathbb{R}^{K\times L}$, $w \in \mathbb{R}^L$. Using the tables in §D.2,

$$\begin{aligned} \operatorname{tr}\big(\nabla_X\, g(X+t\,Y)^T Y\big) &= \operatorname{tr}\big(2ww^T(X^T + t\,Y^T)Y\big) & (1148)\\ &= 2w^T(X^T Y + t\,Y^T Y)w & (1149) \end{aligned}$$

Applying the equivalence (1146),

$$\begin{aligned} \frac{d}{dt} g(X+t\,Y) &= \frac{d}{dt} w^T (X+t\,Y)^T (X+t\,Y) w & (1150)\\ &= w^T\left(X^T Y + Y^T X + 2t\,Y^T Y\right) w & (1151)\\ &= 2w^T(X^T Y + t\,Y^T Y)w & (1152) \end{aligned}$$

which is the same as (1149); hence, the equivalence is demonstrated.

It is easy to extract $\nabla g(X)$ from (1152) knowing only (1146):

$$\begin{aligned} \operatorname{tr}\big(\nabla_X\, g(X+t\,Y)^T Y\big) &= 2w^T(X^T Y + t\,Y^T Y)w\\ &= 2\operatorname{tr}\big(ww^T(X^T + t\,Y^T)Y\big)\\ \operatorname{tr}\big(\nabla_X\, g(X)^T Y\big) &= 2\operatorname{tr}\big(ww^T X^T Y\big)\\ &\Leftrightarrow\\ \nabla_X\, g(X) &= 2Xww^T \end{aligned} \tag{1153}$$

$\square$

D.1.7.2 second-order

Likewise removing the evaluation at $t=0$ from (1135),

$$\overset{\to Y}{dg^2}(X+t\,Y) = \frac{d^2}{dt^2} g(X+t\,Y) \tag{1154}$$

we can find a similar relationship between the second-order gradient and the second derivative: In the general case $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}^{M\times N}$ from (1128) and (1131),

$$\operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla_X\, g_{mn}(X+t\,Y)^T Y\big)^T Y\Big) = \frac{d^2}{dt^2} g_{mn}(X+t\,Y) \tag{1155}$$

In the case of a real function $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}$, we have, of course,

$$\operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla_X\, g(X+t\,Y)^T Y\big)^T Y\Big) = \frac{d^2}{dt^2} g(X+t\,Y) \tag{1156}$$

From (1142), the simpler case, where the real function $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument,

$$Y^T \nabla_X^2 g(X+t\,Y)Y = \frac{d^2}{dt^2} g(X+t\,Y) \tag{1157}$$

D.1.7.2.1 Example. *Second-order gradient.*
Given real function $g(X) = \log\det X$, having domain $X \in \operatorname{int} \mathbb{S}_+^K$, we want to find $\nabla^2 g(X) \in \mathbb{R}^{K\times K\times K\times K}$. From the tables in §D.2,

$$h(X) \triangleq \nabla g(X) = X^{-1} \in \operatorname{int} \mathbb{S}_+^K \tag{1158}$$

so $\nabla^2 g(X) = \nabla h(X)$. By (1145) and (1113), for $Y \in \mathbb{S}^K$,

$$\begin{aligned}
\operatorname{tr}\big(\nabla h_{mn}(X)^T Y\big) &= \left.\frac{d}{dt}\right|_{t=0} h_{mn}(X+t\,Y) &(1159)\\
&= \left(\left.\frac{d}{dt}\right|_{t=0} h(X+t\,Y)\right)_{mn} &(1160)\\
&= \left(\left.\frac{d}{dt}\right|_{t=0} (X+t\,Y)^{-1}\right)_{mn} &(1161)\\
&= -\left(X^{-1}\,Y X^{-1}\right)_{mn} &(1162)
\end{aligned}$$

Setting Y to a member of the standard basis $E_{kl} = e_k e_l^T$, for $k, l \in \{1 \ldots K\}$, and employing a property of the trace function (20), we find

$$\nabla^2 g(X)_{mnkl} = \operatorname{tr}\big(\nabla h_{mn}(X)^T E_{kl}\big) = \nabla h_{mn}(X)_{kl} = -\,(X^{-1} E_{kl}\, X^{-1})_{mn} \tag{1163}$$

$$\nabla^2 g(X)_{kl} = \nabla h(X)_{kl} = -\big(X^{-1} E_{kl}\, X^{-1}\big) \in \mathbb{R}^{K\times K} \tag{1164}$$

□

From all these first- and second-order expressions, we may generate new ones by evaluating both sides at arbitrary t, in some open interval, but only after the differentiation.

D.2 Tables of gradients and derivatives

- [40] [169] When proving results for symmetric matrices algebraically, it is critical to take gradients ignoring symmetry and to then substitute symmetric entries afterward.

- $a\,,b\in\mathbb{R}^n,\ x\,,y\in\mathbb{R}^k,\ A\,,B\in\mathbb{R}^{m\times n},\ X,Y\in\mathbb{R}^{K\times L},\ i\,,j\,,k\,,\ell\,,K,L\,,m\,,n\,,$ M,N are integers, $t\,,\mu\in\mathbb{R}$, unless otherwise noted.

- x^μ means $\delta(\delta(x)^\mu)$ for $\mu\in\mathbb{R}$; *id est*, entry-wise exponentiation. δ is the main-diagonal operator (42) (§A.1). $x^0\triangleq\mathbf{1}$, $X^0\triangleq I$.

- $\frac{d}{dx}\triangleq\begin{bmatrix}\frac{d}{dx_1}\\ \vdots\\ \frac{d}{dx_k}\end{bmatrix}$, $\overset{\to y}{dg}(x)$, $\overset{\to y}{dg^2}(x)$ (directional derivatives §D.1), $\log x$, $\operatorname{sgn} x$, $\sin x$, x/y (entry-wise division), *etcetera*, are maps $f:\mathbb{R}^k\to\mathbb{R}^k$ that maintain dimension; *e.g.*, (§A.1)

$$\frac{d}{dx}x^{-1}\triangleq\nabla_x\,\mathbf{1}^T\delta(x)^{-1}\mathbf{1} \tag{1165}$$

- Given $f(x):\mathcal{X}\to\mathbb{R}$ defined on arbitrary set $\mathcal{X}$, [29, §0.1.2]

$$\begin{aligned}\inf_{x\in\mathcal{X}} f(x) &= -\sup_{x\in\mathcal{X}} -f(x)\\ \sup_{x\in\mathcal{X}} f(x) &= -\inf_{x\in\mathcal{X}} -f(x)\end{aligned} \tag{1166}$$

$$\begin{aligned}\arg\inf_{x\in\mathcal{X}} f(x) &= \arg\sup_{x\in\mathcal{X}} -f(x)\\ \arg\sup_{x\in\mathcal{X}} f(x) &= \arg\inf_{x\in\mathcal{X}} -f(x)\end{aligned} \tag{1167}$$

- Given $g(x,y):\mathcal{X}\times\mathcal{Y}\to\mathbb{R}$ defined on arbitrary sets $\mathcal{X}$ and $\mathcal{Y}$, [29, §0.1.2] and independent variables x and y,

$$\inf_{x\in\mathcal{X},\,y\in\mathcal{Y}} g(x,y) = \inf_{x\in\mathcal{X}}\inf_{y\in\mathcal{Y}} g(x,y) = \inf_{y\in\mathcal{Y}}\inf_{x\in\mathcal{X}} g(x,y) \tag{1168}$$

  The respective arguments of infima are not necessarily unique.

- The standard basis: $\left\{E_{kl}=e_k e_\ell^T \text{ for } k\,,\ell\in\{1\ldots K\}\right\}$ in $\mathbb{R}^{K\times K}$.

- For A a scalar or matrix, we have the Taylor series [170, §3.6]

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k \tag{1169}$$

Further, [26, §5.4]

$$e^A \succ 0\,, \qquad \forall A \in \mathbb{S}^m \tag{1170}$$

- For all square A and integer k,

$$\det^k A = \det A^k \tag{1171}$$

Try to generalize 2X2 cases...

Try $\frac{d}{dt} f(X + t\,Y)^\mu = \ldots\,,\quad -1 \leq \mu \leq 1\,,\; X, Y \in \mathbb{S}_+^M \ldots$ f monotone [24, §2.3.5]

The function X^μ is convex on $\mathbb{S}_+^M$ for $-1 \leq \mu \leq 0$ or $1 \leq \mu \leq 2$ and concave for $0 \leq \mu \leq 1 \ldots$ [1, §3.6.2]

D.2.1 Algebraic

$\nabla_x\, x = \nabla_x\, x^T = I \in \mathbb{R}^{k\times k}$	$\nabla_X X = \nabla_X X^T \triangleq I \in \mathbb{R}^{K\times L\times K\times L}$ (the identity)
$\nabla_x (Ax - b) = A^T$	
$\nabla_x \big(x^TA - b^T\big) = A$	
$\nabla_x (Ax-b)^T(Ax-b) = 2A^T(Ax-b)$	
$\nabla_x^2 (Ax-b)^T(Ax-b) = 2A^TA$	
$\nabla_x \big(x^TAx + 2x^TBy + y^TCy\big) = (A+A^T)x + 2By$	
$\nabla_x^2 \big(x^TAx + 2x^TBy + y^TCy\big) = A + A^T$	
	$\nabla_X\, a^TXb = \nabla_X\, b^TX^Ta = ab^T$
	$\nabla_X\, a^TX^2b = X^Tab^T + ab^TX^T$
	$\nabla_X\, a^TX^{-1}b = -X^{-T}ab^TX^{-T}$
	$\nabla_X (X^{-1})_{kl} = \dfrac{\partial X^{-1}}{\partial X_{kl}} = -X^{-1}E_{kl}\,X^{-1}$, *confer* (1105)(1164)
$\nabla_x\, a^Tx^Txb = 2xa^Tb$	$\nabla_X\, a^TX^TXb = X(ab^T + ba^T)$
$\nabla_x\, a^Txx^Tb = (ab^T + ba^T)x$	$\nabla_X\, a^TXX^Tb = (ab^T + ba^T)X$
$\nabla_x\, a^Tx^Txa = 2xa^Ta$	$\nabla_X\, a^TX^TXa = 2Xaa^T$
$\nabla_x\, a^Txx^Ta = 2aa^Tx$	$\nabla_X\, a^TXX^Ta = 2aa^TX$
$\nabla_x\, a^Tyx^Tb = ba^Ty$	$\nabla_X\, a^TYX^Tb = ba^TY$
$\nabla_x\, a^Ty^Txb = yb^Ta$	$\nabla_X\, a^TY^TXb = Yab^T$
$\nabla_x\, a^Txy^Tb = ab^Ty$	$\nabla_X\, a^TXY^Tb = ab^TY$
$\nabla_x\, a^Tx^Tyb = ya^Tb$	$\nabla_X\, a^TX^TYb = Yba^T$

D.2.1.1 **Algebraic** cont.

$$\frac{d}{dt}(X+t\,Y) = Y$$

$$\frac{d}{dt}B^T(X+t\,Y)^{-1}A = -B^T(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}A$$
$$\frac{d}{dt}B^T(X+t\,Y)^{-T}A = -B^T(X+t\,Y)^{-T}\,Y^T(X+t\,Y)^{-T}A$$
$$\frac{d}{dt}B^T(X+t\,Y)^{\mu}A = \ldots\,, \quad -1 \leq \mu \leq 1\,,\ X,Y \in \mathbb{S}_+^M$$

$$\frac{d^2}{dt^2}B^T(X+t\,Y)^{-1}A = 2B^T(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}A$$

$$\frac{d}{dt}\big((X+t\,Y)^TA(X+t\,Y)\big) = Y^TAX + X^TAY + 2\,t\,Y^TAY$$

$$\frac{d^2}{dt^2}\big((X+t\,Y)^TA(X+t\,Y)\big) = 2\,Y^TAY$$

$$\frac{d}{dt}\big((X+t\,Y)A(X+t\,Y)\big) = YAX + XAY + 2\,t\,YAY$$

$$\frac{d^2}{dt^2}\big((X+t\,Y)A(X+t\,Y)\big) = 2\,YAY$$

D.2.2 Trace

$\nabla_x\, \mu\, x = \mu I$	$\nabla_X \operatorname{tr} \mu X = \nabla_X\, \mu \operatorname{tr} X = \mu I$
$\nabla_x\, \mathbf{1}^T \delta(x)^{-1} \mathbf{1} = \frac{d}{dx} x^{-1} = -x^{-2}$ $\nabla_x\, \mathbf{1}^T \delta(x)^{-1} y = -\delta(x)^{-2} y$ (§A.1)	$\nabla_X \operatorname{tr} X^{-1} = -X^{-2T}$ $\nabla_X \operatorname{tr}(X^{-1} Y) = \nabla_X \operatorname{tr}(Y X^{-1}) = -X^{-T} Y^T X^{-T}$
$\frac{d}{dx} x^{\mu} = \mu x^{\mu-1}$	$\nabla_X \operatorname{tr} X^{\mu} = \mu X^{(\mu-1)T}\,, \qquad X \in \mathbb{R}^{\mathbf{2\times 2}}$
	$\nabla_X \operatorname{tr} X^{j} = j X^{(j-1)T}$
$\nabla_x (b - a^T x)^{-1} = (b - a^T x)^{-2} a$	$\nabla_X \operatorname{tr}((B - AX)^{-1}) = ((B - AX)^{-2} A)^T$
$\nabla_x (b - a^T x)^{\mu} = -\mu (b - a^T x)^{\mu-1} a$	
$\nabla_x\, x^T y = \nabla_x\, y^T x = y$	$\nabla_X \operatorname{tr}(X^T Y) = \nabla_X \operatorname{tr}(Y X^T) = \nabla_X \operatorname{tr}(Y^T X) = \nabla_X \operatorname{tr}(X Y^T) = Y$
	$\nabla_X \operatorname{tr}(A X B X^T) = \nabla_X \operatorname{tr}(X B X^T A) = A^T X B^T + A X B$ $\nabla_X \operatorname{tr}(A X B X) = \nabla_X \operatorname{tr}(X B X A) = A^T X^T B^T + B^T X^T A^T$
	$\nabla_X \operatorname{tr}(AXAXAX) = \nabla_X \operatorname{tr}(XAXAXA) = 3(AXAXA)^T$
	$\nabla_X \operatorname{tr}(Y X^k) = \nabla_X \operatorname{tr}(X^k Y) = \sum_{i=0}^{k-1} \left(X^i Y X^{k-1-i}\right)^T$
	$\nabla_X \operatorname{tr}(Y^T X X^T Y) = \nabla_X \operatorname{tr}(X^T Y Y^T X) = 2\, Y Y^T X$ $\nabla_X \operatorname{tr}(Y^T X^T X Y) = \nabla_X \operatorname{tr}(X Y Y^T X^T) = 2 X Y Y^T$
	$\nabla_X \operatorname{tr}\big((X+Y)^T (X+Y)\big) = 2(X+Y)$ $\nabla_X \operatorname{tr}((X+Y)(X+Y)) = 2(X+Y)^T$
	$\nabla_X \operatorname{tr}(A^T X B) = \nabla_X \operatorname{tr}(X^T A B^T) = A B^T$ $\nabla_X \operatorname{tr}(A^T X^{-1} B) = \nabla_X \operatorname{tr}(X^{-T} A B^T) = -X^{-T} A B^T X^{-T}$
	$\nabla_X\, a^T X b = \nabla_X \operatorname{tr}(b a^T X) = \nabla_X \operatorname{tr}(X b a^T) = a b^T$ $\nabla_X\, b^T X^T a = \nabla_X \operatorname{tr}(X^T a b^T) = \nabla_X \operatorname{tr}(a b^T X^T) = a b^T$ $\nabla_X\, a^T X^{-1} b = \nabla_X \operatorname{tr}(X^{-T} a b^T) = -X^{-T} a b^T X^{-T}$ $\nabla_X\, a^T X^{\mu} b =$

D.2.2.1 Trace cont.

$$\tfrac{d}{dt}\operatorname{tr} g(X+t\,Y) = \operatorname{tr}\tfrac{d}{dt}\, g(X+t\,Y)$$

$$\tfrac{d}{dt}\operatorname{tr}(X+t\,Y) = \operatorname{tr} Y$$

$$\tfrac{d}{dt}\operatorname{tr}^j(X+t\,Y) = j\operatorname{tr}^{j-1}(X+t\,Y)\operatorname{tr} Y$$

$$\tfrac{d}{dt}\operatorname{tr}(X+t\,Y)^j = j\operatorname{tr}((X+t\,Y)^{j-1}\,Y) \qquad (\forall j)$$

$$\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)Y) = \operatorname{tr} Y^2$$

$$\tfrac{d}{dt}\operatorname{tr}\big((X+t\,Y)^k\,Y\big) = \tfrac{d}{dt}\operatorname{tr}(Y(X+t\,Y)^k) = k\operatorname{tr}\big((X+t\,Y)^{k-1}\,Y^2\big)\ , \quad k\in\{0,1,2\}$$

$$\tfrac{d}{dt}\operatorname{tr}\big((X+t\,Y)^k\,Y\big) = \tfrac{d}{dt}\operatorname{tr}(Y(X+t\,Y)^k) = \operatorname{tr}\sum_{i=0}^{k-1}(X+t\,Y)^i\,Y(X+t\,Y)^{k-1-i}\,Y$$

$$\begin{aligned}
\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)^{-1}\,Y) &= -\operatorname{tr}((X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}\,Y)\\
\tfrac{d}{dt}\operatorname{tr}\big(B^T(X+t\,Y)^{-1}A\big) &= -\operatorname{tr}\big(B^T(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}A\big)\\
\tfrac{d}{dt}\operatorname{tr}\big(B^T(X+t\,Y)^{-T}A\big) &= -\operatorname{tr}\big(B^T(X+t\,Y)^{-T}\,Y^T(X+t\,Y)^{-T}A\big)\\
\tfrac{d}{dt}\operatorname{tr}\big(B^T(X+t\,Y)^{-k}A\big) &= \ldots\ k>0\\
\tfrac{d}{dt}\operatorname{tr}\big(B^T(X+t\,Y)^{\mu}A\big) &= \ldots,\quad -1\le\mu\le 1\,,\ X,Y\in\mathbb{S}_+^M
\end{aligned}$$

$$\tfrac{d^2}{dt^2}\operatorname{tr}\big(B^T(X+t\,Y)^{-1}A\big) = 2\operatorname{tr}\big(B^T(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}\,Y(X+t\,Y)^{-1}A\big)$$

$$\tfrac{d}{dt}\operatorname{tr}\big((X+t\,Y)^TA(X+t\,Y)\big) = \operatorname{tr}\big(Y^TAX + X^TAY + 2\,t\,Y^TAY\big)$$

$$\tfrac{d^2}{dt^2}\operatorname{tr}\big((X+t\,Y)^TA(X+t\,Y)\big) = 2\operatorname{tr}\big(Y^TAY\big)$$

$$\tfrac{d}{dt}\operatorname{tr}\big((X+t\,Y)A(X+t\,Y)\big) = \operatorname{tr}(YAX + XAY + 2\,t\,YAY)$$

$$\tfrac{d^2}{dt^2}\operatorname{tr}\big((X+t\,Y)A(X+t\,Y)\big) = 2\operatorname{tr}(YAY)$$

D.2.3 Trace Kronecker

$$\nabla_{\operatorname{vec} X} \operatorname{tr}(AXBX^T) \;=\; \nabla_{\operatorname{vec} X} \operatorname{vec}^T(X)(B^T \otimes A)\operatorname{vec} X \;=\; (B \otimes A^T + \; B^T \otimes A)\operatorname{vec} X$$

$$\nabla^2_{\operatorname{vec} X} \operatorname{tr}(AXBX^T) \;=\; \nabla^2_{\operatorname{vec} X} \operatorname{vec}^T(X)(B^T \otimes A)\operatorname{vec} X \;=\; B \otimes A^T + \; B^T \otimes A$$

D.2.4 Log determinant

$x \succ 0$, $\det X > 0$ on some neighborhood of X, $\det(X + t\,Y) > 0$ on some open interval of t; otherwise, $\log(\cdot)$ is discontinuous.

