# Fundamental Convex Euclidean Geometry and its Applications

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for Jennie Columba

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◊ Antonio

◊

and Sze Wan

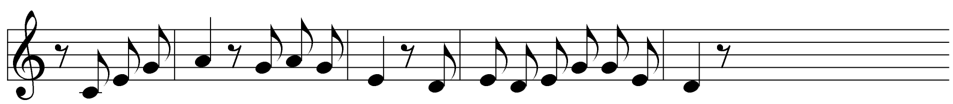
*Sooner or later just like the world first day,*
*Sooner or later we learn to throw the past away.*

−Gordon Sumner

## Preface

Philosophy in Ph.D., to some these pages may seem stark; quite the contrary... Very few places in life is it possible to achieve a glimpse of perfection, *e.g.*, musical performance, sports,...
Why do this... purpose is belief will make life better for others in some respect, reflects hope for the future. Passion...art...what we leave behind...life is short... do this regardless

-Jon Dattorro, Stanford 2003



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# 1 Introduction

There will be a virtual flood of applications with the realization that many problems hitherto believed non-convex can be transformed or relaxed into convexity. example, LMI books [1] [2].

Circuit design: analog/digital filter synthesis [3], chip design