$\frac{d}{dx}\log x = x^{-1}$	$\nabla_X \log\det X = X^{-T}$ $\nabla_X^2 \log\det(X)_{kl} = \dfrac{\partial X^{-T}}{\partial X_{kl}} = -(X^{-1}E_{kl}\,X^{-1})^T$, *confer* (1122)(1164)
$\frac{d}{dx}\log x^{-1} = -x^{-1}$	$\nabla_X \log\det X^{-1} = -X^{-T}$
$\frac{d}{dx}\log x^{\mu} = \mu x^{-1}$	$\nabla_X \log\det^{\mu} X = \mu X^{-T}$
	$\nabla_X \log\det X^{\mu} = \mu X^{-T}$, $X \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$
	$\nabla_X \log\det X^{k} = \nabla_X \log\det^{k} X = kX^{-T}$
	$\nabla_X \log\det^{\mu}(X + t\,Y) = \mu(X + t\,Y)^{-T}$
$\nabla_x \log(a^Tx + b) = a\frac{1}{a^Tx+b}$	$\nabla_X \log\det(AX + B) = A^T(AX + B)^{-T}$
	$\nabla_X \log\det(I \pm A^TXA) = \ldots$
	$\nabla_X \log\det(X + t\,Y)^k = \nabla_X \log\det^k(X + t\,Y) = k(X + t\,Y)^{-T}$
	$\frac{d}{dt}\log\det(X + t\,Y) = \operatorname{tr}\big((X + t\,Y)^{-1}\,Y\big)$
	$\frac{d^2}{dt^2}\log\det(X + t\,Y) = -\operatorname{tr}\big((X + t\,Y)^{-1}\,Y(X + t\,Y)^{-1}\,Y\big)$
	$\frac{d}{dt}\log\det(X + t\,Y)^{-1} = -\operatorname{tr}\big((X + t\,Y)^{-1}\,Y\big)$
	$\frac{d^2}{dt^2}\log\det(X + t\,Y)^{-1} = \operatorname{tr}\big((X + t\,Y)^{-1}\,Y(X + t\,Y)^{-1}\,Y\big)$
	$\frac{d}{dt}\log\det\big(\delta(A(x + t\,y) + a)^2 + \mu I\big)$ $= \operatorname{tr}\Big(\big(\delta(A(x + t\,y) + a)^2 + \mu I\big)^{-1} 2\delta\big(A(x + t\,y) + a\big)\delta(Ay)\Big)$

D.2.5 Determinant

$$\nabla_X \det X = \nabla_X \det X^T = \det(X)X^{-T}$$

$$\nabla_X \det X^{-1} = -\det(X^{-1})X^{-T} = -\det(X)^{-1}X^{-T}$$

$$\nabla_X \det^\mu X = \mu \det^\mu(X)X^{-T}$$

$$\nabla_X \det X^\mu = \mu \det(X^\mu)X^{-T}\,, \qquad X\in\mathbb{R}^{\mathbf{2\times 2}}$$

$$\nabla_X \det X^k = k \det^{k-1}(X)\big(\operatorname{tr}(X)I - X^T\big)\ , \qquad X\in\mathbb{R}^{\mathbf{2\times 2}}$$

$$\nabla_X \det X^k = \nabla_X \det^k X = k\det(X^k)X^{-T} = k\det^k(X)X^{-T}$$

$$\nabla_X \det^\mu(X+t\,Y) = \mu\det^\mu(X+t\,Y)(X+t\,Y)^{-T}$$

$$\nabla_X \det(X+t\,Y)^k = \nabla_X \det^k(X+t\,Y) = k\det^k(X+t\,Y)(X+t\,Y)^{-T}$$

$$\tfrac{d}{dt}\det(X+t\,Y) = \det(X+t\,Y)\operatorname{tr}((X+t\,Y)^{-1}Y)$$

$$\tfrac{d^2}{dt^2}\det(X+t\,Y) = \det(X+t\,Y)\,(\operatorname{tr}^2((X+t\,Y)^{-1}Y) - \operatorname{tr}((X+t\,Y)^{-1}Y(X+t\,Y)^{-1}Y))$$

$$\tfrac{d}{dt}\det(X+t\,Y)^{-1} = -\det(X+t\,Y)^{-1}\operatorname{tr}((X+t\,Y)^{-1}Y)$$

$$\tfrac{d^2}{dt^2}\det(X+t\,Y)^{-1} = \det(X+t\,Y)^{-1}(\operatorname{tr}^2((X+t\,Y)^{-1}Y) + \operatorname{tr}((X+t\,Y)^{-1}Y(X+t\,Y)^{-1}Y))$$

$$\tfrac{d}{dt}\det^\mu(X+t\,Y) =$$

D.2.6 Logarithmic

$$\frac{d}{dt}\log(X+t\,Y)^{\mu} = \ldots\,, \quad -1 \leq \mu \leq 1\,,\ X,Y \in \mathbb{S}^M_+ \text{ [25, §6.6, prob.20]}$$

D.2.7 Exponential

[170, §3.6, §4.5] [26, §5.4]

$$\nabla_X e^{\operatorname{tr}(Y^TX)} = \nabla_X \det e^{Y^TX} = e^{\operatorname{tr}(Y^TX)}Y \qquad (\forall\, X, Y)$$

$$\nabla_X \operatorname{tr} e^{YX} = e^{Y^TX^T}Y^T = Y^Te^{X^TY^T}$$

log-sum-exp & geometric mean [1, p.74]...

$$\frac{d^j}{dt^j}e^{\operatorname{tr}(X+t\,Y)} = e^{\operatorname{tr}(X+t\,Y)}\operatorname{tr}^j(Y)$$

$$\frac{d}{dt}e^{tY} = e^{tY}Y = Ye^{tY}$$

$$\frac{d}{dt}e^{X+t\,Y} = e^{X+t\,Y}Y = Ye^{X+t\,Y}\,, \qquad XY = YX$$

$$\frac{d^2}{dt^2}e^{X+t\,Y} = e^{X+t\,Y}Y^2 = Ye^{X+t\,Y}Y = Y^2e^{X+t\,Y}\,, \quad XY = YX$$

e^X for symmetric X of dimension less than 3 [1, pg.110]...

Appendix E

Pseudoinverse, Projection

For all $A\in\mathbb{R}^{m\times n}$, the pseudoinverse [28, §7.3, prob.9] [44, §5.5.4] [26, App.A] [37, §6.12, prob.19]

$$A^\dagger \;=\; \lim_{t\to 0^+}(A^TA+\,t\,I\,)^{-1}A^T \;=\; \lim_{t\to 0^+}A^T(AA^T+\,t\,I\,)^{-1}\in\mathbb{R}^{n\times m} \tag{1172}$$

is a unique matrix, having[E.1] [171] [99, §III.1, exer.1]

$$\mathcal{R}(A^\dagger)=\mathcal{R}(A^T), \qquad \mathcal{R}(A^{\dagger T})=\mathcal{R}(A) \tag{1173}$$

$$\mathcal{N}(A^\dagger)=\mathcal{N}(A^T), \qquad \mathcal{N}(A^{\dagger T})=\mathcal{N}(A) \tag{1174}$$

that satisfies the *Penrose conditions*: [48] [155, §1.3]

1. $AA^\dagger A \;=A$
2. $A^\dagger AA^\dagger \;=A^\dagger$
3. $(AA^\dagger)^T=AA^\dagger$
4. $(A^\dagger A)^T=A^\dagger A$

The Penrose conditions are necessary and sufficient to establish the pseudoinverse whose principal action is to injectively map $\mathcal{R}(A)$ onto $\mathcal{R}(A^T)$. The following relations are reliably true without qualification:

[E.1] Proof of (1173) and (1174) is by singular value decomposition (§A.6).

a. $A^{T\dagger} = A^{\dagger T}$
b. $A^{\dagger\dagger} = A$
c. $(AA^T)^\dagger = A^{\dagger T}A^\dagger$
d. $(A^TA)^\dagger = A^\dagger A^{\dagger T}$
e. $(AA^\dagger)^\dagger = AA^\dagger$
f. $(A^\dagger A)^\dagger = A^\dagger A$

Yet for arbitrary A,B it is generally true that $(AB)^\dagger \neq B^\dagger A^\dagger$:

Theorem. *Pseudoinverse of product.* [172] [173, exer.7.23]
For $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{n\times k}$,

$$(AB)^\dagger = B^\dagger A^\dagger \tag{1175}$$

if and only if

$$\mathcal{R}(A^TAB) \subseteq \mathcal{R}(B) \quad \text{and} \quad \mathcal{R}(BB^TA^T) \subseteq \mathcal{R}(A^T) \tag{1176}$$

◇

For orthogonal matrices U, Q and arbitrary A , [99, §III.1]

$$(UA\,Q^T)^\dagger = QA^\dagger U^T \tag{1177}$$

E.0.1 Logical deductions

When A is invertible, $A^\dagger = A^{-1}$, of course; so $A^\dagger A = AA^\dagger = I$. Otherwise, for $A \in \mathbb{R}^{m\times n}$, [148, §5.3.3.1] [173, §7] [174]

g. $A^\dagger A = I\,,$ $\quad A^\dagger = (A^TA)^{-1}A^T\,,$ $\quad \operatorname{rank} A = n$
h. $AA^\dagger = I\,,$ $\quad A^\dagger = A^T(AA^T)^{-1}\,,$ $\quad \operatorname{rank} A = m$
i. $A^\dagger A\omega = \omega\,,$ $\quad \omega \in \mathcal{R}(A^T)$
j. $AA^\dagger \upsilon = \upsilon\,,$ $\quad \upsilon \in \mathcal{R}(A)$
k. $A^\dagger A = AA^\dagger\,,$ $\quad A$ normal
l. $A^{k\dagger} = A^{\dagger k}\,,$ $\quad A$ normal, k an integer

When A is symmetric, $A^\dagger$ is symmetric and (§A.6)

$$A \succeq 0 \;\Leftrightarrow\; A^\dagger \succeq 0 \tag{1178}$$

E.1 Idempotent matrices

Projection matrices are square and defined by *idempotence*, $P^2 = P$; [26, §2.6] [155, §1.3] equivalent to the condition that P be diagonalizable [28, §3.3, prob.3] with eigenvalues $\phi_i \in \{0, 1\}$. [45, §4.1, thm.4.1] Idempotent matrices are not necessarily symmetric. The transpose of an idempotent matrix remains idempotent; $P^T P^T = P^T$. Solely excepting $P = I$, all projection matrices are neither orthogonal (§B.5) or invertible. [26, §3.4] The collection of all projection matrices of particular dimension does not form a convex set.

Suppose we wish to project nonorthogonally (obliquely) on the range of any particular matrix $A \in \mathbb{R}^{m\times n}$. All idempotent matrices projecting nonorthogonally on $\mathcal{R}(A)$ may be expressed:

$$P = A(A^\dagger + BZ^T) \tag{1179}$$

where $\mathcal{R}(P) = \mathcal{R}(A)$, [E.2] $B \in \mathbb{R}^{n\times k}$ for $k \in \{1 \ldots m\}$ is otherwise arbitrary, and $Z \in \mathbb{R}^{m\times k}$ is any matrix in $\mathcal{N}(A^T)$; *id est*,

$$A^T Z \;=\; A^\dagger Z \;=\; \mathbf{0} \tag{1180}$$

Evidently, the collection of nonorthogonal projectors on $\mathcal{R}(A)$ is an affine set

$$\mathcal{P}_k = \left\{ A(A^\dagger + BZ^T) \mid B \in \mathbb{R}^{n\times k} \right\} \tag{1181}$$

When matrix A in (1179) is full-rank ($A^\dagger A = I$) or even has orthonormal columns ($A^T A = I$), this characteristic leads to a biorthogonal characterization of nonorthogonal projection:

[E.2] **Proof.** $\mathcal{R}(P) \subseteq \mathcal{R}(A)$ is obvious [26, §3.6]. By (89) and (90),

$$\begin{aligned}\mathcal{R}(A^\dagger + BZ^T) \;&=\; \{(A^\dagger + BZ^T)y \mid y \in \mathbb{R}^m\}\\ &\supseteq\; \{(A^\dagger + BZ^T)y \mid y \in \mathcal{R}(A)\} = \mathcal{R}(A^T)\end{aligned}$$

$$\begin{aligned}\mathcal{R}(P) \;&=\; \{A(A^\dagger + BZ^T)y \mid y \in \mathbb{R}^m\}\\ &\supseteq\; \{A(A^\dagger + BZ^T)y \mid (A^\dagger + BZ^T)y \in \mathcal{R}(A^T)\} = \mathcal{R}(A)\end{aligned}$$

♦

E.1.1 Biorthogonal characterization

Any nonorthogonal projector $P^2 = P \in \mathbb{R}^{m\times m}$ on $\mathcal{R}(U)$ can be defined by a biorthogonality condition $Q^TU = I$; the biorthogonal decomposition of P being (*confer* (1179))

$$P = UQ^T\,, \qquad Q^TU = I \tag{1182}$$

where[E.3] (§B.1.1.1)

$$\mathcal{R}(P) = \mathcal{R}(U)\ , \qquad \mathcal{N}(P) = \mathcal{N}(Q^T) \tag{1183}$$

and where generally (*confer* (1207))[E.4]

$$P^T \neq P\,, \qquad P^\dagger \neq P\,, \qquad \|P\|_2 \neq 1\,, \qquad P \not\succeq 0 \tag{1184}$$

and P is not non-expansive (1208).

($\Longleftarrow$) To verify assertion (1182) we observe: because idempotent matrices are diagonalizable (§A.5), [28, §3.3, prob.3] they must have the form (913)

$$P \;=\; S\Phi S^{-1} \;=\; \sum_{i=1}^{m} \phi_i\, s_i w_i^T \;=\; \sum_{i=1}^{k\,\leq\, m} s_i w_i^T \tag{1185}$$

that is a sum of $k = \operatorname{rank} P$ independent *projector dyads* (idempotent dyad §B.1.1) where $\phi_i \in \{0,1\}$ are the eigenvalues of P [45, §4.1, thm.4.1] in diagonal matrix $\Phi \in \mathbb{R}^{m\times m}$ arranged in nonincreasing order, and where $s_i\,, w_i \in \mathbb{R}^m$ are the right and left-eigenvectors of P , respectively, which are independent and real.[E.5] Therefore

$$U \;\triangleq\; S(:\,,1\!:\!k) \;=\; \left[\, s_1 \cdots s_k \,\right] \in \mathbb{R}^{m\times k} \tag{1186}$$

[E.3] **Proof.** Obviously, $\mathcal{R}(P) \subseteq \mathcal{R}(U)$. Because $Q^TU = I$,

$$\begin{aligned} \mathcal{R}(P) \;&=\; \{UQ^Tx \mid x \in \mathbb{R}^m\} \\ &\supseteq\; \{UQ^TUy \mid y \in \mathbb{R}^k\} \;=\; \mathcal{R}(U) \end{aligned}$$

♦

[E.4] Orthonormal decomposition (1204) (§E.3.4) is a special case of biorthogonal decomposition (1182), so these characteristics (1184) are not necessary conditions for biorthogonality.

[E.5] Eigenvectors of a real matrix corresponding to real eigenvalues must be real. (§A.5.0.0.1) is the full-rank matrix $S \in \mathbb{R}^{m\times m}$ having $m-k$ columns truncated (corresponding to 0 eigenvalues), while

$$Q^T \triangleq S^{-1}(1\!:\!k\,,:) = \begin{bmatrix} w_1^T \\ \vdots \\ w_k^T \end{bmatrix} \in \mathbb{R}^{k\times m} \tag{1187}$$

is matrix S^{-1} having the corresponding $m-k$ rows truncated. By the 0 *eigenvalues theorem* (§A.7.2.0.1), $\mathcal{R}(U)=\mathcal{R}(P)$, $\mathcal{R}(Q)=\mathcal{R}(P^T)$, and

$$\begin{aligned} \mathcal{R}(P) &= \operatorname{span}\{s_i \mid \phi_i = 1,\ \forall i\} \\ \mathcal{N}(P) &= \operatorname{span}\{s_i \mid \phi_i = 0,\ \forall i\} \\ \mathcal{R}(P^T) &= \operatorname{span}\{w_i \mid \phi_i = 1,\ \forall i\} \\ \mathcal{N}(P^T) &= \operatorname{span}\{w_i \mid \phi_i = 0,\ \forall i\} \end{aligned} \tag{1188}$$

Thus biorthogonality $Q^TU = I$ is a necessary condition for idempotence, and so the collection of nonorthogonal projectors on $\mathcal{R}(U)$ is the affine set $\mathcal{P}_k = U\mathcal{Q}_k^T$ where $\mathcal{Q}_k = \{Q \mid Q^TU = I\,,\ Q\in\mathbb{R}^{m\times k}\}$.

($\Longrightarrow$) Biorthogonality is a sufficient condition for idempotence;

$$P^2 = \sum_{i=1}^k s_i w_i^T \sum_{j=1}^k s_j w_j^T = P \tag{1189}$$

id est, if the cross-products are annihilated, then $P^2 = P$. ♦

The nonorthogonal projection of x on $\mathcal{R}(P)$ can be expressed in a biorthogonal expansion of the projection,

$$Px = UQ^Tx = \sum_{i=1}^k w_i^T x\, s_i \tag{1190}$$

When the domain is restricted to the range of P, say $x = U\xi$ for $\xi\in\mathbb{R}^k$, then $x = Px = UQ^TU\xi = U\xi$ and the expansion is unique because the eigenvectors are linearly independent. Otherwise, any component of x in $\mathcal{N}(Q^T)$ will be ignored by the expansion. The direction of nonorthogonal projection is orthogonal to $\mathcal{R}(Q) \Leftrightarrow Q^TU = I$; *id est*, for $Px\in\mathcal{R}(U)$,

$$Px - x \perp \mathcal{R}(Q) \text{ in } \mathbb{R}^m \tag{1191}$$

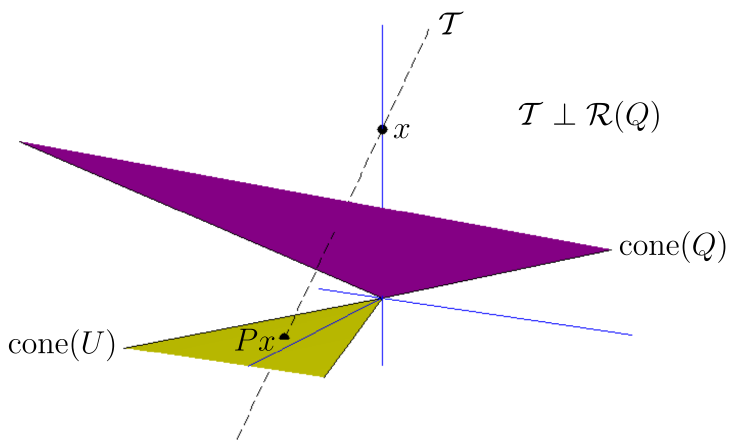


Figure E.1: Nonorthogonal projection of $x \in \mathbb{R}^3$ on $\mathcal{R}(U) = \mathbb{R}^2$ under biorthogonality condition; $Px = UQ^Tx$ such that $Q^TU = I$. Any point along imaginary line $\mathcal{T}$ connecting x to Px will be projected nonorthogonally on Px with respect to horizontal plane constituting $\mathbb{R}^2$ in this example. Extreme directions of cone(U) correspond to two columns of U; likewise for cone(Q). For purpose of illustration, we truncate each conic hull by truncating coefficients of conic combination at unity. Conic hull cone(Q) is headed upward at an angle, out of plane of page. Nonorthogonal projection would fail were $\mathcal{N}(Q^T)$ in $\mathcal{R}(U)$ (were $\mathcal{T}$ parallel to $\mathcal{R}(U)$).

E.1.1.0.1 Example. *Illustration of nonorthogonal projector.*
Figure **E.1** shows $\text{cone}(U)$, the conic hull of the columns of

$$U = \begin{bmatrix} 1 & 1 \\ -0.5 & 0.3 \\ 0 & 0 \end{bmatrix} \tag{1192}$$

from nonorthogonal projector $P = UQ^T$. Matrix U has a limitless number of left inverses because $\mathcal{N}(U^T)$ is nontrivial. Left inverse Q^T from (1179),

$$\begin{aligned} Q = U^{\dagger T} + ZB^T &= \begin{bmatrix} 0.3750 & 0.6250 \\ -1.2500 & 1.2500 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} [\,0.5 \;\; 0.5\,] \\ &= \begin{bmatrix} 0.3750 & 0.6250 \\ -1.2500 & 1.2500 \\ 0.5000 & 0.5000 \end{bmatrix} \end{aligned} \tag{1193}$$

where $Z \in \mathcal{N}(U^T)$ and matrix B is selected arbitrarily, is similarly depicted; *id est*, $Q^T U = I$ because U is full-rank.

Direction of projection on $\mathcal{R}(U)$ is orthogonal to $\mathcal{R}(Q)$. Any point along line $\mathcal{T}$ in the figure, for example, will have the same projection. Were matrix Z instead equal to $\mathbf{0}$, then $\text{cone}(Q)$ would become the relative dual to $\text{cone}(U)$ sharing the same affine hull. (§2.9.1, *confer* Figure **2.23**) In that case, projection $Px = UU^\dagger x$ of x on $\mathcal{R}(U)$ becomes orthogonal (unique in the sense, minimum distance). □

E.1.2 Idempotence summary

Summarizing, nonorthogonal projector P is a linear operator defined by idempotence or biorthogonal decomposition (1182), but characterized not by symmetry nor positive semidefiniteness nor non-expansiveness (1208).

E.2 $I-P$, Projection on algebraic complement

It follows from the diagonalizability of idempotent matrices that $I-P$ must also be a projection matrix because it too is idempotent, and because it may be expressed

$$I - P \;=\; S(I - \Phi)S^{-1} \;=\; \sum_{i=1}^{m}(1 - \phi_i)\, s_i w_i^T \tag{1194}$$

where $(1-\phi_i)\in\{1,0\}$ are the eigenvalues of $I-P$ (849) whose eigenvectors $s_i\,, w_i$ are identical to those of P in (1185). A consequence of that complementary relationship is the fact, [175, §2] [176, §2] for subspace projector $P=P^2\in\mathbb{R}^{m\times m}$,

$$\begin{array}{rl}\mathcal{R}(P) = \operatorname{span}\{s_i \mid \phi_i=1,\ \forall i\} = \operatorname{span}\{s_i \mid (1-\phi_i)=0,\ \forall i\} = \mathcal{N}(I-P)\\ \mathcal{N}(P) = \operatorname{span}\{s_i \mid \phi_i=0,\ \forall i\} = \operatorname{span}\{s_i \mid (1-\phi_i)=1,\ \forall i\} = \mathcal{R}(I-P)\\ \mathcal{R}(P^T) = \operatorname{span}\{w_i \mid \phi_i=1,\ \forall i\} = \operatorname{span}\{w_i \mid (1-\phi_i)=0,\ \forall i\} = \mathcal{N}(I-P^T)\\ \mathcal{N}(P^T) = \operatorname{span}\{w_i \mid \phi_i=0,\ \forall i\} = \operatorname{span}\{w_i \mid (1-\phi_i)=1,\ \forall i\} = \mathcal{R}(I-P^T)\end{array} \tag{1195}$$

that is easy to see from (1185) and (1194). Idempotent $I-P$ therefore projects vectors on its range, $\mathcal{N}(P)$. Because all eigenvectors of a real idempotent matrix are real and independent, the *algebraic complement* [38, §3.3] of $\mathcal{R}(P)$ is equivalent to $\mathcal{N}(P)$;[E.6] *id est*,

$$\mathcal{R}(P)\oplus\mathcal{N}(P) = \mathcal{R}(P^T)\oplus\mathcal{N}(P^T) = \mathcal{R}(P^T)\oplus\mathcal{N}(P) = \mathcal{R}(P)\oplus\mathcal{N}(P^T) = \mathbb{R}^m \tag{1196}$$

because $\mathcal{R}(P)\oplus\mathcal{R}(I-P)=\mathbb{R}^m$. For idempotent $P\in\mathbb{R}^{m\times m}$, consequently,

$$\operatorname{rank} P + \operatorname{rank}(I-P) = m \tag{1197}$$

E.2.0.0.1 Theorem. *Rank/Trace.* [45, §4.1, prob.9] (*confer* (1212))

$$\begin{array}{c}P^2=P\\ \Leftrightarrow\\ \operatorname{rank} P = \operatorname{tr} P \quad\text{and}\quad \operatorname{rank}(I-P)=\operatorname{tr}(I-P)\end{array} \tag{1198}$$

⋄

E.3 Symmetric idempotent matrices

When idempotent matrix P is symmetric, P is an orthogonal projector. In other words, the projection Px of vector $x\in\mathbb{R}^m$ on subspace $\mathcal{R}(P)$ is orthogonal; [48] *id est*, for $P^2=P\in\mathbb{S}^m$ and $Px\in\mathcal{R}(P)$,

$$Px-x \perp \mathcal{R}(P) \text{ in } \mathbb{R}^m \tag{1199}$$

[E.6] The same phenomenon occurs with symmetric (non-idempotent) matrices, for example. When the summands in $A\oplus B=\mathbb{R}^m$ are orthogonal vector spaces, the algebraic complement is called an orthogonal complement.

which is a necessary and sufficient perpendicularity condition for orthogonal projection on a subspace.

Any norm is a convex function. [37, §7.8] A condition equivalent to (1199) is: The norm of vector $x-Px$ is the infimum of all nonorthogonal projections of x on $\mathcal{R}(P)$; [37, §3.3] for $P^2=P\in\mathbb{S}^m$, $\mathcal{R}(P)=\mathcal{R}(A)$, matrices $A\,,B\,,Z$ and integer k as defined for (1179), and any given $x\in\mathbb{R}^m$,

$$\|x-Px\|_2 \;=\; \inf_{B\in\mathbb{R}^{n\times k}} \|x-A(A^\dagger+BZ^T)x\|_2 \tag{1200}$$

The infimum is attained for $\mathcal{R}(B)\subseteq\mathcal{N}(A)$ over any affine set of nonorthogonal projectors (1181) indexed by k . The proof is straightforward, applying gradients from §D.2, setting the gradient of the norm-square to $\mathbf{0}$,

$$\begin{gathered}\big(A^TABZ^T - A^T(I-AA^\dagger)\big)\,xx^TA \;=\; \mathbf{0}\\ \Leftrightarrow\\ A^TABZ^Txx^TA=\mathbf{0}\end{gathered} \tag{1201}$$

In any case, $P=AA^\dagger$ so the projection matrix must be symmetric. Then for any $A\in\mathbb{R}^{m\times n}$, $P=AA^\dagger$ projects any vector x in $\mathbb{R}^m$ orthogonally on $\mathcal{R}(A)$. Under either condition (1199) or (1200), the projection Px is unique (minimum distance).

E.3.1 Four subspaces

We summarize the orthogonal projectors on the four fundamental subspaces:

$$\begin{array}{lll} A^\dagger A & :\mathbb{R}^n \text{ on } \mathcal{R}(A^\dagger A) & =\mathcal{R}(A^T)\\ AA^\dagger & :\mathbb{R}^m \text{ on } \mathcal{R}(AA^\dagger) & =\mathcal{R}(A)\\ I-A^\dagger A & :\mathbb{R}^n \text{ on } \mathcal{R}(I-A^\dagger A) & =\mathcal{N}(A)\\ I-AA^\dagger & :\mathbb{R}^m \text{ on } \mathcal{R}(I-AA^\dagger) & =\mathcal{N}(A^T)\end{array} \tag{1202}$$

For completeness:[E.7] (1195)

$$\begin{array}{ll} \mathcal{N}(A^\dagger A) & =\mathcal{N}(A)\\ \mathcal{N}(AA^\dagger) & =\mathcal{N}(A^T)\\ \mathcal{N}(I-A^\dagger A) & =\mathcal{R}(A^T)\\ \mathcal{N}(I-AA^\dagger) & =\mathcal{R}(A)\end{array} \tag{1203}$$

[E.7]**Proof** is by singular value decomposition (§A.6.2): $\mathcal{N}(A^\dagger A)\subseteq\mathcal{N}(A)$ is obvious. Conversely, suppose $A^\dagger Ax=0$. Then $x^TA^\dagger Ax=x^TQQ^Tx=\|Q^Tx\|^2=0$ where $A=U\Sigma Q^T$ is the subcompact singular value decomposition. Because $\mathcal{R}(Q)=\mathcal{R}(A^T)$, then $x\in\mathcal{N}(A)$ that implies $\mathcal{N}(A^\dagger A)\supseteq\mathcal{N}(A)$. ♦

E.3.2 Orthogonal characterization

Any symmetric projector $P^2 = P \in \mathbb{S}^m$ on $\mathcal{R}(Q)$ can be defined by the *orthonormality condition* $Q^TQ = I$. When skinny matrix $Q \in \mathbb{R}^{m\times k}$ has orthonormal columns, then $Q^\dagger = Q^T$ by the Penrose conditions. Hence, any P having an *orthonormal decomposition* (§E.3.4)

$$P = QQ^T\,, \qquad Q^TQ = I \tag{1204}$$

where [26, §3.3] (958)

$$\mathcal{R}(P) = \mathcal{R}(Q)\ , \qquad \mathcal{N}(P) = \mathcal{N}(Q^T) \tag{1205}$$

is an orthogonal projector on $\mathcal{R}(Q)$ having, for $Px \in \mathcal{R}(Q)$, (*confer* (1191)))

$$Px - x \;\perp\; \mathcal{R}(Q) \text{ in } \mathbb{R}^m \tag{1206}$$

From (1204), orthogonal projector P is obviously positive semidefinite (§A.3.1.0.6); necessarily,

$$P^T = P\,, \qquad P^\dagger = P\,, \qquad \|P\|_2 = 1\,, \qquad P \succeq 0 \tag{1207}$$

and $\|Px\| = \|QQ^Tx\| = \|Q^Tx\|$ because $\|Qy\| = \|y\|\ \forall\, y \in \mathbb{R}^k$. All orthogonal projectors are therefore *non-expansive* because, from Bessel's inequality [38],

$$\|Px\| \;=\; \|Q^Tx\| \;\leq\; \|x\| \quad \forall\, x \in \mathbb{R}^m \tag{1208}$$

with equality when $x \in \mathcal{R}(Q)$.

From the diagonalization of idempotent matrices (1185) on page 386,

$$P \;=\; S\Phi S^T \;=\; \sum_{i=1}^{m} \phi_i\, s_i s_i^T \;=\; \sum_{i=1}^{k\,\leq\, m} s_i s_i^T \tag{1209}$$

orthogonal projection of point x on $\mathcal{R}(P)$ can be expressed in an orthogonal expansion of the projection,

$$Px \;=\; QQ^Tx \;=\; \sum_{i=1}^{k} s_i^T x\, s_i \tag{1210}$$

where

$$Q \;=\; S(:\,,1\!:\!k) \;=\; \left[\, s_1 \cdots s_k \,\right] \in \mathbb{R}^{m\times k} \tag{1211}$$

and where the s_i [*sic*] are orthonormal eigenvectors of symmetric idempotent P. When the domain is restricted to the range of P, say $x = Q\xi$ for $\xi \in \mathbb{R}^k$, then $x = Px = QQ^TQ\xi = Q\xi$ and the expansion is unique because the eigenvectors are linearly independent. Otherwise, any component of x in $\mathcal{N}(Q^T)$ will be ignored by the expansion.

E.3.2.0.1 Theorem. *Symmetric rank/trace.* (*confer* (1198) (847))

$$P^T = P\,, \quad P^2 = P$$
$$\Leftrightarrow$$
$$\operatorname{rank} P \;=\; \operatorname{tr} P \;=\; \|P\|_{\mathrm{F}}^2 \quad \text{and} \quad \operatorname{rank}(I-P) \;=\; \operatorname{tr}(I-P) \;=\; \|I-P\|_{\mathrm{F}}^2 \tag{1212}$$
$\diamond$

Proof. We take as given Theorem E.2.0.0.1 that establishes idempotence. We only have left to show $\operatorname{tr} P = \|P\|_{\mathrm{F}}^2 \Rightarrow P^T = P$. [45, §7.1] ♦

E.3.3 Symmetric idempotence summary

In summary, orthogonal projector P is a linear operator defined [29, §A.3.1] by idempotence and symmetry, and characterized by positive semidefiniteness and non-expansiveness.

E.3.4 Orthonormal decomposition

When $Z = \mathbf{0}$ in the general nonorthogonal projector $A(A^\dagger + BZ^T)$ (1179), an orthogonal projector results (for any matrix A) characterized principally by idempotence and symmetry. Any real orthogonal projector may, in fact, be represented by an orthonormal decomposition such as (1204). [155, §1, prob.42]

To verify that assertion for the four fundamental subspaces (1202), we need only to express A using the compact singular value decomposition (§A.6.1) [44, §2.5.4]: From (935) and the compact SVD we have

$$\begin{array}{rlrl} AA^\dagger \;=\; U\Sigma\Sigma^\dagger U^T \;=\; \hat{U}\hat{U}^T, & & A^\dagger A \;=\; Q\Sigma^\dagger\Sigma Q^T \;=\; \hat{Q}\hat{Q}^T \\ I - AA^\dagger \;=\; I - \hat{U}\hat{U}^T \;=\; \hat{U}^\perp\hat{U}^{\perp T}, & & I - A^\dagger A \;=\; I - \hat{Q}\hat{Q}^T \;=\; \hat{Q}^\perp\hat{Q}^{\perp T} \end{array} \tag{1213}$$

where $\hat{U} \in \mathbb{R}^{m\times \operatorname{rank} A}$ is the SVD matrix U having $\eta - \operatorname{rank} A$ of its orthonormal columns (corresponding to 0 singular values) truncated, likewise for $\hat{Q} \in \mathbb{R}^{n\times \operatorname{rank} A}$, and where $\hat{U}^\perp \in \mathbb{R}^{m\times m-\operatorname{rank} A}$ holds a columnar orthonormal basis for the orthogonal complement of $\mathcal{R}(\hat{U})$, and likewise for $\hat{Q}^\perp \in \mathbb{R}^{n\times n-\operatorname{rank} A}$. The existence of an orthonormal decomposition is sufficient to establish idempotence and symmetry of P (1204). ♦

E.3.4.1 Unifying trait of all projectors: direction

The relation (1213) shows that orthogonal projectors simultaneously possess a biorthogonal decomposition (§E.1.1; *e.g.*, $AA^\dagger$ for skinny-or-square A full-rank) and an orthonormal decomposition (*e.g.*, $\hat{U}\hat{U}^T$, whence the orthogonal expansion of $Px=\hat{U}\hat{U}^Tx$).

E.3.4.1.1 orthogonal projector, orthonormal decomposition

Consider orthogonal expansion of $x\in\mathcal{R}(\hat{U})$:

$$x \;=\; \hat{U}\hat{U}^Tx \;=\; \sum_{i=1}^n \hat{u}_i\hat{u}_i^Tx \tag{1214}$$

a sum of one-dimensional orthogonal projections (§E.6.3), where

$$\hat{U} \triangleq [\,\hat{u}_1 \cdots \hat{u}_n\,] \tag{1215}$$

and where the orthogonal projector has two expressions, (1213)

$$AA^\dagger \triangleq \hat{U}\hat{U}^T \tag{1216}$$

where $A\in\mathbb{R}^{m\times n}$ has rank n. The direction of projection of x on $\hat{u}_j$ for some $j\in\{1\ldots n\}$, for example, is orthogonal to $\hat{u}_j$ but parallel to the span of all the remaining vectors constituting the columns of $\hat{U}$;

$$\begin{aligned} \hat{u}_j^T(\hat{u}_j\hat{u}_j^Tx-x)&=0\\ \hat{u}_j\hat{u}_j^Tx-x \;=\; \hat{u}_j\hat{u}_j^Tx-\hat{U}\hat{U}^Tx \;&\in\; \mathcal{R}(\{\hat{u}_i\,|\,i=1\ldots n\,,\; i\neq j\}) \end{aligned} \tag{1217}$$

E.3.4.1.2 orthogonal projector, biorthogonal decomposition

We get a similar result for the biorthogonal expansion of $x\in\mathcal{R}(A)$. Define

$$A \triangleq [\,a_1 \;\; a_2 \;\cdots\; a_n\,] \in \mathbb{R}^{m\times n} \tag{1218}$$

and the rows of the pseudoinverse

$$A^\dagger \triangleq \begin{bmatrix} a_1^\dagger \\ a_2^\dagger \\ \vdots \\ a_n^\dagger \end{bmatrix} \in \mathbb{R}^{n\times m} \tag{1219}$$

under the biorthogonality condition $A^\dagger A = I$. In the biorthogonal expansion (§2.9.1)

$$x = AA^\dagger x = \sum_{i=1}^{n} a_i a_i^\dagger x \tag{1220}$$

the direction of projection of x on a_j for some particular $j \in \{1 \ldots n\}$, for example, is orthogonal to $a_j^\dagger$ and parallel to the span of all the remaining vectors constituting the columns of A;

$$\begin{aligned} a_j^\dagger(a_j a_j^\dagger x - x) &= 0 \\ a_j a_j^\dagger x - x = a_j a_j^\dagger x - AA^\dagger x &\in \mathcal{R}(\{a_i \mid i=1 \ldots n\,,\ i \neq j\}) \end{aligned} \tag{1221}$$

E.3.4.1.3 nonorthogonal projector, biorthogonal decomposition

Because this foregoing result is independent of symmetry $AA^\dagger = (AA^\dagger)^T$, we must have the same result for any nonorthogonal projector characterized by a biorthogonality condition; namely, for nonorthogonal projector $P = UQ^T$ (1182) under biorthogonality condition $Q^T U = I$ and $x \in \mathcal{R}(U)$, in the biorthogonal expansion

$$x = UQ^T x = \sum_{i=1}^{k} u_i q_i^T x \tag{1222}$$

where

$$\begin{aligned} U &\triangleq \begin{bmatrix} u_1 \cdots u_k \end{bmatrix} \in \mathbb{R}^{m\times k} \\ Q^T &\triangleq \begin{bmatrix} q_1^T \\ \vdots \\ q_k^T \end{bmatrix} \in \mathbb{R}^{k\times m} \end{aligned} \tag{1223}$$

the direction of projection of x on u_j is orthogonal to q_j and parallel to the span of the remaining u_i:

$$\begin{aligned} q_j^T(u_j q_j^T x - x) &= 0 \\ u_j q_j^T x - x = u_j q_j^T x - UQ^T x &\in \mathcal{R}(\{u_i \mid i=1 \ldots k\,,\ i \neq j\}) \end{aligned} \tag{1224}$$

E.4 Algebra of projection on affine subsets

Let $P_{\mathcal{A}}x$ denote projection of x on affine subset $\mathcal{A} \triangleq \mathcal{R} + \alpha$ where $\mathcal{R}$ is a subspace and $\alpha \in \mathcal{A}$. Then, because $\mathcal{R}$ is parallel to $\mathcal{A}$, it holds:

$$\begin{aligned} P_{\mathcal{A}}x \;=\; P_{\mathcal{R}+\alpha}x \;&=\; (I - P_{\mathcal{R}})(\alpha) + P_{\mathcal{R}}x \\ &=\; P_{\mathcal{R}}(x - \alpha) + \alpha \end{aligned} \tag{1225}$$

Subspace projector $P_{\mathcal{R}}$ is a linear operator, and $P_{\mathcal{R}}(x + y) = P_{\mathcal{R}}x$ whenever $y \perp \mathcal{R}$ and $P_{\mathcal{R}}$ is an orthogonal projector.

Theorem. *Orthogonal projection on affine subset.* [70, §9.26]
Let $\mathcal{A} = \mathcal{R} + \alpha$ be an affine subset where $\alpha \in \mathcal{A}$, and let $\mathcal{R}^{\perp}$ be the orthogonal complement of subspace $\mathcal{R}$. Then $P_{\mathcal{A}}x$ is the orthogonal projection of $x \in \mathbb{R}^n$ on $\mathcal{A}$ if and only if

$$P_{\mathcal{A}}x \in \mathcal{A}\,, \quad \langle P_{\mathcal{A}}x - x\,,\, a - \alpha\rangle = 0\,,\;\; \forall\, a \in \mathcal{A} \tag{1226}$$

or if and only if

$$P_{\mathcal{A}}x \in \mathcal{A}\,, \quad P_{\mathcal{A}}x - x \in \mathcal{R}^{\perp} \tag{1227}$$

$\diamond$

E.5 Projection examples

E.5.0.1.1 Example. *Orthogonal projection on orthogonal basis.*
Orthogonal projection on a subspace can instead be accomplished by orthogonally projecting on the individual members of an orthogonal basis for that subspace. Suppose, for example, matrix $A \in \mathbb{R}^{m \times n}$ holds an orthonormal basis for $\mathcal{R}(A)$ in its columns; $A \triangleq [\, a_1 \; a_2 \; \cdots \; a_n \,]$. Then orthogonal projection of vector x on $\mathcal{R}(A)$ is a sum of one-dimensional orthogonal projections

$$Px \;=\; AA^{\dagger}x \;=\; A(A^TA)^{-1}A^Tx \;=\; AA^Tx \;=\; \sum_{i=1}^{n} a_i a_i^T x \tag{1228}$$

where each symmetric dyad $a_i a_i^T$ is an orthogonal projector on $\mathcal{R}(a_i)$. (§E.6.3) $\square$

E.5.0.1.2 Example. *Orthogonal projection on span of nonorthogonal basis.* Orthogonal projection on a subspace can also be accomplished by projecting nonorthogonally on the individual members of any nonorthogonal basis for that subspace. This interpretation is in fact the principal function of the pseudoinverse we discussed. Now suppose matrix A holds a nonorthogonal basis for $\mathcal{R}(A)$ in its columns;

$$A \triangleq [\,a_1 \;\; a_2 \;\cdots\; a_n\,] \in \mathbb{R}^{m\times n} \tag{1229}$$

and define the rows of the pseudoinverse

$$A^\dagger \triangleq \begin{bmatrix} a_1^{\dagger} \\ a_2^{\dagger} \\ \vdots \\ a_n^{\dagger} \end{bmatrix} \in \mathbb{R}^{n\times m} \tag{1230}$$

with $A^\dagger A = I$. Then orthogonal projection of vector x on $\mathcal{R}(A)$ is a sum of one-dimensional nonorthogonal projections

$$Px \;=\; AA^\dagger x \;=\; \sum_{i=1}^{n} a_i a_i^{\dagger} x \tag{1231}$$

where each nonsymmetric dyad $a_i a_i^{\dagger}$ is a nonorthogonal projector on $\mathcal{R}(a_i)$, (§E.6.1) idempotent because of the biorthogonality condition $A^\dagger A = I$.

□

E.5.0.1.3 Example. *Biorthogonal expansion as nonorthogonal projection.* Biorthogonal expansion can be viewed as a sum of components, each a nonorthogonal projection on the range of an extreme direction of a pointed polyhedral cone $\mathcal{K}$; *e.g.*, Figure **E.2**.

Suppose matrix $A \in \mathbb{R}^{m\times n}$ holds a nonorthogonal basis for $\mathcal{R}(A)$ in its columns as in (1229), and the rows of pseudoinverse $A^\dagger$ are defined as in (1230). Assuming the most general biorthogonality condition $(A^\dagger + BZ^T)A = I$ with BZ^T defined as for (1179), then biorthogonal expansion of vector x is a sum of one-dimensional nonorthogonal projections; for $x \in \mathcal{R}(A)$,

$$x \;=\; A(A^\dagger + BZ^T)x \;=\; AA^\dagger x \;=\; \sum_{i=1}^{n} a_i a_i^{\dagger} x \tag{1232}$$

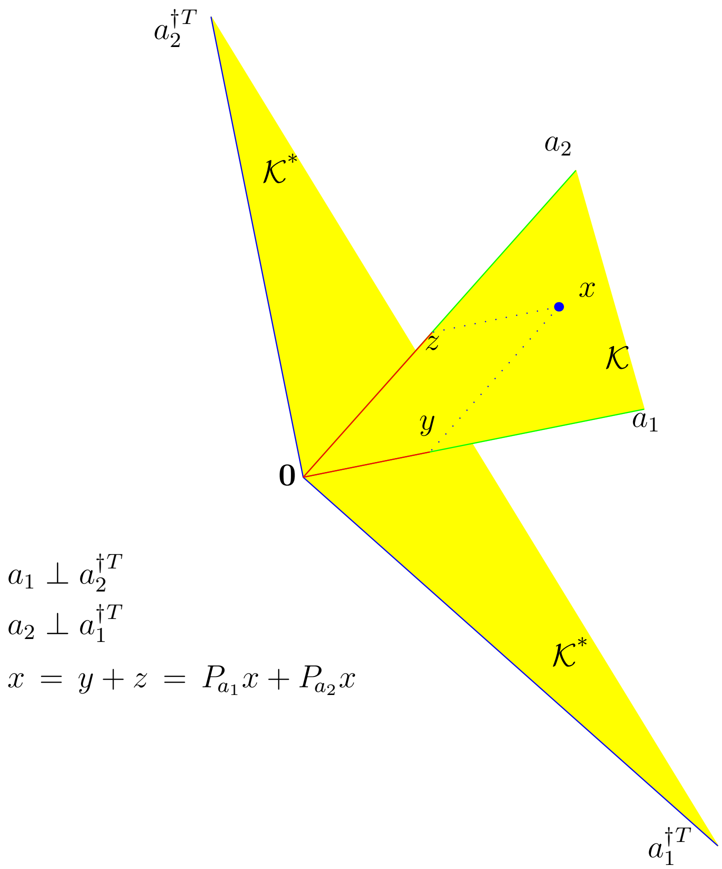


Figure E.2: (*confer* Figure **2.23**) Biorthogonal expansion of point $x \in \operatorname{aff} \mathcal{K}$ is found by projecting x nonorthogonally on range of extreme directions of polyhedral cone $\mathcal{K} \subset \mathbb{R}^{\mathbf{2}}$. Direction of projection on extreme direction a_1 is orthogonal to extreme direction $a_1^{\dagger T}$ of dual cone $\mathcal{K}^*$ and parallel to a_2 (§E.3.4.1); similarly, direction of projection on a_2 is orthogonal to $a_2^{\dagger T}$ and parallel to a_1. Point x is sum of nonorthogonal projections: x on $\mathcal{R}(a_1)$ and x on $\mathcal{R}(a_2)$. Expansion is unique because extreme directions of $\mathcal{K}$ are linearly independent. Were a_1 orthogonal to a_2, then $\mathcal{K}$ would be identical to $\mathcal{K}^*$ and nonorthogonal projections would become orthogonal.

where each dyad $a_i a_i^\dagger$ is a nonorthogonal projector on $\mathcal{R}(a_i)$. (§E.6.1) The extreme directions of $\mathcal{K} = \text{cone}(A)$ are $\{a_1, \ldots, a_n\}$ the linearly independent columns of A while $\{a_1^{\dagger T}, \ldots, a_n^{\dagger T}\}$ the extreme directions of relative dual cone $\mathcal{K}^* \cap \text{aff}\, \mathcal{K} = \text{cone}(A^{\dagger T})$ (§2.9.1) correspond to the linearly independent (§B.1.1.1) rows of $A^\dagger$. The directions of nonorthogonal projection are determined by the pseudoinverse; *id est*, direction of projection $a_i a_i^\dagger x - x$ on $\mathcal{R}(a_i)$ is orthogonal to $a_i^{\dagger T}$.[E.8]

Because the extreme directions of this cone $\mathcal{K}$ are linearly independent, the component projections are unique in the sense:

- there is only one linear combination of extreme directions of $\mathcal{K}$ that yields a particular point $x \in \mathcal{R}(A)$ whenever

$$\mathcal{R}(A) \;=\; \text{aff}\, \mathcal{K} \;=\; \mathcal{R}(a_1) \oplus \mathcal{R}(a_2) \oplus \ldots \oplus \mathcal{R}(a_n) \tag{1233}$$

□

E.5.0.1.4 Example. *Nonorthogonal projection on elementary matrix.* Suppose $P_\mathcal{Y}$ is a linear nonorthogonal projector on subspace $\mathcal{Y} \subset \mathcal{M}$, and suppose the range of a vector u is linearly independent of $\mathcal{Y}$; *id est*, for some other subspace $\mathcal{M}$,

$$\mathcal{M} = \mathcal{R}(u) \oplus \mathcal{Y} \tag{1234}$$

Assuming $P_\mathcal{M} x = P_u x + P_\mathcal{Y} x$ holds, then it follows for vector $x \in \mathcal{M}$,

$$P_u x = x - P_\mathcal{Y} x\ , \qquad P_\mathcal{Y} x = x - P_u x \tag{1235}$$

the nonorthogonal projection of x on $\mathcal{R}(u)$ can be determined from the nonorthogonal projection of x on $\mathcal{Y}$, and *vice versa.*

Such a scenario is realizable were there some arbitrary basis for $\mathcal{Y}$ populating a full-rank skinny-or-square matrix A,

$$A \triangleq [\,\text{basis}\, \mathcal{Y} \quad u\,] \in \mathbb{R}^{n+1} \tag{1236}$$

Then $P_\mathcal{M} = AA^\dagger$ fulfills the requirements, with $P_u = A(:\,, n+1)A^\dagger(n+1\,,:)$ and $P_\mathcal{Y} = A(:\,,1 : n)A^\dagger(1 : n\,,:)$. Observe, $P_\mathcal{M}$ is an orthogonal projector whereas $P_\mathcal{Y}$ and P_u are nonorthogonal projectors.

[E.8] This remains true in high dimension although only a little more difficult to visualize in $\mathbb{R}^3$; *confer*, Figure **2.24**.

Now suppose, for example, $P_{\mathcal{Y}}$ is an elementary matrix (§B.3); in particular,

$$P_{\mathcal{Y}} = I - e_1\mathbf{1}^T = \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} \in \mathbb{R}^{N\times N} \tag{1237}$$

where $\mathcal{Y} = \mathcal{N}(\mathbf{1}^T)$. We have $\mathcal{M} = \mathbb{R}^N$, $A = [\sqrt{2}V_{\mathcal{N}} \;\; e_1]$, and $u = e_1$. Thus $P_u = e_1\mathbf{1}^T$ is a nonorthogonal projector on $\mathcal{R}(u)$ projecting in a direction parallel to $\mathcal{Y}$ (§E.3.4.1), and $P_{\mathcal{Y}}x = x - e_1\mathbf{1}^Tx$ is a nonorthogonal projection of x on $\mathcal{Y}$ in a direction parallel to $\mathcal{R}(u)$. □

E.5.0.1.5 Example. *Projecting the origin on a hyperplane.*
(*confer* §2.3.2.1) Given the hyperplane representation having $b \in \mathbb{R}$ and nonzero normal $a \in \mathbb{R}^m$,

$$\partial\mathcal{H} = \{y \mid a^Ty = b\} \subset \mathbb{R}^m \tag{75}$$

the orthogonal projection of the origin $P\mathbf{0}$ on that hyperplane is the solution to a minimization problem: (1200)

$$\begin{aligned} \|P\mathbf{0} - \mathbf{0}\|_2 &= \inf_{y\in\partial\mathcal{H}} \|y - \mathbf{0}\|_2 \\ &= \inf_{\xi\in\mathbb{R}^{m-1}} \|Z\xi + x\|_2 \end{aligned} \tag{1238}$$

where x is any solution to $a^Ty = b$, and where the columns of $Z \in \mathbb{R}^{m\times m-1}$ constitute a basis for $\mathcal{N}(a^T)$ so that $y = Z\xi + x \in \partial\mathcal{H}$ for all $\xi \in \mathbb{R}^{m-1}$.

The infimum can be found by setting the gradient (with respect to ξ) of the strictly convex norm-square to $\mathbf{0}$. We find the minimizing argument,

$$\xi^\star = -(Z^TZ)^{-1}Z^Tx \tag{1239}$$

so

$$y^\star = \big(I - Z(Z^TZ)^{-1}Z^T\big)x \tag{1240}$$

and from (1202),

$$P\mathbf{0} = y^\star = a(a^Ta)^{-1}a^Tx = \frac{a}{\|a\|}\frac{a^T}{\|a\|}x \triangleq AA^\dagger x = a\frac{b}{\|a\|^2} \tag{1241}$$

In words, any point x in the hyperplane $\partial\mathcal{H}$ projected on its normal a (*confer* (1265)) yields that point $y^\star$ in the hyperplane closest to the origin.

□

E.5.0.1.6 Example. *Projection on affine subset.*
The technique of Example E.5.0.1.5 is extensible. Given an intersection of hyperplanes

$$\mathcal{A} = \{y \mid Ay = b\} \subset \mathbb{R}^m \tag{1242}$$

where each row of $A \in \mathbb{R}^{m\times n}$ is nonzero and $b \in \mathcal{R}(A)$, then the orthogonal projection Px of any point $x \in \mathbb{R}^n$ on $\mathcal{A}$ is the solution to a minimization problem:

$$\begin{aligned}\|Px - x\|_2 &= \inf_{y\in\mathcal{A}} \|y - x\|_2 \\ &= \inf_{\xi\in\mathbb{R}^{n-\operatorname{rank} A}} \|Z\xi + y_p - x\|_2\end{aligned} \tag{1243}$$

where y_p is any solution to $Ay = b$, and where the columns of $Z \in \mathbb{R}^{n\times n-\operatorname{rank} A}$ constitute a basis for $\mathcal{N}(A)$ so that $y = Z\xi + y_p \in \mathcal{A}$ for all $\xi \in \mathbb{R}^{n-\operatorname{rank} A}$.

The infimum is found by setting the gradient of the strictly convex norm-square to $\mathbf{0}$. The minimizing argument is

$$\xi^\star = -(Z^TZ)^{-1}Z^T(y_p - x) \tag{1244}$$

so

$$y^\star = \big(I - Z(Z^TZ)^{-1}Z^T\big)(y_p - x) + x \tag{1245}$$

and from (1202),

$$\begin{aligned}Px \;=\; y^\star \;&=\; x - A^\dagger(Ax - b) \\ &=\; (I - A^\dagger A)x + A^\dagger A y_p\end{aligned} \tag{1246}$$

which is a projection of x on $\mathcal{N}(A)$ then translated perpendicularly with respect to the nullspace until it meets the affine subset $\mathcal{A}$. □

E.5.0.1.7 Example. *Projection on affine subset, vertex-description.*
Suppose now we instead describe the affine subset $\mathcal{A}$ in terms of some given minimal set of generators arranged columnar in $X \in \mathbb{R}^{n\times N}$ (54); *id est*,

$$\mathcal{A} \stackrel{\Delta}{=} \operatorname{aff} X \;=\; \{Xa \mid a^T\mathbf{1} = 1\} \subseteq \mathbb{R}^n \tag{1247}$$

Here a minimal set means $XV_{\mathcal{N}} = [\,x_2 - x_1\,,\; x_3 - x_1 \;\cdots\; x_N - x_1\,]/\sqrt{2}$ is full-rank (§2.3.2.3) where $V_{\mathcal{N}} \in \mathbb{R}^{N\times N-1}$ is the auxiliary matrix from §B.4.2.

Then the orthogonal projection Px of any point $x \in \mathbb{R}^n$ on $\mathcal{A}$ is, as before, the solution to a minimization problem:

$$\begin{aligned} \|Px - x\|_2 &= \inf_{a^T\mathbf{1}=1} \|Xa - x\|_2 \\ &= \inf_{\xi\in\mathbb{R}^{N-1}} \|X(V_{\mathcal{N}}\xi + a_p) - x\|_2 \end{aligned} \tag{1248}$$

where a_p is any solution to $a^T\mathbf{1}=1$. We find the minimizing argument

$$\xi^\star = -(V_{\mathcal{N}}^T X^T X V_{\mathcal{N}})^{-1} V_{\mathcal{N}}^T X^T (Xa_p - x) \tag{1249}$$

and so the orthogonal projection is [54, §3]

$$Px \;=\; Xa^\star = \big(I - XV_{\mathcal{N}}(XV_{\mathcal{N}})^\dagger\big)Xa_p + XV_{\mathcal{N}}(XV_{\mathcal{N}})^\dagger x \tag{1250}$$

a projection of point x on $\mathcal{R}(XV_{\mathcal{N}})$ then translated perpendicularly with respect to that range until it meets the affine subset $\mathcal{A}$. □

E.5.0.1.8 Example. *Projecting on hyperplane, halfspace.*
Given the hyperplane representation having $b \in \mathbb{R}$ and nonzero normal $a \in \mathbb{R}^m$,

$$\partial\mathcal{H} = \{y \mid a^T y = b\} \subset \mathbb{R}^m \tag{75}$$

the orthogonal projection of any point $x \in \mathbb{R}^m$ on that hyperplane is

$$Px \;=\; x - a(a^Ta)^{-1}(a^Tx - b) \tag{1251}$$

Similarly, orthogonal projection of x on the halfspace

$$\mathcal{H}_- = \{y \mid a^T y \le b\} \subset \mathbb{R}^m \tag{65}$$

is the point

$$Px = x - a(a^Ta)^{-1}\max\{0\,,\; a^Tx - b\} \tag{1252}$$

□

E.6 Vectorization interpretation, projection on a matrix

E.6.1 Nonorthogonal projection on a vector

Nonorthogonal projection of vector x on the range of vector y is accomplished using a normalized dyad P_0 (§B.1); *videlicet*,

$$\frac{\langle z, x\rangle}{\langle z, y\rangle}\, y \;=\; \frac{z^T x}{z^T y}\, y \;=\; \frac{y z^T}{z^T y}\, x \;\triangleq\; P_0\, x \tag{1253}$$

where $\langle z, x\rangle / \langle z, y\rangle$ is the coefficient of projection on y. Because $P_0^2 = P_0$ and $\mathcal{R}(P_0) = \mathcal{R}(y)$, rank-one matrix P_0 is a nonorthogonal projector on y. The direction of nonorthogonal projection is orthogonal to z; *id est*,

$$P_0\, x - x \;\perp\; \mathcal{R}(P_0^T) \tag{1254}$$

E.6.2 Nonorthogonal projection on vectorized matrix

Formula (1253) is extensible. Given $X, Y, Z \in \mathbb{R}^{m\times n}$, we have the one-dimensional nonorthogonal projection of X in isomorphic $\mathbb{R}^{mn}$ on the range of vectorized Y: (§2.1.1)

$$\frac{\langle Z\,,\, X\rangle}{\langle Z\,,\, Y\rangle}\, Y\;, \qquad \langle Z\,,\, Y\rangle \neq 0 \tag{1255}$$

where $\langle Z\,,\, X\rangle / \langle Z\,,\, Y\rangle$ is the coefficient of projection. The inequality accounts for the fact: projection on $\operatorname{vec} Y$ is in a direction orthogonal to $\operatorname{vec} Z$.

E.6.2.1 Nonorthogonal projection on dyad

Now suppose we have nonorthogonal projector dyad

$$P_0 = \frac{y z^T}{z^T y} \in \mathbb{R}^{m\times m} \tag{1256}$$

Analogous to (1253), for $X \in \mathbb{R}^{m\times m}$,

$$P_0 X P_0 = \frac{y z^T}{z^T y}\, X\, \frac{y z^T}{z^T y} \;=\; \frac{z^T X y}{(z^T y)^2}\, y z^T \;=\; \frac{\langle z y^T,\, X\rangle}{\langle z y^T,\, y z^T\rangle}\, y z^T \tag{1257}$$

is the nonorthogonal projection of matrix X on the range of vectorized dyad P_0 ; from which it follows:

$$P_0 X P_0 = \frac{z^T X y}{z^T y} \frac{y z^T}{z^T y} = \left\langle \frac{z y^T}{z^T y}, X \right\rangle \frac{y z^T}{z^T y} = \langle P_0^T, X \rangle P_0 = \frac{\langle P_0^T, X \rangle}{\langle P_0^T, P_0 \rangle} P_0 \tag{1258}$$

When nonsymmetric projector P_0 is rank-one as in (1256), therefore,

$$\mathcal{R}(\operatorname{vec} P_0 X P_0) = \mathcal{R}(\operatorname{vec} P_0) \text{ in } \mathbb{R}^{m^2} \tag{1259}$$

and

$$P_0 X P_0 - X \perp P_0^T \text{ in } \mathbb{R}^{m^2} \tag{1260}$$

E.6.2.1.1 Example. *λ as coefficients of nonorthogonal projection.*
Any diagonalization (913)

$$X = S \Lambda S^{-1} = \sum_{i=1}^{m} \lambda_i \, s_i w_i^T \in \mathbb{R}^{m \times m} \tag{1261}$$

may be expressed as a sum of nonorthogonal projections on the range of its vectorized eigenmatrices $P_j \triangleq s_j w_j^T$;

$$\begin{aligned} X &= \sum_{i,j=1}^{m} \langle (S e_i e_j^T S^{-1})^T, X \rangle \, S e_i e_j^T S^{-1} \\ &= \sum_{j=1}^{m} \langle (s_j w_j^T)^T, X \rangle \, s_j w_j^T \;+\; \sum_{\substack{i,j=1 \\ j \neq i}}^{m} \langle (S e_i e_j^T S^{-1})^T, S \Lambda S^{-1} \rangle \, S e_i e_j^T S^{-1} \\ &= \sum_{j=1}^{m} \langle (s_j w_j^T)^T, X \rangle \, s_j w_j^T \\ &\triangleq \sum_{j=1}^{m} \langle P_j^T, X \rangle \, P_j = \sum_{j=1}^{m} s_j w_j^T X s_j w_j^T = \sum_{j=1}^{m} P_j X P_j \\ &= \sum_{j=1}^{m} \lambda_j \, s_j w_j^T \end{aligned} \tag{1262}$$

Matrix X is a sum of one-dimensional nonorthogonal projections because the term outside the projection coefficient $\langle \cdot \rangle$ differs from the term inside. (§E.6.4) The eigenvalues λ_j are coefficients of nonorthogonal projection of

X, while the remaining $M(M-1)/2$ coefficients (for $i \neq j$) are zeroed by the projection. When P_j is rank-one as in (1262),

$$\mathcal{R}(\text{vec}\, P_j X P_j) \;=\; \mathcal{R}(\text{vec}\, s_j w_j^T) \;=\; \mathcal{R}(\text{vec}\, P_j) \text{ in } \mathbb{R}^{m^2} \tag{1263}$$

and

$$P_j X P_j - X \;\perp\; P_j^T \text{ in } \mathbb{R}^{m^2} \tag{1264}$$

Were X a symmetric matrix, then the eigenmatrices would also be symmetric. So the one-dimensional projections would become orthogonal.

□

E.6.3 Orthogonal projection on a vector

The formula for orthogonal projection of vector x on the range of vector y (*one-dimensional projection*) is basic analytic geometry; [177, §3.3] [26, §3.2] [43, §2.2] [90, §1-8]

$$\frac{\langle y, x\rangle}{\langle y, y\rangle}\, y \;=\; \frac{y^T x}{y^T y}\, y \;=\; \frac{y y^T}{y^T y}\, x \;\triangleq\; P_1 x \tag{1265}$$

where $\langle y, x\rangle/\langle y, y\rangle$ is the coefficient of projection on y. An equivalent description is: Vector $P_1 x$ is the orthogonal projection of vector x on $\mathcal{R}(P_1) = \mathcal{R}(y)$. Rank-one matrix P_1 is a projection matrix because $P_1^2 = P_1$. The projection is orthogonal

$$P_1 x - x \;\perp\; \mathcal{R}(P_1) \tag{1266}$$

because $P_1^T = P_1$.

E.6.4 Orthogonal projection on a vectorized matrix

From (1265), given instead $X, Y \in \mathbb{R}^{m\times n}$, we have the one-dimensional orthogonal projection of matrix X in isomorphic $\mathbb{R}^{mn}$ on the range of vectorized Y: (§2.1.1)

$$\frac{\langle Y, X\rangle}{\langle Y, Y\rangle}\, Y \tag{1267}$$

where $\langle Y, X\rangle/\langle Y, Y\rangle$ is the coefficient of projection.

For orthogonal projection, the term outside the inner products $\langle\cdot\rangle$ must equal the terms inside in three places.

E.6.4.1 Orthogonal projection on dyad

There is opportunity for insight when Y is a dyad yz^T (§B.1): Instead given $X\in\mathbb{R}^{m\times n}$, $y\in\mathbb{R}^m$, and $z\in\mathbb{R}^n$,

$$\frac{\langle yz^T,\, X\rangle}{\langle yz^T,\, yz^T\rangle}\, yz^T \;=\; \frac{y^TXz}{y^Ty\, z^Tz}\, yz^T \tag{1268}$$

is the one-dimensional orthogonal projection of X in isomorphic $\mathbb{R}^{mn}$ on the range of vectorized yz^T. To reveal the obscured symmetric projection matrices P_1 and P_2 we rewrite (1268):

$$\frac{y^TXz}{y^Ty\, z^Tz}\, yz^T \;=\; \frac{yy^T}{y^Ty}\, X\, \frac{zz^T}{z^Tz} \;\triangleq\; P_1XP_2 \tag{1269}$$

So for projector dyads, the projection (1269) in $\mathbb{R}^{mn}$ is orthogonal if and only if projectors P_1 and P_2 are symmetric;[E.9]

- for orthogonal projection on the range of a vectorized dyad yz^T, in other words, the term outside the inner products $\langle\cdot\rangle$ in (1268) must equal the terms inside in three places.

When P_1 and P_2 are rank-one symmetric projectors as in (1269), (18)

$$\mathcal{R}(\operatorname{vec} P_1XP_2) = \mathcal{R}(\operatorname{vec} yz^T) \text{ in } \mathbb{R}^{mn} \tag{1270}$$

and

$$P_1XP_2 - X \;\perp\; yz^T \text{ in } \mathbb{R}^{mn} \tag{1271}$$

When $y=z$ then $P_1=P_2=P_2^T$ and

$$P_1XP_1 \;=\; \langle P_1\,,X\rangle\, P_1 \;=\; \frac{\langle P_1\,,X\rangle}{\langle P_1\,,P_1\rangle}\, P_1 \tag{1272}$$

meaning, P_1XP_1 is equivalent to orthogonal projection of matrix X on the vectorized range of projector dyad P_1.

[E.9] For diagonalizable $X\in\mathbb{R}^{m\times m}$ (§A.5), its orthogonal projection in isomorphic $\mathbb{R}^{m^2}$ on $yz^T\in\mathbb{R}^{m\times m}$ becomes:

$$P_1XP_2 = \sum_{i=1}^{m} \lambda_i\, P_1\, s_i w_i^T P_2$$

When $\mathcal{R}(P_1)=\mathcal{R}(w_j)$ and $\mathcal{R}(P_2)=\mathcal{R}(s_j)$, the j^{th} dyad term from the diagonalization is isolated but only, in general, to within a scale factor because neither set of left or right eigenvectors is necessarily orthonormal unless X is normal [45, §3.2]. Yet when $\mathcal{R}(P_2)=\mathcal{R}(s_k)$, $k\neq j\in\{1\ldots m\}$, then $P_1XP_2=\mathbf{0}$.

E.6.4.1.1 Example. *Eigenvalues λ as coefficients of orthogonal projection.* Let $\mathcal{C}$ represent any convex subset of subspace $\mathbb{S}^M$, and let $\mathcal{C}_1$ be any element of $\mathcal{C}$. Then $\mathcal{C}_1$ can be written as the orthonormal series:

$$\mathcal{C}_1 = \sum_{i=1}^{M} \sum_{\substack{j=1 \\ j \geq i}}^{M} \langle E_{ij} \,,\, \mathcal{C}_1 \rangle \, E_{ij} \;\in \mathcal{C} \subset \mathbb{S}^M \tag{1273}$$

where $E_{ij} \in \mathbb{S}^M$ is a member of the standard orthonormal basis for $\mathbb{S}^M$ (38); $\langle E_{ij} \,,\, E_{ij} \rangle = 1$. This series is a sum of one-dimensional orthogonal projections; each projection on the range of a vectorized standard basis matrix. The vector inner product $\langle E_{ij} \,,\, \mathcal{C}_1 \rangle$ (§2.1.1) is the coefficient of projection of $\operatorname{vec} \mathcal{C}_1$ on $\operatorname{vec} E_{ij}$.

When $\mathcal{C}_1$ is any member of a convex set $\mathcal{C}$ whose dimension is L, *Caratheodory's theorem* [50] [30] [29] [65] [33] guarantees that no more than $L+1$ affinely independent members from $\mathcal{C}$ are required to faithfully represent it by some linear combination of those members. Because any symmetric matrix can be diagonalized [27, §6.4], for example, $\mathcal{C}_1 \in \mathbb{S}^M$ has a decomposition in terms of its eigenmatrices $q_i q_i^T$ (§A.5) and eigenvalues λ_i;

$$\mathcal{C}_1 \;=\; Q \Lambda Q^T = \sum_{i=1}^{M} \lambda_i \, q_i q_i^T \in \mathbb{S}^M \tag{1274}$$

where $\Lambda \in \mathbb{S}^M$ is a diagonal matrix having $\delta(\Lambda)_i = \lambda_i$, and $Q = [q_1 \cdots q_M]$ is an orthogonal matrix in $\mathbb{R}^{M \times M}$ containing corresponding eigenvectors. Yet the dimension of $\mathbb{S}^M$ is $M(M+1)/2$ in isometrically isomorphic $\mathbb{R}^{M(M+1)/2}$.

To derive eigen-decomposition (1274) from (1273), M standard basis matrices E_{ij} are rotated (§B.5) into alignment with the M eigenmatrices $q_i q_i^T$ of $\mathcal{C}_1$ by applying a traditional *similarity transformation*; [26, §5.6]

$$\{Q E_{ij} Q^T\} = \left\{ \begin{array}{ll} q_i q_i^T \,, & i = j = 1 \ldots M \\ \frac{1}{\sqrt{2}}\big(q_i q_j^T + q_j q_i^T\big) \,, & 1 \leq i < j \leq M \end{array} \right\} \tag{1275}$$

This set remains an orthonormal basis for $\mathbb{S}^M$, and a remarkable thing happens to the series:

$$\begin{aligned}
\mathcal{C}_1 &= \sum_{\substack{i,j=1\\ j\geq i}}^{M} \langle QE_{ij}Q^T,\, \mathcal{C}_1\rangle\, QE_{ij}Q^T \\
&= \sum_{i=1}^{M} \langle q_i q_i^T,\, \mathcal{C}_1\rangle\, q_i q_i^T \;+\; \sum_{\substack{i,j=1\\ j>i}}^{M} \langle QE_{ij}Q^T,\, Q\Lambda Q^T\rangle\, QE_{ij}Q^T \\
&= \sum_{i=1}^{M} \langle q_i q_i^T,\, \mathcal{C}_1\rangle\, q_i q_i^T \\
&\triangleq \sum_{i=1}^{M} \langle P_i\,,\, \mathcal{C}_1\rangle\, P_i \;=\; \sum_{i=1}^{M} q_i q_i^T \mathcal{C}_1\, q_i q_i^T \;=\; \sum_{i=1}^{M} P_i\, \mathcal{C}_1 P_i \\
&= \sum_{i=1}^{M} \lambda_i\, q_i q_i^T
\end{aligned} \tag{1276}$$

The eigenvalues

$$\lambda_i = \langle q_i q_i^T,\, \mathcal{C}_1\rangle \tag{1277}$$

are clearly coefficients of orthogonal projection of $\mathcal{C}_1$ on the range of its vectorized eigenmatrices; (*confer* §E.6.2.1.1) $\mathcal{C}_1$ still is a sum of one-dimensional projections. The remaining $M(M-1)/2$ coefficients ($i\neq j$) are zeroed by the projection. When P_i is rank-one symmetric as it is in (1276),

$$\mathcal{R}(\operatorname{vec} P_i\, \mathcal{C}_1 P_i) \;=\; \mathcal{R}(\operatorname{vec} q_i q_i^T) \;=\; \mathcal{R}(\operatorname{vec} P_i) \text{ in } \mathbb{R}^{M^2} \tag{1278}$$

and

$$P_i\, \mathcal{C}_1 P_i - \mathcal{C}_1 \;\perp\; P_i \text{ in } \mathbb{R}^{M^2} \tag{1279}$$

□

E.6.4.2 Positive semidefiniteness test as orthogonal projection

For any given $X\in\mathbb{R}^{m\times m}$, the familiar quadratic construct $y^TXy\geq 0$, over broad domain, is a fundamental test of positive semidefiniteness. (§A.2) It is a fact that y^TXy is always proportional to a coefficient of orthogonal projection; letting z in formula (1268) become $y\in\mathbb{R}^m$, then $P_2=P_1=yy^T/y^Ty=yy^T/\|yy^T\|_2$ $\big($*confer* (961)$\big)$ and formula (1269) becomes

$$\frac{\langle yy^T,\, X\rangle}{\langle yy^T,\, yy^T\rangle}\, yy^T = \frac{y^TXy}{y^Ty}\,\frac{yy^T}{y^Ty} \;=\; \frac{yy^T}{y^Ty}\, X\, \frac{yy^T}{y^Ty} \;\triangleq\; P_1 X P_1 \tag{1280}$$

By (1267), the product $P_1 X P_1$ is the one-dimensional orthogonal projection of X in isomorphic $\mathbb{R}^{m^2}$ on the range of vectorized P_1 because, for $\operatorname{rank} P_1 = 1$ and $P_1^2 = P_1 \in \mathbb{S}^m$, (*confer* (1258))

$$P_1 X P_1 = \frac{y^T X y}{y^T y}\frac{yy^T}{y^T y} = \left\langle \frac{yy^T}{y^T y}\,,\, X\right\rangle \frac{yy^T}{y^T y} = \langle P_1\,,\, X\rangle\, P_1 = \frac{\langle P_1\,,\, X\rangle}{\langle P_1\,,\, P_1\rangle}\, P_1 \tag{1281}$$

The coefficient of orthogonal projection $\langle P_1\,,\, X\rangle = y^T X y/(y^T y)$ is also known as *Rayleigh's quotient.*[E.10] When P_1 is rank-one symmetric as in (1280),

$$\mathcal{R}(\operatorname{vec} P_1 X P_1) = \mathcal{R}(\operatorname{vec} P_1) \text{ in } \mathbb{R}^{m^2} \tag{1282}$$

and

$$P_1 X P_1 - X \perp P_1 \text{ in } \mathbb{R}^{m^2} \tag{1283}$$

The test for positive semidefiniteness, then, is a test for nonnegativity of the coefficient of orthogonal projection of X on the range of each and every vectorized extreme direction yy^T (§2.6.4) from the positive semidefinite cone in the ambient space of symmetric matrices.

[E.10] When y becomes the j^{th} eigenvector s_j of diagonalizable X, for example, $\langle P_1\,,\, X\rangle$ becomes the j^{th} eigenvalue: [58, §III]

$$\langle P_1\,,\, X\rangle|_{y=s_j} = \frac{s_j^T\left(\sum\limits_{i=1}^m \lambda_i\, s_i w_i^T\right) s_j}{s_j^T s_j} = \lambda_j$$

Similarly for $y = w_j$, the j^{th} left-eigenvector,

$$\langle P_1\,,\, X\rangle|_{y=w_j} = \frac{w_j^T\left(\sum\limits_{i=1}^m \lambda_i\, s_i w_i^T\right) w_j}{w_j^T w_j} = \lambda_j$$

A quandary may arise regarding the potential annihilation of the antisymmetric part of X when $s_j^T X s_j$ is formed. Were annihilation to occur, it would imply the eigenvalue thus found came instead from the symmetric part of X. The quandary is resolved recognizing that diagonalization of real X admits complex eigenvectors; hence, annihilation could only come about by forming $\operatorname{Re}(s_j^H X s_j) = s_j^H (X + X^T) s_j / 2$ [28, §7.1] where $(X + X^T)/2$ is the symmetric part of X, and s_j^H denotes the conjugate transpose.

E.6.4.2.1 $PXP \succeq 0$

In some circumstances, it may be desirable to limit the domain of test $y^T X y \geq 0$ for positive semidefiniteness; *e.g.*, $\|y\|=1$. Another example of limiting the domain-of-test is central to Euclidean distance geometry: For $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$, the test $-VDV \succeq 0$ determines whether $D \in \mathbb{S}_{\mathbf{0}}^N$ is a Euclidean distance matrix. The same test may be stated: For $D \in \mathbb{S}_{\mathbf{0}}^N$ (and optionally $\|y\|=1$),

$$D \in \mathbb{EDM}^N \Leftrightarrow -y^T D y = \langle yy^T, -D \rangle \geq 0 \quad \forall y \in \mathcal{R}(V) \tag{1284}$$

The test $-VDV \succeq 0$ is therefore equivalent to a test for nonnegativity of the coefficient of orthogonal projection of $-D$ on the range of each and every vectorized extreme direction yy^T from the positive semidefinite cone $\mathbb{S}_+^N$ such that $\mathcal{R}(yy^T) = \mathcal{R}(y) \subseteq \mathcal{R}(V)$. (The validity of this result is independent of whether V is itself a projection matrix.)

E.6.4.3 PXP misinterpretation for higher rank P

For a projection matrix P of rank greater than 1, PXP is generally not commensurate with $\frac{\langle P, X \rangle}{\langle P, P \rangle} P$ as is the case for projector dyads (1281). Yet for a symmetric idempotent matrix P of any rank we are tempted to say " PXP is an orthogonal projection of $X \in \mathbb{S}^m$ on $\operatorname{vec} P$ ". The fallacy is: $\operatorname{vec} PXP$ does not necessarily belong to the range of vectorized P; the most basic requirement for projection on $\operatorname{vec} P$.

E.7 Range/Rowspace interpretation

For projection matrices P_1 and P_2 of any rank, $P_1 X P_2^T$ is a projection of $\mathcal{R}(X)$ on $\mathcal{R}(P_1)$ and a projection of $\mathcal{R}(X^T)$ on $\mathcal{R}(P_2)$: For any $X = U\Sigma Q^T \in \mathbb{R}^{m \times p}$ as in compact singular value decomposition (922) where here $\eta \triangleq \min\{m, p\}$,

$$P_1 X P_2^T = \sum_{i=1}^{\eta} \sigma_i P_1 u_i q_i^T P_2^T = \sum_{i=1}^{\eta} \sigma_i P_1 u_i (P_2 q_i)^T \tag{1285}$$

Recall $u_i \in \mathcal{R}(X)$ and $q_i \in \mathcal{R}(X^T)$ when the corresponding singular values are nonzero. (§A.6.1) So P_1 projects u_i on $\mathcal{R}(P_1)$ while P_2 projects q_i on

$\mathcal{R}(P_2)$; *id est*, the range and rowspace of any X are respectively projected on the ranges of P_1 and P_2.[E.11]

E.7.1 Projection on vectorized matrices of higher rank

With $A_1, B_1, Z_1, A_2, B_2, Z_2$ as defined for nonorthogonal projector (1179), for $P_1 \triangleq A_1A_1^\dagger \in \mathbb{S}^m$ where $A_1 \in \mathbb{R}^{m\times n}$, $Z_1 \in \mathbb{R}^{m\times k}$, and for $P_2 \triangleq A_2A_2^\dagger \in \mathbb{S}^p$ where $A_2 \in \mathbb{R}^{p\times n}$, $Z_2 \in \mathbb{R}^{p\times k}$, and any given X,

$$\|X - P_1XP_2\|_{\mathrm{F}} = \inf_{B_1,\, B_2 \in \mathbb{R}^{n\times k}} \|X - A_1(A_1^\dagger + B_1Z_1^T)X(A_2^{\dagger T} + Z_2B_2^T)A_2^T\|_{\mathrm{F}} \tag{1286}$$

As for all projectors, the range of the projector is the subspace upon which projection is made; $\{P_1YP_2\}$. Altogether this means

$$P_1XP_2 - X \perp \{P_1YP_2 \mid Y \in \mathbb{R}^{m\times p}\} \text{ in } \mathbb{R}^{mp} \tag{1287}$$

and projectors P_1 and P_2 must each be symmetric (*confer* (1269)) to achieve the infimum, but may be of any rank:

E.7.1.0.1 Proof. *Minimum Frobenius norm* (1286).

$$\inf_{B_1,\, B_2} \|X - A_1(A_1^\dagger + B_1Z_1^T)X(A_2^{\dagger T} + Z_2B_2^T)A_2^T\|_{\mathrm{F}} \tag{1288}$$

Defining $P \triangleq A_1(A_1^\dagger + B_1Z_1^T)$,

$$\begin{aligned}
&\inf_{B_1,\, B_2} \|X - PX(A_2^{\dagger T} + Z_2B_2^T)A_2^T\|_{\mathrm{F}}^2 \\
&\quad = \inf_{B_1,\, B_2} \operatorname{tr}\Big((X^T - A_2(A_2^\dagger + B_2Z_2^T)X^TP^T)(X - PX(A_2^{\dagger T} + Z_2B_2^T)A_2^T)\Big) \\
&\quad = \inf_{B_1,\, B_2} \operatorname{tr}\Big(X^TX - X^TPX(A_2^{\dagger T} + Z_2B_2^T)A_2^T - A_2(A_2^\dagger + B_2Z_2^T)X^TP^TX \\
&\qquad\qquad + A_2(A_2^\dagger + B_2Z_2^T)X^TP^TPX(A_2^{\dagger T} + Z_2B_2^T)A_2^T\Big)
\end{aligned} \tag{1289}$$

[E.11] When P_1 and P_2 are symmetric and $\mathcal{R}(P_1) = \mathcal{R}(u_j)$ and $\mathcal{R}(P_2) = \mathcal{R}(q_j)$, then the j^{th} dyad term from the singular value decomposition of X is isolated by the projection. Yet if $\mathcal{R}(P_2) = \mathcal{R}(q_\ell)$, $\ell \neq j \in \{1 \ldots \eta\}$, then $P_1XP_2 = \mathbf{0}$.

The Frobenius norm is a convex function. [1, §8.1] Necessary and sufficient conditions for a global minimum are $\nabla_{B_1}=\mathbf{0}$ and $\nabla_{B_2}=\mathbf{0}$. (§D.1.3.1) Terms not containing B_2 in (1289) will vanish from the gradient ∇_{B_2} ; (§D.2.2)

$$\begin{aligned}
\nabla_{B_2}\operatorname{tr}\Big(&-X^TPXZ_2B_2^TA_2^T-A_2B_2Z_2^TX^TP^TX+A_2A_2^\dagger X^TP^TPXZ_2B_2^TA_2^T\\
&\qquad +A_2B_2Z_2^TX^TP^TPXA_2^{\dagger T}A_2^T+A_2B_2Z_2^TX^TP^TPXZ_2B_2^TA_2^T\Big)\\
&= -2A_2^TX^TPXZ_2+2A_2^TA_2A_2^\dagger X^TP^TPXZ_2+2A_2^TA_2B_2Z_2^TX^TP^TPXZ_2\\
&= A_2^T\Big(-X^T+A_2A_2^\dagger X^TP^T+A_2B_2Z_2^TX^TP^T\Big)PXZ_2\\
&= \mathbf{0}\\
&\Leftrightarrow\\
&\mathcal{R}(B_1)\subseteq\mathcal{N}(A_1) \text{ and } \mathcal{R}(B_2)\subseteq\mathcal{N}(A_2)
\end{aligned}\tag{1290}$$

The same conclusion is obtained were instead $P^T\triangleq(A_2^{\dagger T}+Z_2B_2^T)A_2^T$ and the gradient with respect to B_1 observed. ♦

E.7.1.0.2 Example. PXP redux, *nullspace.*
Suppose we define a subspace of all $m\times n$ matrices, each matrix having columns constituting a list whose geometric center (§4.5.1.0.1) is the origin in $\mathbb{R}^m$:

$$\begin{aligned}
\mathbb{R}_g^{m\times n} &\triangleq \{Y\in\mathbb{R}^{m\times n} \mid Y\mathbf{1}=\mathbf{0}\}\\
&=\{Y\in\mathbb{R}^{m\times n} \mid \mathcal{N}(Y)\supseteq\mathbf{1}\} = \{Y\in\mathbb{R}^{m\times n} \mid \mathcal{R}(Y^T)\subseteq\mathcal{N}(\mathbf{1}^T)\}
\end{aligned}\tag{1291}$$

Further suppose $V\in\mathbb{S}^n$ is a projection matrix having $\mathcal{N}(V)=\mathcal{R}(\mathbf{1})$ and $\mathcal{R}(V)=\mathcal{N}(\mathbf{1}^T)$. Then linear operator $T(X)=XV$ is an orthogonal projector, projecting any $X\in\mathbb{R}^{m\times n}$ on $\mathbb{R}_g^{m\times n}$ in the sense (1287) because V is symmetric, $XV\mathbf{1}=\mathbf{0}$, $\mathcal{N}(XV)\supseteq\mathbf{1}$, and $\mathcal{R}(VX^T)\subseteq\mathcal{N}(\mathbf{1}^T)$.

Now suppose we define a subspace of all symmetric $n\times n$ matrices each of whose columns constitute a list having the origin in $\mathbb{R}^n$ as their geometric center,

$$\begin{aligned}
\mathbb{S}_g^n &\triangleq \{Y\in\mathbb{S}^n \mid Y\mathbf{1}=\mathbf{0}\}\\
&=\{Y\in\mathbb{S}^n \mid \mathcal{N}(Y)\supseteq\mathbf{1}\} = \{Y\in\mathbb{S}^n \mid \mathcal{R}(Y)\subseteq\mathcal{N}(\mathbf{1}^T)\}
\end{aligned}\tag{1292}$$

the *geometric center subspace.* Further suppose $V\in\mathbb{S}^n$ is a projection matrix, the same as before. Then geometric centering operator $\mathbf{V}(X)=VXV$

(§4.6.1) is an orthogonal projector, projecting any $X \in \mathbb{S}^n$ on $\mathbb{S}_g^n$ in the sense (1287) because V is symmetric, $VXV\mathbf{1} = \mathbf{0}$, $\mathcal{N}(VXV) \supseteq \mathbf{1}$, and $\mathcal{R}(VXV) \subseteq \mathcal{N}(\mathbf{1}^T)$. Two-sided projection is necessary only to remain in the ambient symmetric subspace. Then

$$\mathbb{S}_g^n = \{VXV \mid X \in \mathbb{S}^n\} \subset \mathbb{S}^n \tag{1293}$$

We find its orthogonal complement as the aggregate of all directions of orthogonal projection on $\mathbb{S}_g^n$:

$$\begin{aligned} \mathbb{S}_g^{n\perp} &\triangleq \{VXV - X \mid X \in \mathbb{S}^n\} \subset \mathbb{S}^n \\ &= \{u\mathbf{1}^T + \mathbf{1}u^T \mid u \in \mathbb{R}^n\} \end{aligned} \tag{1294}$$

characterized by the doublet $u\mathbf{1}^T + \mathbf{1}u^T$ (§B.2).[E.12] Analogously to vector projectors (§E.2), $\mathcal{N}(\mathbf{V}) = \mathcal{R}(I - \mathbf{V})$; *id est*,

$$\mathcal{N}(\mathbf{V}) = \mathbb{S}_g^{n\perp} \tag{1295}$$

Now compare the subspace of symmetric matrices having all zeros in the first row and column

$$\begin{aligned} \mathbb{S}_{\mathbf{1}}^n &\triangleq \{Y \in \mathbb{S}^n \mid Ye_1 = \mathbf{0}\} \\ &= \left\{ \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} X \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} \mid X \in \mathbb{S}^n \right\} \end{aligned} \tag{1296}$$

[E.12] **Proof.**

$$\begin{aligned} \{VXV - X \mid X \in \mathbb{S}^n\} &= \{(I - \tfrac{1}{n}\mathbf{1}\mathbf{1}^T)X(I - \mathbf{1}\mathbf{1}^T\tfrac{1}{n}) - X \mid X \in \mathbb{S}^n\} \\ &= \{-\tfrac{1}{n}\mathbf{1}\mathbf{1}^T X \;-\; X\mathbf{1}\mathbf{1}^T\tfrac{1}{n} \;+\; \tfrac{1}{n}\mathbf{1}\mathbf{1}^T X\mathbf{1}\mathbf{1}^T\tfrac{1}{n} \mid X \in \mathbb{S}^n\} \end{aligned}$$

Because $\{X\mathbf{1} \mid X \in \mathbb{S}^n\} = \mathbb{R}^n$,

$$\begin{aligned} \{VXV - X \mid X \in \mathbb{S}^n\} &= \{-\mathbf{1}\zeta^T - \zeta\mathbf{1}^T + \mathbf{1}\mathbf{1}^T(\mathbf{1}^T\zeta\tfrac{1}{n}) \mid \zeta \in \mathbb{R}^n\} \\ &= \left\{-\mathbf{1}\zeta^T\left(I - \mathbf{1}\mathbf{1}^T\frac{1}{2n}\right) - \left(I - \frac{1}{2n}\mathbf{1}\mathbf{1}^T\right)\zeta\mathbf{1}^T \mid \zeta \in \mathbb{R}^n\right\} \end{aligned}$$

where $I - \frac{1}{2n}\mathbf{1}\mathbf{1}^T$ is invertible. ♦

where $\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix}$ is an orthogonal projector. Then similarly,

$$\begin{aligned} \mathbb{S}_{\mathbf{1}}^{n\perp} &\triangleq \left\{\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} X \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & I \end{bmatrix} - X \mid X\in\mathbb{S}^n\right\} \subset \mathbb{S}^n \\ &= \left\{u e_1^T + e_1 u^T \mid u\in\mathbb{R}^n\right\} \end{aligned} \tag{1297}$$

and obviously $\mathbb{S}_{\mathbf{1}}^n \oplus \mathbb{S}_{\mathbf{1}}^{n\perp} = \mathbb{S}^n$. □

E.8 Projection on convex set

Thus far we have discussed only projection on subspaces. Now we generalize, considering projection on arbitrary convex sets in Euclidean space; convex because projection is then unique.

If $\mathcal{C}\subseteq\mathbb{R}^n$ is a closed convex set, then for each and every $x\in\mathbb{R}^n$ there exists a unique point Px belonging to $\mathcal{C}$ that is closest to x in the Euclidean sense. Like before (1200), the unique projection Px of a point x on convex set $\mathcal{C}$ is that point in $\mathcal{C}$ closest to x; [37, §3.12]

$$\|x - Px\|_2 \;=\; \inf_{y\in\mathcal{C}} \|x-y\|_2 \tag{1298}$$

There exists a converse:

Bunt-Motzkin Theorem. *Convex set if projections unique.* [32, §7.5] [178] If $\mathcal{C}\subseteq\mathbb{R}^n$ is a nonempty closed set and if for each and every x in $\mathbb{R}^n$ there is a unique Euclidean projection of x on $\mathcal{C}$ belonging to $\mathcal{C}$, then $\mathcal{C}$ is convex. ◇

Also like before, there is a well-known equivalent characterization of projection on a convex set; a generalization of the perpendicularity condition (1199) for projection on a subspace:

E.8.0.0.1 Theorem. *Unique projection.*
[29, §A.3.1] [37, §3.12] [70, §4.1] [179] (Figure **E.6**(b), p.425) Point Px is the unique projection of a point $x\in\mathbb{R}^n$ on the closed convex set $\mathcal{C}\subseteq\mathbb{R}^n$ if and only if,

$$Px\in\mathcal{C}\,,\qquad \langle x-Px\,,\,y-Px\rangle\leq 0\quad\forall\,y\in\mathcal{C} \tag{1299}$$

In other words, Px is that point in $\mathcal{C}$ nearest some given x. ⋄

Yet unlike before, the operator P is not linear; projector P is a linear operator if and only if convex set $\mathcal{C}$ (on which projection is made) is a subspace.

E.8.0.0.2 Fact. *Non-expansivity.* When $\mathcal{C}\subset\mathbb{R}^n$ is an arbitrary closed convex set, projector P on $\mathcal{C}$ is non-expansive in the sense: [180, §2] for any $x\,,y\in\mathbb{R}^n$,

$$\|Px-Py\|\leq\|x-y\| \tag{1300}$$

with equality when $x-Px=y-Py$.[E.13] ⋄

Proof. [181]

$$\begin{aligned}\|x-y\|^2 =\;& \|Px-Py\|^2+\|(I-P)x-(I-P)y\|^2\\ &+2\langle x-Px\,,\,Px-Py\rangle+2\langle y-Py\,,\,Py-Px\rangle\end{aligned} \tag{1301}$$

Nonnegativity of the last two terms follows directly from the *unique projection theorem.* ♦

E.8.1 Projection on cone

When the convex set $\mathcal{C}$ is a cone, there is a finer statement of optimality conditions:

[E.13] This condition for equality corrects an error in [179] (where the norm is applied to each side of the condition given here) easily revealed by counter-example.

E.8.1.0.1 Theorem. *Unique projection on cone.* [29, §A.3.2]
Let $\mathcal{K}\subseteq\mathbb{R}^n$ be a closed convex cone, and $\mathcal{K}^*$ its dual (§2.8.1). Then Px is the unique (minimum distance) projection of $x\in\mathbb{R}^n$ on $\mathcal{K}$ if and only if

$$Px\in\mathcal{K}\,,\quad \langle Px-x\,,\,Px\rangle=0\,,\quad Px-x\in\mathcal{K}^* \tag{1302}$$

◇

In words, Px is the unique projection of x on $\mathcal{K}$ if and only if

1) projection Px lies in $\mathcal{K}$,

2) direction $Px-x$ is orthogonal to the projection Px,

3) direction $Px-x$ lies in the dual cone $\mathcal{K}^*$.

As stated, the theorem admits projection on $\mathcal{K}$ having empty interior; *id est*, convex cones in a proper subspace of $\mathbb{R}^n$. Projection on $\mathcal{K}$ of any point $x\in-\mathcal{K}^*$ belonging to the negative dual cone is on the origin.

E.8.1.1 Relation to subspace projection

The first and second conditions of the theorem are common with orthogonal projection on a subspace $\mathcal{R}(P)$: The first is the most basic requirement; namely, $Px\in\mathcal{R}(P)$, the projection belongs to the subspace. Invoking perpendicularity condition (1199), we recall the second requirement for projection on a subspace:

$$Px-x\perp\mathcal{R}(P)\quad\text{or}\quad Px-x\in\mathcal{R}(P)^\perp \tag{1303}$$

Yet condition 3 is a generalization of subspace projection; *id est*, for unique projection on a closed convex cone, $\mathcal{K}^*$ plays the role $\mathcal{R}(P)^\perp$ plays for subspace projection. Indeed, orthogonal vector sum (p.447) $\mathcal{K}\boxplus-\mathcal{K}^*=\mathbb{R}^n\Rightarrow$ cone $\mathcal{K}$ is closed and convex. [31, §2.7] Recalling that any subspace is a closed convex cone (but a proper subspace is not a proper cone (§2.6.2.0.2)),

$$\mathcal{K}=\mathcal{R}(P)\ \Leftrightarrow\ \mathcal{K}^*=\mathcal{R}(P)^\perp \tag{1304}$$

meaning, when a cone is a subspace $\mathcal{R}(P)$ then the dual cone becomes its orthogonal complement $\mathcal{R}(P)^\perp$. [1, §2.6.1] In this circumstance, condition 3 becomes coincident with condition 2.

By analogy to projection on the algebraic complement via $I-P$ in §E.2, given unique projection Px on convex cone $\mathcal{K}$ satisfying Theorem E.8.1.0.1,

$$\mathcal{K}^*=\{Px-x\mid x\in\mathbb{R}^n\} \tag{1305}$$

E.8.1.2 Salient properties: projection Px on closed convex cone $\mathcal{K}$

[29, §A.3.2]

1. $Px = \mathbf{0} \;\Leftrightarrow\; x \in -\mathcal{K}^*$
2. $P\alpha x = \alpha\, Px \;\; \forall\, \alpha \geq 0$
3. $P(-x)$ (on $\mathcal{K}$) $= -(Px$ on $-\mathcal{K})$
4. (Jean-Jacques Moreau)

$$\begin{gathered} x = x_1 + x_2\,, \quad x_1 \in \mathcal{K}\,, \quad x_2 \in -\mathcal{K}^*, \quad x_1 \perp x_2 \\ \Leftrightarrow \\ x_1 = Px \;\; (\text{on } \mathcal{K}) \quad \text{and} \quad x_2 = Px \;\; \text{on } -\mathcal{K}^* \end{gathered}$$

E.8.1.2.1 Example. *Unique projection on nonnegative orthant.*
(*confer* (712)) From the *unique projection on cone theorem*, to uniquely project matrix $H \in \mathbb{R}^{m\times n}$ on the self-dual orthant (§2.8.3.2) of nonnegative matrices $\mathbb{R}_+^{m\times n}$ in isomorphic $\mathbb{R}^{mn}$, the necessary and sufficient conditions are:

$$\begin{aligned} &H^\star \geq \mathbf{0} \\ &\operatorname{tr}\big((H^\star - H)^T H^\star\big) = 0 \\ &H^\star - H \geq \mathbf{0} \end{aligned} \tag{1306}$$

where the inequalities denote entry-wise comparison. The optimal solution $H^\star$ is simply H having all its negative entries zeroed. □

Example. *Unique projection on truncated convex cone.* Consider the problem of projecting a point x on a pointed closed convex cone that is artificially bounded; really, a bounded convex polyhedron having a vertex at the origin:

$$\begin{array}{cl} \underset{y\succeq 0}{\text{minimize}} & \|x - Ay\|_2 \\ \text{subject to} & \|y\|_\infty \leq 1 \end{array} \tag{1307}$$

where the (unbounded) cone has vertex-description (§2.7.2),

$$\mathcal{K} = \{Ay \mid y \succeq 0\} \tag{1308}$$

This is an optimization problem having no closed-form solution, in general. It arises, for example, in the fitting of hearing aids that are designed around a programmable graphic equalizer (a filter bank whose only adjustable parameters are gain). [182] The problem is equivalent to a Schur-form semidefinite program (§A.4.1),

$$\begin{array}{cl}\underset{y\succeq 0,\; t\in\mathbb{R}}{\text{minimize}} & t\\ \text{subject to} & \begin{bmatrix} tI & \operatorname{vec}(x-Ay)\\ \operatorname{vec}^T(x-Ay) & t\end{bmatrix}\succeq 0\\ & y\preceq \mathbf{1}\end{array}\tag{1309}$$

perhaps easier to solve numerically. □

E.8.2 Easy projections

- Projecting any matrix $H\in\mathbb{R}^{n\times n}$ orthogonally in the Euclidean/Frobenius sense on the subspace of symmetric matrices $\mathbb{S}^n$ in isomorphic $\mathbb{R}^{n^2}$ amounts to taking the symmetric part of H; (§2.1.2) *id est*, $(H+H^T)/2$ is the projection.

- To project any $H\in\mathbb{R}^{n\times n}$ orthogonally on the symmetric hollow subspace $\mathbb{S}^n_{\mathbf{0}}$ in isomorphic $\mathbb{R}^{n^2}$ (§2.1.2.2), we may take the symmetric part and then zero all entries along the main diagonal, or *vice versa* (because this is projection on the intersection of two subspaces); *id est*, $(H+H^T)/2-\delta^2(H)$.

- To project uniquely on the nonnegative orthant $\mathbb{R}^{m\times n}_+$, simply clip all negative entries to 0.

- Clipping in excess of $|1|$ each entry of a point $x\in\mathbb{R}^n$ is equivalent to unique projection of x on the unit hypercube centered at the origin. (*confer* §E.9.3.1.1)

- Projection of $x\in\mathbb{R}^n$ on a hyper-rectangle: [1, §8.1.1]

$$\mathcal{C}=\{y\in\mathbb{R}^n \mid l\preceq y\preceq u\,,\; l\prec u\}\tag{1310}$$

$$P(x)_k=\begin{cases} l_k\;, & x_k\leq l_k\\ x_k\;, & l_k\leq x_k\leq u_k\\ u_k\;, & x_k\geq u_k\end{cases}\tag{1311}$$

- Unique projection of $H \in \mathbb{S}^n$ in the Euclidean/Frobenius sense on the positive semidefinite cone $\mathbb{S}^n_+$ is accomplished by eigen-decomposition (diagonalization) followed by clipping all negative eigenvalues to 0.

  Unique projection on all rank ρ matrices belonging to $\mathbb{S}^n_+$ is accomplished by clipping all negative eigenvalues to 0 and zeroing the smallest nonnegative eigenvalues keeping only ρ largest. (§7.1.2)

- Unique projection of $H \in \mathbb{R}^{m\times n}$ in the Euclidean/Frobenius sense on the set of all $m\times n$ matrices of rank no greater than k is the singular value decomposition (§A.6) of H having all singular values beyond the k^{th} zeroed. [99, p.208] This solution is identical to the projection in the sense of spectral norm. [1, §8.1]

- Unique projection on ellipsoid (Figure **2.1**(c)) [164]...

- Unique projection on set of all matrices whose largest singular value does not exceed 1...

- Projection on Lorentz cone... [1, exer.8.3(c)]

Yet projecting matrix $H \in \mathbb{R}^{n\times n}$ uniquely on convex cone $\mathcal{K} = \mathbb{R}^{n\times n}_+ \cap \mathbb{S}^n$ in isomorphic $\mathbb{R}^{n^2}$ can be accomplished by first projecting on $\mathbb{S}^n$ and only then projecting the result on $\mathbb{R}^{n\times n}_+$: (*confer* §7.0.2)

E.8.3 Projection on convex set in subspace

Suppose a convex set $\mathcal{C}$ is contained in some subspace $\mathbb{R}^n$. Then unique (minimum distance) projection of any point in $\mathbb{R}^n \oplus \mathbb{R}^{n\perp}$ on $\mathcal{C}$ can be accomplished by first projecting orthogonally on that subspace, and then uniquely projecting the result on $\mathcal{C}$; [70, §5.14] *id est*, the ordered product of two individual projections.

To show that, suppose Px on $\mathcal{C}$ is y as illustrated in Figure **E.3**;

$$\|x-y\| \leq \|x-q\| \quad \forall\, q \in \mathcal{C} \tag{1312}$$

Further suppose Px on $\mathbb{R}^n$ equals z . By the *Pythagorean theorem*

$$\|x-y\|^2 = \|x-z\|^2 + \|z-y\|^2 \tag{1313}$$

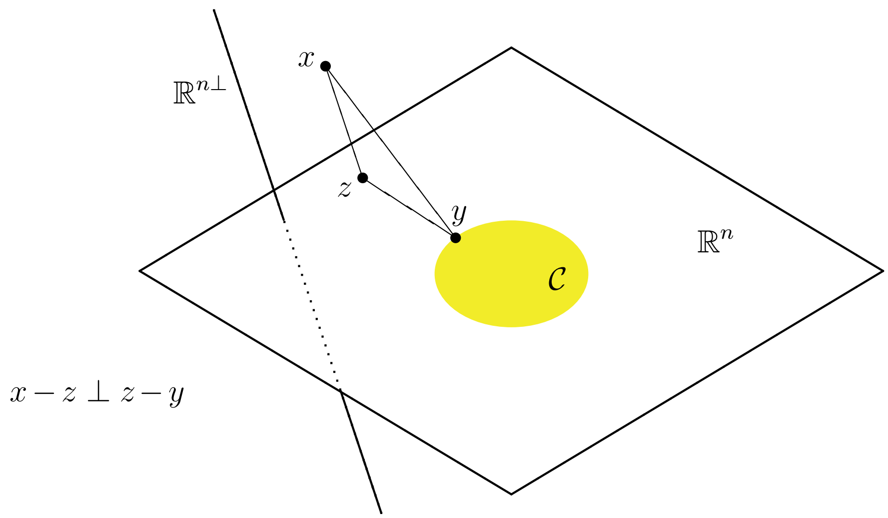


Figure E.3: Closed convex set $\mathcal{C}$, whose relative boundary is drawn, belongs to subspace $\mathbb{R}^n$ represented in sketch by the diamond (drawn without proper perspective). Point y is unique projection of x on $\mathcal{C}$; equivalent to product of orthogonal projection of x on $\mathbb{R}^n$ and unique projection of result z on $\mathcal{C}$.

because $x-z \perp z-y$. (1199) [37, §3.3] Then point y is also the projection of z on $\mathcal{C}$ because

$$\|z-y\|^2 \;=\; \|x-y\|^2 - \|x-z\|^2 \;\leq\; \|z-q\|^2 \;=\; \|x-q\|^2 - \|x-z\|^2 \quad \forall\, q \in \mathcal{C} \tag{1314}$$

The converse also holds. ♦

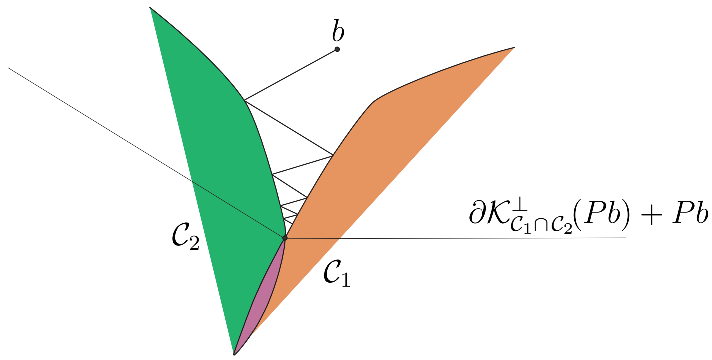


Figure E.4: First several iterations (1324) in the von Neumann-style projection of point b converging on the closest point Pb in the intersection of two closed convex sets in $\mathbb{R}^2$; $\mathcal{C}_1$ and $\mathcal{C}_2$ are partially drawn in the vicinity of their intersection. The pointed normal cone $\mathcal{K}^{\perp}$ (1345) is translated to Pb, the unique projection of b on the intersection. For this particular example, it is possible to start anywhere in a large neighborhood of b and still converge to Pb. The iterates are themselves robust with respect to some significant amount of noise because they belong to the translated normal cone.

E.9 Alternating projection

The method of alternating projection is an iterative technique for finding a point in the intersection of a number of arbitrary closed convex sets $\mathcal{C}_k$, or for finding the distance between two nonintersecting closed convex sets. Because it can sometimes be difficult or inefficient to compute the intersection or express it analytically, one naturally asks whether it is possible to instead sequentially project uniquely (minimum distance) on the individual $\mathcal{C}_k$, often easier. Once a sequence of projections (an *iteration*) is complete, we then cyclically repeat (*iterate*) the sequence until convergence, as we shall show. If the intersection of two closed convex sets is empty, then by *convergence* we mean the iterates settle to a point of minimum distance. (§E.9.2)

Given, in particular, two convex sets $\mathcal{C}_1$ and $\mathcal{C}_2$ and their respective projection operators P_1 and P_2, one considers alternating projection whenever those projectors do not commute; *id est*, when $P_1P_2 \neq P_2P_1$. When $\mathcal{C}_1$ and $\mathcal{C}_2$ are subspaces, projectors P_1 and P_2 commute if and only if $P_1P_2 = P_{\mathcal{C}_1\cap\mathcal{C}_2}$ or if and only if P_1P_2 is the orthogonal projection on a Euclidean subspace. [70, lem.9.2] Subspace projectors will commute, for example, when $\mathcal{C}_1 \subset \mathcal{C}_2$

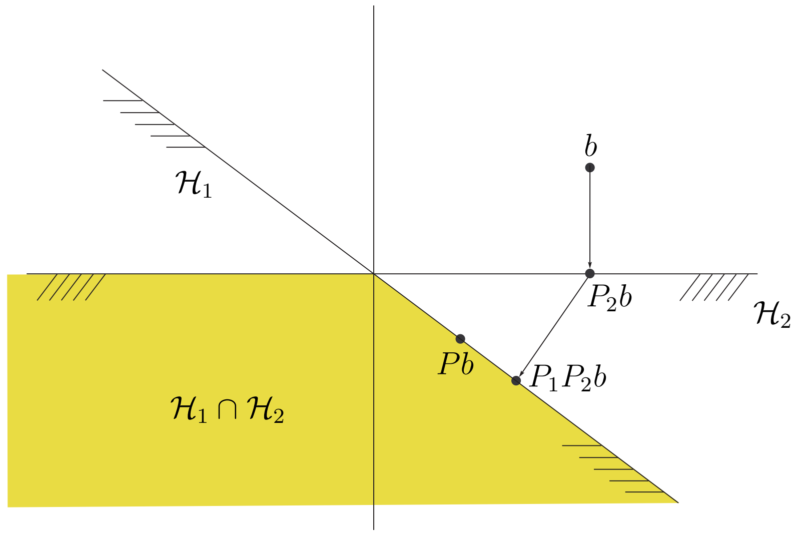


Figure E.5: The sets $\{\mathcal{C}_k\}$ in this example comprise two halfspaces $\mathcal{H}_1$ and $\mathcal{H}_2$. The von Neumann-style alternating projection in $\mathbb{R}^{\mathbf{2}}$ quickly converges to $P_1 P_2 b$ (feasibility). The unique projection on the intersection is, of course, Pb.

or $\mathcal{C}_2 \subset \mathcal{C}_1$ or $\mathcal{C}_1 \perp \mathcal{C}_2$. When the projectors commute, this means we can find a point in the intersection in a finite number of steps; in fact, the closest point.

The iconic example for non-commutative projectors illustrated in Figure **E.4** shows the iterates converging to the closest point in the intersection of two arbitrary convex sets. Yet simple examples like Figure **E.5** reveal that non-commutative alternating projection does not always yield the closest point, although we shall show it always yields some point in the intersection or a point that attains the distance between two convex sets.

Alternating projection is also known as *successive projection* [183] [180] [184], *cyclic projection* [137], *successive approximation* [179], or simply *projection on convex sets* [185, §6.4]. It is traced back to von Neumann (1933) [186] and later Wiener [187] who showed that higher iterates of a product of two orthogonal projections on subspaces converge at each point in the ambient space to the unique projection on the intersection of the two subspaces. More precisely, if $\mathcal{R}_1$ and $\mathcal{R}_2$ are closed subspaces of a Euclidean space and P_1 and P_2 respectively denote orthogonal projection on $\mathcal{R}_1$ and

$\mathcal{R}_2$, then for each vector b in that space,

$$\lim_{i\to\infty}(P_1P_2)^i b = P_{\mathcal{R}_1\cap\mathcal{R}_2} b \tag{1315}$$

Deutsch [70, thm.9.8, thm.9.35] shows that rate of convergence for subspaces is *geometric* [4, §1.4.4]; bounded above by $\kappa^{2i+1}\|b\|$, $i=0,1,2\ldots$, where $0\leq\kappa<1$:

$$\|\,(P_1P_2)^i b - P_{\mathcal{R}_1\cap\mathcal{R}_2} b\,\| \;\leq\; \kappa^{2i+1}\|b\| \tag{1316}$$

This means convergence can be slow when κ is close to 1.

This von Neumann sense of alternating projection may be applied to convex sets that are not subspaces, although convergence is not necessarily to the unique projection on the intersection. Figure **E.4** illustrates one application where convergence is reasonably geometric and the result is the unique projection. Figure **E.5**, in contrast, demonstrates convergence in one iteration to a *fixed point* (of the projection product)[E.14] in the intersection of two halfspaces; `a.k.a.`, feasibility problem.

Alternating projection has different meaning depending on the field of study; specifically, it may be interpreted as a distance problem, a feasibility problem (von Neumann), or an optimization problem (Dykstra):

- **Distance.** Figure **E.6**. Find a unique point of projection $P_1b\in\mathcal{C}_1$ that attains the distance between any two closed convex sets $\mathcal{C}_1$ and $\mathcal{C}_2$;

$$\|P_1b - b\| \;=\; \operatorname{dist}(\mathcal{C}_1\,,\,\mathcal{C}_2) \;\stackrel{\Delta}{=}\; \inf_{z\in\mathcal{C}_2}\|P_1z - z\| \tag{1317}$$

- **Feasibility.** Figure **E.6**(c), $\bigcap\mathcal{C}_k \neq \emptyset$. Given a number of indexed closed convex sets $\mathcal{C}_k\subset\mathbb{R}^n$, find any fixed point in their intersection by iterating (i) a projection product starting from b ;

$$\left(\prod_{i,k} P_k\right) b \;\in\; \bigcap_k \mathcal{C}_k \tag{1318}$$

- **Optimization.** Figure **E.6**(c), $\bigcap\mathcal{C}_k\neq\emptyset$. Given a number of indexed closed convex sets $\mathcal{C}_k\subset\mathbb{R}^n$, project a given point b on $\bigcap\mathcal{C}_k$;

$$\|Pb - b\| \;=\; \inf_{x\in\bigcap\mathcal{C}_k}\|x - b\| \tag{1319}$$

[E.14] A fixed point of a mapping $T:\mathbb{R}^n\to\mathbb{R}^n$ is a point x whose image is identical under the map; *id est*, $Tx=x$.

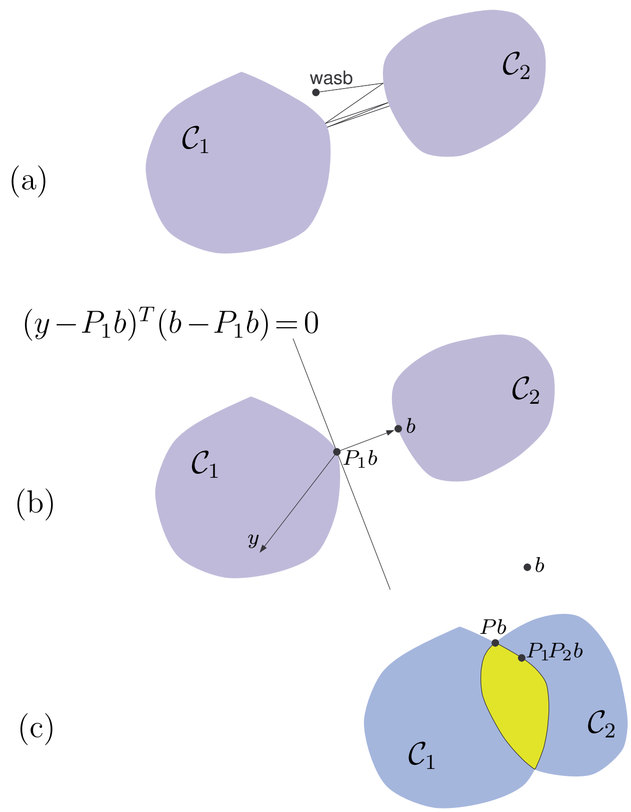


Figure E.6:
(a) (**distance**) Intersection of two convex sets in $\mathbb{R}^{\mathbf{2}}$ is empty. Method of alternating projection would be applied to find that point in $\mathcal{C}_1$ nearest $\mathcal{C}_2$.
(b) (**distance**) Given $b \in \mathcal{C}_2$, then $P_1b \in \mathcal{C}_1$ is nearest b iff $(y-P_1b)^T(b-P_1b) \leq 0 \ \forall\, y \in \mathcal{C}_1$ by the *unique projection theorem* (§E.8.0.0.1). When b attains the distance between the two sets, the hyperplane $\{y \mid (b-P_1b)^T(y-P_1b)=0\}$ separates $\mathcal{C}_1$ from $\mathcal{C}_2$. [1, §2.5.1]
(c) (**0 distance**) Intersection is nonempty. (**optimization**) We may want the point Pb in $\bigcap \mathcal{C}_k$ nearest point b, or (**feasibility**) we may instead be satisfied with a fixed point $x = P_1P_2b$ in $\bigcap \mathcal{C}_k$ of the projection product.

E.9.1 Distance and existence

The existence of a fixed point is established:

Theorem. *Distance.* [179] Given any two closed convex sets $\mathcal{C}_1$ and $\mathcal{C}_2$ in $\mathbb{R}^n$, then $P_1 b \in \mathcal{C}_1$ is a fixed point of the projection product $P_1 P_2$ if and only if $P_1 b$ is a point of $\mathcal{C}_1$ nearest $\mathcal{C}_2$. $\diamond$

Proof. ($\Longrightarrow$) Given fixed point $a = P_1 P_2 a \in \mathcal{C}_1$ with $b \overset{\Delta}{=} P_2 a \in \mathcal{C}_2$ in tandem so that $a = P_1 b$, then by the *unique projection theorem* (§E.8.0.0.1)

$$\begin{gathered}(u-a)^T(b-a) \leq 0 \quad \forall\, u \in \mathcal{C}_1 \\ (v-b)^T(a-b) \leq 0 \quad \forall\, v \in \mathcal{C}_2 \\ \Leftrightarrow \\ \|a-b\| \leq \|u-v\|\end{gathered} \tag{1320}$$

by the Schwarz inequality [38] [30].
($\Longleftarrow$) Suppose $a \in \mathcal{C}_1$ and $\|a - P_2 a\| \leq \|u - P_2 u\|\ \forall\, u \in \mathcal{C}_1$. Now suppose we choose $u = P_1 P_2 a$. Then

$$\|u - P_2 u\| = \|P_1 P_2 a - P_2 P_1 P_2 a\| \leq \|a - P_2 a\| \ \Leftrightarrow\ a = P_1 P_2 a \tag{1321}$$

Thus $a = P_1 b$ (with $b \overset{\Delta}{=} P_2 a \in \mathcal{C}_2$) is a fixed point in $\mathcal{C}_1$ of the projection product $P_1 P_2$.[E.15] ♦

E.9.2 Feasibility and convergence

The set of all fixed points of any non-expansive mapping is a closed convex set. [188, lem.3.4] [189, §1] The projection product $P_1 P_2$ is non-expansive by Fact E.8.0.0.2 because, for any $x, a \in \mathbb{R}^n$,

$$\|P_1 P_2 x - P_1 P_2 a\| \ \leq\ \|P_2 x - P_2 a\| \ \leq\ \|x - a\| \tag{1322}$$

If the intersection of two closed convex sets $\mathcal{C}_1 \cap \mathcal{C}_2$ is empty, then the iterates converge to a point of minimum distance, a fixed point of the projection product. Otherwise, convergence is to some fixed point in their intersection (a feasible point) whose existence is guaranteed by virtue of the fact that each

[E.15] Point $b = P_2 a$ can be shown similarly to be a fixed point of the product $P_2 P_1$.

and every point in the convex intersection is in one-to-one correspondence with fixed points of the non-expansive projection product.

Bauschke & Borwein [189, §2] argue that any sequence monotone in the sense of Fejér is convergent.[E.16]

Definition. *Fejér monotonicity.* [190] Given closed convex set $\mathcal{C} \neq \emptyset$, then a sequence $[\, x_i \in \mathbb{R}^n \mid i \geq 0 \,]$ is monotone in the sense of Fejér with respect to $\mathcal{C}$ iff

$$\|x_{i+1} - c\| \leq \|x_i - c\| \quad \text{for every } i \geq 0 \;\text{ and }\; \forall\, c \in \mathcal{C} \tag{1323}$$

$\triangle$

Given $x_0 \stackrel{\Delta}{=} b$, if we express each iteration of alternating projection by

$$x_{i+1} = P_1 P_2\, x_i \;, \quad i = 0, 1, 2 \ldots \tag{1324}$$

and define any fixed point $a = P_1 P_2\, a$, then the sequence x_i is Fejér monotone with respect to fixed point a because

$$\|P_1 P_2\, x_i - a\| \leq \|x_i - a\| \quad \forall\, i \geq 0 \tag{1325}$$

by non-expansivity. The nonincreasing sequence $\|P_1 P_2\, x_i - a\|$ is bounded below hence convergent because any bounded monotone sequence in $\mathbb{R}$ is convergent; [36, §1.2] [33, §1.1] $P_1 P_2\, x_{i+1} = P_1 P_2\, x_i = x_{i+1}$. Sequence x_i therefore converges to some fixed point. If the intersection $\mathcal{C}_1 \cap \mathcal{C}_2$ is nonempty, convergence is to some point there by the *distance theorem.* Otherwise, x_i converges to a point in $\mathcal{C}_1$ of minimum distance to $\mathcal{C}_2$.

E.9.2.0.1 Example. *Hyperplane/orthant intersection.* Find a feasible point $(\prod P_k) b$ belonging to the nonempty intersection of two convex sets:

$$\mathcal{C}_1 \cap \mathcal{C}_2 \;=\; \mathbb{R}^n_+ \cap \mathcal{A} \;=\; \{y \mid y \succeq 0\} \cap \{y \mid Ay = \beta\} \subset \mathbb{R}^n \tag{1326}$$

the nonnegative orthant with affine subset $\mathcal{A}$ an intersection of hyperplanes $\big(A \in \mathbb{R}^{m\times n},\; \beta \in \mathcal{R}(A)\big)$. Projection of an iterate $x_i \in \mathbb{R}^n$ on $\mathcal{A}$ is calculated

$$P_2\, x_i \;=\; x_i - A^T (AA^T)^{-1} (Ax_i - \beta) \qquad (1246)$$

while, thereafter, projection of the result on the orthant is simply

$$x_{i+1} \;=\; P_1 P_2\, x_i \;=\; \max\{\mathbf{0}, P_2\, x_i\} \tag{1327}$$

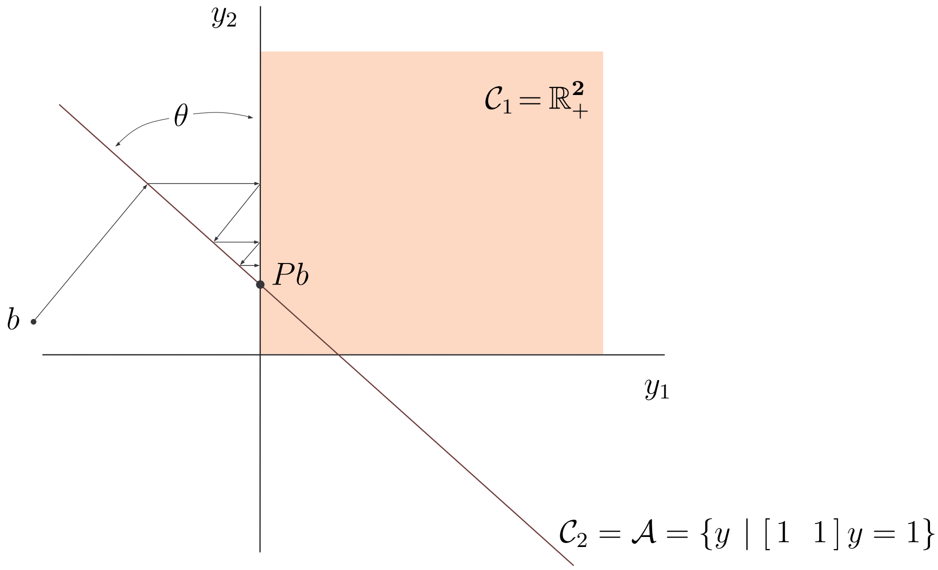


Figure E.7: From Example E.9.2.0.1 in $\mathbb{R}^{\mathbf{2}}$, showing von Neumann-style iterations to find feasible point belonging to intersection of nonnegative orthant with hyperplane. Point Pb lies at intersection of hyperplane with ordinate. In this particular example, the feasible point found is coincidentally optimal. The rate of convergence depends upon angle θ; as it becomes more acute, convergence slows. [180, §3]

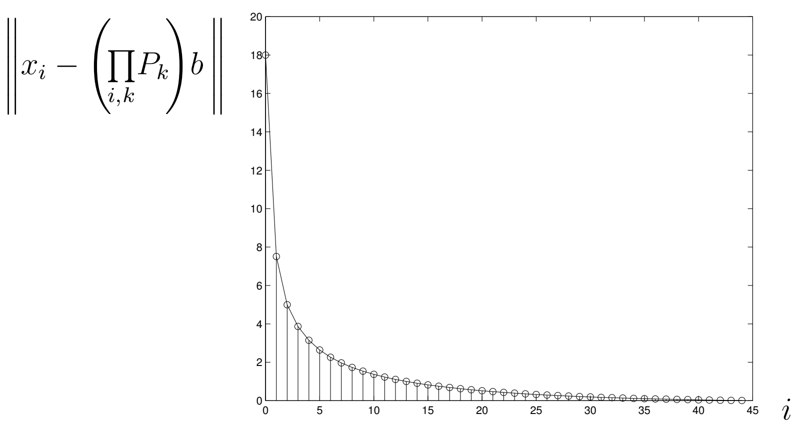


Figure E.8: Geometric convergence of iterates in norm, for Example E.9.2.0.1 in $\mathbb{R}^{\mathbf{1000}}$.

where the maximum is entry-wise (§E.8.1.2.1).

One realization of this problem in $\mathbb{R}^2$ is illustrated in Figure **E.7**: For $A=[\,1\;\;1\,]$, $\beta=1$, and $x_0=b=[\,-3\;\;1/2\,]^T$, the iterates converge to the feasible point $Pb=[\,0\;\;1\,]^T$.

To give a more palpable sense of convergence in higher dimension, we do this example again but now we compute an alternating projection for the case $A\in\mathbb{R}^{400\times1000}$, $\beta\in\mathbb{R}^{400}$, and $b\in\mathbb{R}^{1000}$, all of whose entries are independently and randomly set to a uniformly distributed real number in the interval $[-1,1]$. The sequence $\|x_i-(\prod\limits_{i,k}P_k)b\|$ is plotted in Figure **E.8**.

$\square$

This application of alternating projection to feasibility is extensible to any finite number of closed convex sets.

E.9.2.1 Relative measure of convergence

The algorithm we used in the Example illustrated in Figure **E.8** required two passes; the first estimates point $\lim\limits_{i\to\infty}(\prod\limits_{i,\ell}P_\ell)b$ in the presumably nonempty intersection, a technique motivated by Fejér monotonicity. *A priori* knowledge of a feasible point to monitor convergence is impractical and antithetical, so we need an alternative measure. Non-expansiveness implies

$$\left\|\left(\prod_\ell^k P_\ell\right)x_{k,i-1}-\left(\prod_\ell^k P_\ell\right)x_{ki}\right\| \;=\; \|x_{ki}-x_{k,i+1}\| \;\le\; \|x_{k,i-1}-x_{ki}\| \tag{1328}$$

where $x_{ki}\in\mathbb{R}^n$ represents unique projection of $x_{k+1,i}$ on convex set k at iteration i. So a good convergence measure is the total monotonic sequence

$$\varepsilon_i \;\triangleq\; \sum_k \|x_{ki}-x_{k,i+1}\| \tag{1329}$$

where $\lim\limits_{i\to\infty}\varepsilon_i=0$ whether or not the intersection is nonempty.

E.9.2.1.1 Example. *Affine subset of positive semidefinite cone.* Consider the problem of finding $X\in\mathbb{S}^n$ that satisfies

$$X\succeq 0\,,\qquad \langle A_j\,,X\rangle=b_j\,,\quad j=1\ldots m \tag{1330}$$

[E.16] Other authors prove convergence by different means. [180] [184]

given nonzero $A_j \in \mathbb{S}^n$ and real b_j. Here we take $\mathcal{C}_1$ to be the positive semidefinite cone $\mathbb{S}^n_+$ while $\mathcal{C}_2$ is the affine subset of $\mathbb{S}^n$

$$\begin{aligned}\mathcal{C}_2 \;=\; \mathcal{A} &\triangleq \{X \mid \operatorname{tr}(A_j X) = b_j\;,\; j=1\ldots m\} \subseteq \mathbb{S}^n \\ &= \{X \mid \begin{bmatrix}\operatorname{vec}(A_1)^T \\ \vdots \\ \operatorname{vec}(A_m)^T\end{bmatrix} \operatorname{vec} X = b\} \\ &\triangleq \{X \mid A \operatorname{vec} X = b\}\end{aligned} \tag{1331}$$

where $b = [b_j] \in \mathbb{R}^m$, $A \in \mathbb{R}^{m\times n^2}$, and vectorization vec is defined in (18). Projection of iterate $X_i \in \mathbb{S}^n$ on $\mathcal{A}$ is: (§E.5.0.1.6)

$$P_2 \operatorname{vec} X_i = \operatorname{vec} X_i - A^\dagger(A \operatorname{vec} X_i - b) \tag{1332}$$

The Euclidean distance from X_i to $\mathcal{A}$ is therefore

$$\operatorname{dist}(X_i\,, \mathcal{A}) \;=\; \|X_i - P_2 X_i\|_{\mathrm{F}} \;=\; \|A^\dagger(A \operatorname{vec} X_i - b)\|_2 \tag{1333}$$

Projection on the positive semidefinite cone (§7.1) is found from the eigendecomposition $P_2 X_i = \sum\limits_j \lambda_j\, q_j q_j^T$;

$$P_1 P_2 X_i = \sum_{j=1}^{n} \max\{0\,, \lambda_j\} q_j q_j^T \tag{1334}$$

The distance from $P_2 X_i$ to the positive semidefinite cone is therefore

$$\operatorname{dist}(P_2 X_i\,, \mathbb{S}^n_+) \;=\; \|P_2 X_i - P_1 P_2 X_i\|_{\mathrm{F}} \;=\; \sqrt{\sum_{j=1}^{n} \min\{0\,, \lambda_j\}^2} \tag{1335}$$

When the intersection is empty $\mathcal{A} \cap \mathbb{S}^n_+ = \emptyset$, the alternating projections converge to that positive semidefinite matrix closest to $\mathcal{A}$ in the Euclidean sense. Otherwise, the alternation converges to some point in the nonempty intersection.

Barvinok (§2.6.6.4.1) shows that if a point feasible with (1330) exists, then there exists an $X \in \mathcal{A} \cap \mathbb{S}^n_+$ such that

$$\operatorname{rank} X \leq \left\lfloor \frac{\sqrt{8m+1} - 1}{2} \right\rfloor \tag{148}$$

$\square$

E.9.2.1.2 Example. *Semidefinite matrix completion.*
Continuing Example E.9.2.1.1: When $m \le n(n+1)/2$ and the A_j matrices are unique members of the standard orthonormal basis $\{E_{\ell q} \in \mathbb{S}^n\}$ (38),

$$\{A_j \in \mathbb{S}^n,\ j=1\ldots m\} \subseteq \{E_{\ell q}\} = \left\{ \begin{array}{ll} e_\ell e_\ell^T\,, & \ell = q = 1\ldots n \\ \frac{1}{\sqrt{2}}(e_\ell e_q^T + e_q e_\ell^T)\,, & 1 \le \ell < q \le n \end{array} \right\} \tag{1336}$$

and when the constants b_j are set to constrained entries of variable X,

$$\{b_j\,,\ j=1\ldots m\} \subseteq \left\{ \begin{array}{ll} X_{\ell q}\,, & \ell = q = 1\ldots n \\ X_{\ell q}\sqrt{2}\,, & 1 \le \ell < q \le n \end{array} \right\} = \{\langle X, E_{\ell q}\rangle\} \tag{1337}$$

then the equality constraints in (1330) fix individual entries of $X \in \mathbb{S}^n$. Thus the feasibility problem becomes a *positive semidefinite matrix completion problem.* Projection of iterate $X_i \in \mathbb{S}^n$ on $\mathcal{A}$ simplifies to (*confer* (1332))

$$P_2 \operatorname{vec} X_i = \operatorname{vec} X_i - A^T(A \operatorname{vec} X_i - b) \tag{1338}$$

From this we can see that orthogonal projection is achieved simply by setting corresponding entries of $P_2 X_i$ to the known entries of X, while the remaining entries of $P_2 X_i$ are set to corresponding entries of the current iterate X_i.

Using this technique, we find a positive semidefinite completion for

$$\begin{bmatrix} 4 & 3 & ? & 2 \\ 3 & 4 & 3 & ? \\ ? & 3 & 4 & 3 \\ 2 & ? & 3 & 4 \end{bmatrix} \tag{1339}$$

Initializing the unknown entries to 0, they all converge geometrically to 1.5858 (rounded) after about 42 iterations.

Laurent gives a problem for which no positive semidefinite completion exists: [191]

$$\begin{bmatrix} 1 & 1 & ? & 0 \\ 1 & 1 & 1 & ? \\ ? & 1 & 1 & 1 \\ 0 & ? & 1 & 1 \end{bmatrix} \tag{1340}$$

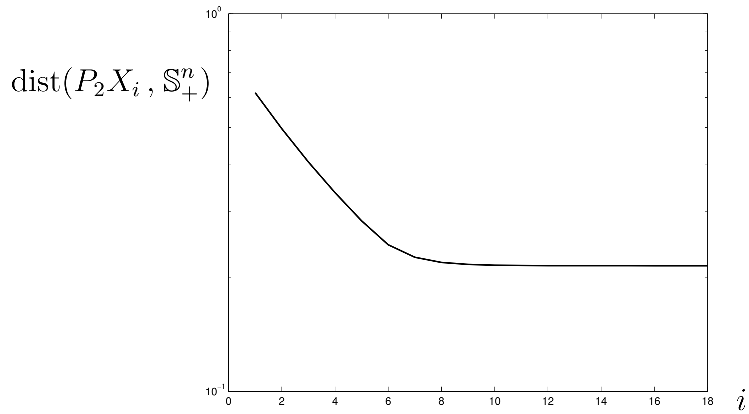


Figure E.9: Distance between iterate in $\mathcal{A}$ (1331) and PSD cone for Laurent's problem; initially decreasing geometrically.

By alternating projection we find the constrained matrix closest to the positive semidefinite cone,

$$\begin{bmatrix} 1 & 1 & 0.5454 & 0 \\ 1 & 1 & 1 & 0.5454 \\ 0.5454 & 1 & 1 & 1 \\ 0 & 0.5454 & 1 & 1 \end{bmatrix} \tag{1341}$$

and we find the positive semidefinite matrix closest to the affine subset $\mathcal{A}$ (1331):

$$\begin{bmatrix} 1.0521 & 0.9409 & 0.5454 & 0.0292 \\ 0.9409 & 1.0980 & 0.9451 & 0.5454 \\ 0.5454 & 0.9451 & 1.0980 & 0.9409 \\ 0.0292 & 0.5454 & 0.9409 & 1.0521 \end{bmatrix} \tag{1342}$$

These matrices (1341) and (1342) achieve the Euclidean distance $\operatorname{dist}(\mathcal{A}\,,\,\mathbb{S}^n_+)$. Convergence is illustrated in Figure **E.9**. □

E.9.3 Optimization

Unique projection on the nonempty intersection of arbitrary convex sets to find the closest point therein is a convex optimization problem. The first successful application of alternating projection to this problem is attributed to Dykstra [192] [193] who in 1983 provided an elegant algorithm that prevails

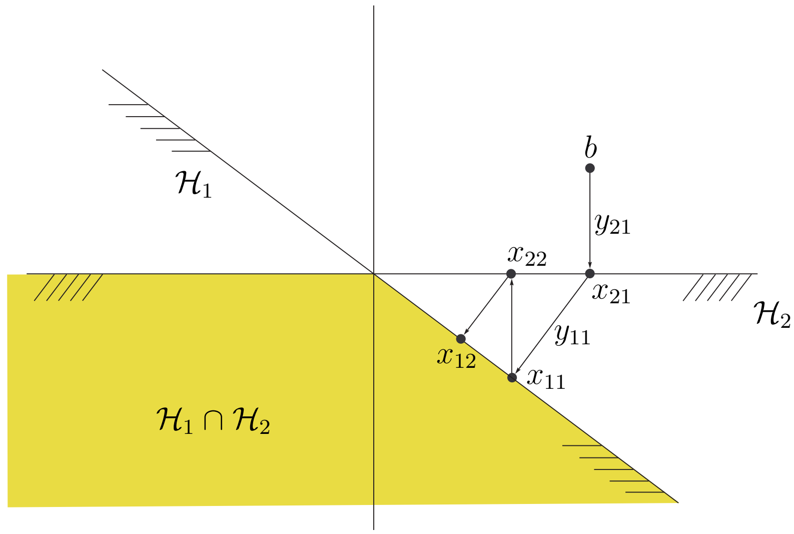


Figure E.10: $\mathcal{H}_1$ and $\mathcal{H}_2$ are the same halfspaces as in Figure **E.5**. Dykstra's alternating projection algorithm generates the sequence $[\, b\,, x_{21}\,, x_{11}\,, x_{22}\,, x_{12}\,, x_{12} \ldots]$. The path illustrated from b to x_{12} in $\mathbb{R}^{\mathbf{2}}$ terminates at the desired result, Pb. The iterates are not so robust in the presence of noise as for the example in Figure **E.4**.

today. In 1988, Han [183] rediscovered the algorithm and provided a primal-dual convergence proof. A synopsis of the history of alternating projection can be found in [194] where it becomes apparent that Dykstra's work is seminal.[E.17]

E.9.3.1 Dykstra's algorithm

Given some point $b \in \mathbb{R}^n$ and closed convex sets $\{\mathcal{C}_k \subset \mathbb{R}^n \mid k = 1 \ldots L\}$, let $x_{ki} \in \mathbb{R}^n$ and $y_{ki} \in \mathbb{R}^n$ respectively denote a primal and dual vector associated with set k at iteration i. Initialize $y_{k0} = 0 \;\; \forall\, k = 1 \ldots L$, and $x_{1,0} = b$. Denoting by $P_k t$ the unique projection of t on $\mathcal{C}_k$, and for convenience

[E.17]For a synopsis of alternating projection applied to distance geometry, see [73, §3.1].

$x_{L+1,i} \stackrel{\Delta}{=} x_{1,i-1}$, calculation of the iterates proceeds:[E.18]

$$\begin{array}{l}
\texttt{for } i=1,2,\ldots \texttt{until convergence } \{ \\
\quad \texttt{for } k=L\ldots 1 \ \{ \\
\qquad t = x_{k+1,i} - y_{k,i-1} \\
\qquad x_{ki} = P_k t \\
\qquad y_{ki} = P_k t - t \\
\quad \} \\
\}
\end{array} \tag{1343}$$

Assuming a nonempty intersection, then the iterates converge to the unique projection of point b on that intersection; [70, §9.24]

$$Pb = \lim_{i\to\infty} x_{1i} \tag{1344}$$

In the case all the $\mathcal{C}_k$ are affine, then calculation of y_{ki} is superfluous and the algorithm becomes identical to alternating projection. [70, §9.26] [137, §1] Dykstra's algorithm is so simple, elegant, and represents such a tiny increment in computational intensity over alternating projection, that it is nearly always arguably cost-effective.

E.9.3.1.1 Normal cone. Glunt [136, §4] observes that the overall effect of this iterative procedure is to drive t toward the translated *normal cone* to $\bigcap \mathcal{C}_k$ at the solution Pb (translated to Pb).

The normal cone to any set $\mathcal{S} \subseteq \mathbb{R}^n$ at any particular $a \in \mathbb{R}^n$ is defined as the closed cone [29, §A.5]

$$\mathcal{K}_{\mathcal{S}}^{\perp}(a) \stackrel{\Delta}{=} \{z \in \mathbb{R}^n \mid z^T(y-a) \leq 0\,,\ \forall\, y \in \mathcal{S}\} \tag{1345}$$

an intersection of halfspaces about the origin, hence convex regardless of the convexity of $\mathcal{S}$. Projection on $\mathcal{S}$ of any point in the translated normal cone $\mathcal{K}_{\mathcal{S}}^{\perp}(a) + a$ (translated to any $a \in \mathcal{S}$) is identical to a .

The normal cone to $\bigcap \mathcal{C}_k$ at Pb in Figure **E.5** is the ray $\{\xi(b-Pb) \mid \xi \geq 0\}$. Applying Dykstra's algorithm to that example, convergence to the desired result is achieved in two iterations as illustrated in Figure **E.10**. Yet applying Dykstra's algorithm to the example in Figure **E.4** does not improve the rate of convergence, unfortunately, because the given point b and all the iterates already belong to the translated normal cone at the vertex of intersection.

[E.18] We reverse order of projection ($k = L \ldots 1$) for continuity of exposition.

Appendix F

MATLAB programs...

These programs are available on the author's website:
http://www.stanford.edu/~dattorro/...

F.1 `isedm()`

...

F.1.1 Subroutines for `isedm()`

F.1.1.1 `chop()`

F.1.1.2 `Vn()`

F.1.1.3 `signeig()`

F.1.1.4 `Dx()`

F.1.1.5 `modchol()` [148]

```
% modified Cholesky factorization.
% -Walter Murray
% A = R^T R - E
function [r,e] = modchol(a)

n = size(a,2);
r = zeros(n,n); e = zeros(n,n);
delta = eps*n*norm(a);

gamma = max(abs(diag(a,0)));
xi = max(max(abs(a - diag(diag(a,0)))));
beta = sqrt(max([gamma, xi/sqrt(n^2-1), eps]));

for k = 1:n
   if k+1<=n, mu(k)=max(abs(a(k,k+1:n))); else mu(k)=0; end;

   r(k,k) = max([delta, sqrt(abs(a(k,k))), mu(k)/beta]);
   e(k,k) = r(k,k)^2 - a(k,k);

   for j=k+1:n
      r(k,j) = a(k,j)/r(k,k);
      for i=k+1:j
         a(i,j) = a(i,j) - r(k,j)*r(k,i);
      end
   end
end
```

F.2 conic independence

The recommended subroutine `lp()` is a linear program solver from MATLAB's *Optimization Toolbox* v2.0 (R11). Later releases of MATLAB replace `lp()` with `linprog()` that we find quite inferior to `lp()` on a wide range of problems.

```
% Test for c.i. of arbitrary directions. -Jon Dattorro 2001
function [indep, how_many_depend, Xci] = conici(X);
[n, N] = size(X);

indep = 'conically independent';
how_many_depend = 0;
if rank(X) == N, Xci = X; return, end

count = 1;
new_N = N;
for i=1:N
   A = [X(:,1:count-1) X(:,count+1:new_N); -eye(new_N-1)];
   b = [X(:,count); zeros(new_N-1,1)];
   [a, lambda, how] = lp(zeros(new_N-1,1),A,b,[ ],[ ],[ ],n,-1);
   if ~strcmp(how,'infeasible')
      how_many_depend = how_many_depend + 1;
      indep = 'conically Dependent';
      X(:,count) = [ ];
      new_N = new_N - 1;
   else
      count = count + 1;
   end
end
Xci = X;
```

F.2.1 lp()

```
LP     Linear programming.
X=LP(f,A,b) solves the linear programming problem:

            min f'x    subject to:   Ax <= b
             x

X=LP(f,A,b,VLB,VUB) defines a set of lower and upper
bounds on the design variables, X, so that the solution is
always in the range VLB <= X <= VUB.

X=LP(f,A,b,VLB,VUB,X0) sets the initial starting point to X0.

X=LP(f,A,b,VLB,VUB,X0,N) indicates that the first N constraints
defined by A and b are equality constraints.

X=LP(f,A,b,VLB,VUB,X0,N,DISPLAY) controls the level of warning
messages displayed.  Warning messages can be turned off with
DISPLAY = -1.

[X,LAMBDA]=LP(f,A,b) returns the set of Lagrangian multipliers,
LAMBDA, at the solution.

[X,LAMBDA,HOW] = LP(f,A,b) also returns a string how that
indicates error conditions at the final iteration.

LP produces warning messages when the solution is either
unbounded or infeasible.
```

F.3 Map of the USA

F.3.1 EDM

```
%Find map of USA using only distance information.
% -Jon Dattorro 2001
%EDM reconstruction problem.
clear all;
close all;

load usalo; %From Matlab Mapping Toolbox
%http://www-ccs.ucsd.edu/matlab/toolbox/map/usalo.html

%To speed-up execution (decimate map data), make
%'factor' bigger positive integer.
factor = 2;
Mg = 2*factor; %Relative decimation factors
Ms = factor;
Mu = 2*factor;

gtlakelat  = decimate(gtlakelat,Mg);
gtlakelon  = decimate(gtlakelon,Mg);
statelat   = decimate(statelat,Ms);
statelon   = decimate(statelon,Ms);
uslat      = decimate(uslat,Mu);
uslon      = decimate(uslon,Mu);

lat = [gtlakelat; statelat; uslat]*pi/180;
lon = [gtlakelon; statelon; uslon]*pi/180;
phi = pi/2 - lat;
theta = lon;
x = sin(phi).*cos(theta);
y = sin(phi).*sin(theta);
z = cos(phi);


%plot original data
plot3(x,y,z), axis equal, axis off
```

```
lengthNaN = length(lat);
id = find(isfinite(x));
X = [x(id)'; y(id)'; z(id)'];
N = length(X(1,:))

% Construct the distance matrix
clear gtlakelat gtlakelon statelat statelon
clear factor x y z phi theta conus
clear uslat uslon Mg Ms Mu lat lon
D = diag(X'*X)*ones(1,N) + ones(N,1)*diag(X'*X)' - 2*X'*X;

%destroy input data
clear X

Vn = [-ones(1,N-1); speye(N-1)];
VDV = (-Vn'*D*Vn)/2;

clear D Vn
pack

[evec evals flag] = eigs(VDV, speye(size(VDV)), 10, 'LR');
if flag, disp('convergence problem'), return, end;
evals = real(diag(evals));

index = find(abs(evals) > eps*normest(VDV)*N);
n = sum(evals(index) > 0);
Xs = [zeros(n,1)  diag(sqrt(evals(index)))*evec(:,index)'];

warning off; Xsplot=zeros(3,lengthNaN)*(0/0); warning on;
Xsplot(:,id) = Xs;
figure(2)

%plot map found via EDM.
plot3(Xsplot(1,:), Xsplot(2,:), Xsplot(3,:))
axis equal, axis off
```

F.3.1.1 USA map input-data decimation subroutine

```
function xd = decimate(x,m)
roll = 0;
rock = 1;
for i=1:length(x)
   if isnan(x(i))
      roll = 0;
      xd(rock) = x(i);
      rock=rock+1;
   else
      if ~mod(roll,m)
         xd(rock) = x(i);
         rock=rock+1;
      end
      roll=roll+1;
   end
end
xd = xd';
```

F.3.2 EDM using ordinal data

```
%Find map of USA using ORDINAL distance information.
% -Jon Dattorro 2003
%EDM reconstruction problem.
clear all;
close all;

load usalo; %From Matlab Mapping Toolbox
%http://www-ccs.ucsd.edu/matlab/toolbox/map/usalo.html

factor = 2;    %Execution time factor=2 approx. 18 minutes.
Mg = 2*factor; %Relative decimation factors
Ms = factor;
Mu = 2*factor;

gtlakelat  = decimate(gtlakelat,Mg);
gtlakelon  = decimate(gtlakelon,Mg);
```

```
statelat   = decimate(statelat,Ms);
statelon   = decimate(statelon,Ms);
uslat      = decimate(uslat,Mu);
uslon      = decimate(uslon,Mu);

lat = [gtlakelat; statelat; uslat]*pi/180;
lon = [gtlakelon; statelon; uslon]*pi/180;
phi = pi/2 - lat;
theta = lon;
x = sin(phi).*cos(theta);
y = sin(phi).*sin(theta);
z = cos(phi);

%plot original data
plot3(x,y,z), axis equal, axis off

lengthNaN = length(lat);
id = find(isfinite(x));
X = [x(id)'; y(id)'; z(id)'];
N = length(X(1,:))

% Construct the distance matrix
clear gtlakelat gtlakelon statelat statelon
clear factor x y z phi theta conus
clear uslat uslon Mg Ms Mu lat lon
D = diag(X'*X)*ones(1,N) + ones(N,1)*diag(X'*X)' - 2*X'*X;

%ORDINAL MDS - vectorize D
count = 1;
f = zeros(N*(N-1)/2,1);
for j=1:N
   for i=1:N
      if i<j
         f(count) = D(i,j);
         count = count + 1;
      end
   end
end
```

```
%sorted = f(idx)
[sorted idx] = sort(f);
clear D sorted X
M = (N*(N-1))/2;
f(idx)=((1:M).^2)/M^2;

%Create ordinal data matrix
O = zeros(N,N);
count = 1;
for j=1:N
   for i=1:N
      if i<j
         O(i,j) = f(count);
         O(j,i) = f(count);
         count = count+1;
      end
   end
end

Vn = [-ones(1,N-1); speye(N-1)];
VOV = (-Vn'*O*Vn)/2;

clear O Vn f idx
pack

[evec evals flag] = eigs(VOV, speye(size(VOV)), 10, 'LR');
if flag, disp('convergence problem'), return, end;
evals = real(diag(evals));

Xs = [zeros(3,1)  diag(sqrt(evals(1:3)))*evec(:,1:3)'];

warning off; Xsplot=zeros(3,lengthNaN)*(0/0); warning on;
Xsplot(:,id) = Xs;
figure(2)

%plot map found via Ordinal MDS.
plot3(Xsplot(1,:), Xsplot(2,:), Xsplot(3,:))
axis equal, axis off
```

Appendix G

Notation and some definitions

b	vector, scalar, or logical condition
g'	first derivative of possibly multidimensional function with respect to real argument
g''	second derivative with respect to real argument
b^T	vector b transpose
b^H	vector b Hermitian (conjugate) transpose
$\overset{\to Y}{dg}$	first directional derivative of possibly multidimensional function g in direction $Y \in \mathbb{R}^{K\times L}$ (maintains dimensions of g)
$\overset{\to Y}{dg^2}$	second directional derivative of g in direction Y
$b_{i:j}$	truncated vector comprising i^{th} through j^{th} entry of vector b
A	matrix, vector, scalar, or logical condition
fat	a fat matrix, meaning more columns than rows; $\begin{bmatrix} \quad\quad\quad\quad \end{bmatrix}$
skinny	a skinny matrix, meaning more rows than columns; $\begin{bmatrix} \\ \\ \\ \end{bmatrix}$

$\mathcal{A}$	some set (calligraphic $\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$)
$\mathcal{F}(\mathcal{C}\ni A)$	smallest face of set $\mathcal{C}$ containing element A
$A^\dagger$	Moore-Penrose pseudoinverse of matrix A
$A^{1/2}$ or $\sqrt{A}$	any matrix such that $\sqrt{A}\sqrt{A}=A$. For $A\in\mathbb{S}_+^n$, $\sqrt{A}\in\mathbb{S}_+^n$ is unique. [39, §1.2]
$A(:,i)$	i^{th} column of matrix A [44, §1.1.8]
$A(j,:)$	j^{th} row of matrix A
a.i.	affinely independent
c.i.	conically independent
l.i.	linearly independent
Re	real part
Im	imaginary part
PSD	positive semidefinite
SDP	semidefinite program
EDM	Euclidean distance matrix
$\mathbb{EDM}^N$	cone of $N\times N$ Euclidean distance matrices in symmetric hollow subspace
$\in$	membership, *belongs to*
$\ni$	membership, *contains* as in $\mathcal{C}\ni y$
$\subset$ $\supset$ $\cap$ $\cup$	from standard set theory, *subset, superset, intersection, union*
$\equiv$	*equivalent to*
$\triangleq$	*defined equal to*
$\approx$	*approximately equal to*

$\simeq$ *isomorphic to* or *with*

$\cong$ *congruent to* or *with*

$\therefore$ *therefore*

$\circ$ Hadamard product of matrices

$\otimes$ Kronecker product of matrices

$\oplus$ vector sum of sets $\mathcal{X} = \mathcal{Y} \oplus \mathcal{Z}$ where every element $x \in \mathcal{X}$ has a unique representation $x = y + z$ where $y \in \mathcal{Y}$ and $z \in \mathcal{Z}$. [30, p.19] $\mathcal{X} = \mathcal{Y} \oplus \mathcal{Z} \Rightarrow \mathcal{X} = \mathcal{Y} + \mathcal{Z}$. Each element in a vector sum of a collection of subspaces has a unique representation when the basis from each subspace is linearly independent with respect to all the others.

$\boxplus$ orthogonal vector sum of sets $\mathcal{X} = \mathcal{Y} \boxplus \mathcal{Z}$ where every element $x \in \mathcal{X}$ has a unique orthogonal decomposition $x = y + z$ where $y \in \mathcal{Y}$, $z \in \mathcal{Z}$, and $y \perp z$. [31, p.51] $\mathcal{X} = \mathcal{Y} \boxplus \mathcal{Z} \Rightarrow \mathcal{X} = \mathcal{Y} + \mathcal{Z}$.

$A \perp B$ A *is orthogonal to* B, where A and B are sets, vectors, or matrices

$\backslash A$ logical *not* A, or *relative complement of* A; *e.g.*, $B \backslash A = \{x \in B \mid x \notin A\}$

$\Leftrightarrow$ *if and only if* or *corresponds to* or *necessary and sufficient*

$\Rightarrow$ or $\Leftarrow$ *implies*; *e.g.*, $A \Rightarrow B \Leftrightarrow \backslash A \Leftarrow \backslash B$

$\nRightarrow$ or $\nLeftarrow$ *does not imply*

$\rightarrow$ *goes to*

$\downarrow$ *goes to from above*; *e.g.*, *above* might mean *positive* in some context [29, p.2]

$\leftarrow$ *is replaced with*

$|$ as in $f(x) \mid x \in \mathcal{C}$ means *with the condition(s)* or *such that* or *evaluated at*, or as in $\{f(x) \mid x \in \mathcal{C}\}$ means *evaluated at each and every* x *belonging to* $\mathcal{C}$

$g|_{x_p}$ *expression* g *evaluated at* x_p

$:$	as in $f : \mathbb{R}^n \to \mathbb{R}^m$ meaning f *is a mapping*
$f : \mathcal{A} \to \mathcal{B}$	meaning f *is a mapping from ambient space* $\mathcal{A}$ *to ambient* $\mathcal{B}$; not necessarily denoting either domain or range
$\ni$	*such that*
$\exists$	*there exists*
$\forall$	*for all*
$\overline{AB}$	closed line segment AB
$[A, B]$	closed interval or line segment between A and B in $\mathbb{R}$
$[\ \ ]$	square brackets denote a matrix or sequence; *e.g.*, respectively $[A\ \ B]$ or $[A_i]$
$\lfloor\ \ \rfloor$	floor function, $\lfloor x \rfloor$ is greatest integer not exceeding x
$\|\ \ \|$	entry-wise absolute value of scalars, vectors, and matrices
det	matrix determinant
(A, B)	open interval between A and B in $\mathbb{R}$
$\{\ \}$	curly braces denote a set or list, *e.g.*, $\{Xa \mid a \succeq 0\}$ *the set of all* Xa *for each and every* $a \succeq 0$ where membership of a to some space is implicit, a union
$\emptyset$	empty set
$\langle\, , \rangle$	angle brackets denote vector inner product
x_p	particular value of x
x_0	particular instance of x , or initial value of a sequence $[x_i]$
x_1	first entry of vector x , or first element or a set or list $\{x_i\}$
$x^\star$	optimal value of variable x
x^*	complex conjugate

f^*	convex conjugate function
$\mathcal{K}^*$	dual cone or set
$P_{\mathcal{C}}x$ or Px	projection of point x on set $\mathcal{C}$
$P_k x$	projection of point x on set $\mathcal{C}_k$
$\delta(A)$	*vector made from the main diagonal of* A if A is a matrix; otherwise, *the diagonal matrix made from the vector* A. $\delta^2(\cdot) \equiv \delta\delta(\cdot)$
$\lambda(A)$	*vector of eigenvalues of matrix* A, typically arranged in nonincreasing order
$\sqrt{d_{ij}}$	(absolute) distance scalar
dist	distance between point or set arguments
d_{ij}	distance-square scalar
$\overline{d_{ij}}$	upper bound on distance-square d_{ij}
$\overline{\mathcal{C}}$	*closure of set* $\mathcal{C}$
$\underline{d_{ij}}$	lower bound on distance-square d_{ij}
$\underline{d}$	vector of distance-square
Δ	distance scalar, or matrix of absolute distance, or difference operator, or diagonal matrix
V	$N\times N$ symmetric elementary, auxiliary, and geometric centering matrix
$V_{\mathcal{N}}$	$N\times N-1$ Schoenberg auxiliary matrix
X	point list, set of generators, or extreme directions in $\mathbb{R}^{n\times N}$, or matrix variable
D	matrix of distance square, or Euclidean distance matrix
$\mathbf{D}$	Euclidean distance matrix function, EDM definition
r	affine dimension

n	list X dimension, or integer
N	cardinality of list X , or integer
∂	*boundary* or *partial derivative* or matrix of distance-square squared
∂y	partial differential of y
$\partial\mathcal{K}$	boundary of set $\mathcal{K}$
dom	domain of function argument
epi	epigraph of function
$\mathcal{R}(A)$	range of A
basis $\mathcal{R}(A)$	columnar basis for range of A
$\mathcal{N}(A)$	nullspace of A
$\mathbb{R}^n$ or $\mathbb{R}^{n\times n}$	Euclidean vector space
$\imath$ or $\jmath$	$\sqrt{-1}$
$\mathbb{C}^n$ or $\mathbb{C}^{n\times n}$	complex Euclidean vector space
$\mathbb{R}^n_+$ or $\mathbb{R}^{n\times n}_+$	nonnegative orthant in Euclidean vector space
$\mathbb{R}^n_-$ or $\mathbb{R}^{n\times n}_-$	nonpositive orthant
$\mathbb{R}^n_{i-}$	orthant whose only negative coordinate is the i^{th}
$\mathbb{S}^n$	subspace comprising all real symmetric $n\times n$ matrices, the *symmetric subspace*
$\mathbb{S}^{n\perp}$	orthogonal complement of $\mathbb{S}^n$ in $\mathbb{R}^{n\times n}$
$\mathbb{S}^n_+$	convex cone comprising all real symmetric positive semidefinite $n\times n$ matrices, the *positive semidefinite cone*
$\operatorname{int}\mathbb{S}^n_+$	interior of convex cone comprising all real symmetric positive semidefinite $n\times n$ matrices; *id est*, positive definite matrices

$\mathbb{S}^n_{\mathbf{1}}$	subspace comprising all symmetric $n\times n$ matrices having all zeros in first row and column
$\mathbb{S}^n_{\mathbf{0}}$	subspace comprising all real symmetric hollow $n\times n$ matrices ($\mathbf{0}$ main diagonal), the *symmetric hollow subspace*
$\mathbb{R}^{m\times n}_g$	subspace comprising all geometrically centered $m\times n$ matrices
$\mathbb{S}^n_g$	subspace comprising all geometrically centered symmetric $n\times n$ matrices, the *geometric center subspace*
$\mathbb{S}^{n\perp}_g$	orthogonal complement of $\mathbb{S}^n_g$ in $\mathbb{S}^n$
$X^\perp$	basis $\mathcal{N}(X^T)$
$x^\perp$	$\mathcal{N}(x^T)$
$\mathcal{R}(P)^\perp$	$\mathcal{N}(P^T)$
$\mathcal{R}^\perp$	set orthogonal to set $\mathcal{R}\subseteq\mathbb{R}^n$; $\mathcal{R}^\perp \triangleq \{y\in\mathbb{R}^n \mid \langle x,y\rangle=0 \quad \forall x\in\mathcal{R}\}$
$\mathcal{K}^\perp$	normal cone
$\mathcal{K}_{\mathcal{M}+}$	monotone nonnegative cone
$\mathcal{K}_{+\mathcal{M}}$	monotone nonnegative cone with reversed indices
$\mathcal{K}^*_{\lambda\delta}$	cone of majorization
$\mathcal{H}$	halfspace
$\partial\mathcal{H}$	hyperplane; *id est*, partial boundary of halfspace
$\underline{\partial\mathcal{H}}$	supporting hyperplane
$\underline{\partial\mathcal{H}}_+$	supporting hyperplane having inward-normal with respect to $\mathcal{H}$
$\underline{\partial\mathcal{H}}_-$	supporting hyperplane having outward-normal with respect to $\mathcal{H}$
I	identity matrix
$\mathbf{0}$	vector or matrix of zeros
$\mathbf{1}$	vector of ones

e_i vector whose i^{th} entry is 1, otherwise 0, or *member of the standard basis for* $\mathbb{R}^n$

arg argument of operator or function

sup supremum, *least upper bound* [29, §0.1.1] (this *bound*, as in *boundary* (5), is not necessarily a member of the set that is argument)

max maximum [29, §0.1.1]

inf infimum, *greatest lower bound* [29, §0.1.1] (this *bound*, as in *boundary* (5), is not necessarily a member of the set that is argument)

min minimum [29, §0.1.1]

iff *if and only if, necessary and sufficient,* meaning typically attached to appearance of the word "if" in a definition; a practice requiring abolition because of ambiguity thus conferred

rel relative

int interior

sgn signum function

mod modulus operator

tr matrix trace

rank A rank of matrix A; $\dim \mathcal{R}(A)$

dim dimension, $\dim \mathbb{R}^n = n$, $\dim(x \in \mathbb{R}^n) = n$, $\dim \mathcal{R}(x \in \mathbb{R}^n) = 1$, $\dim \mathcal{R}(A \in \mathbb{R}^{m \times n}) = \operatorname{rank}(A)$

aff affine hull

conv convex hull

cenv convex envelope

cone conic hull

content content of high-dimensional bounded polyhedron, it is volume in 3 dimensions, area in 2, and so on cof matrix of cofactors corresponding to matrix argument

vec vectorization of matrix, Euclidean dimension n^2

svec vectorization of symmetric matrix, Euclidean dimension $n(n+1)/2$

dvec vectorization of symmetric hollow matrix, Euclidean dimension $n(n-1)/2$

$\succeq$ generalized inequality, for example, $A \succeq 0$ means vector or matrix A *can be expressed in a biorthogonal expansion having nonnegative coordinates with respect to some implicit pointed closed convex cone* $\mathcal{K}$, or *comparison to the origin with respect to some implicit pointed closed convex cone*, or when $\mathcal{K} = \mathbb{S}^n_+$ *matrix* A *belongs to the positive semidefinite cone of symmetric matrices*

$\geq$ *greater than or equal to*; comparison of scalars or entry-wise comparison of vectors or matrices with respect to $\mathbb{R}$

$\|x\|$ vector 2-norm or Euclidean norm $\|x\|_2$

$\|x\|_\ell$ $= \sqrt[\ell]{\sum_{j=1}^{n} |x_j|^\ell}$ vector ℓ-norm

$\|x\|_2^2$ $= x^T x$

$\|x\|_\infty$ $= \max\{|x_j|\,, \forall j\}$ infinity-norm

$\|x\|_1$ $= \mathbf{1}^T|x|$ 1-norm, dual infinity-norm

$\|X\|_2$ $= \sup\limits_{\|a\|=1} \|Xa\|_2 = \sigma_1 = \sqrt{\lambda(X^TX)_{\mathbf{1}}}$ matrix 2-norm (spectral norm), greatest singular value

$\|X\|$ $= \|X\|_\mathrm{F}$ Frobenius' matrix norm

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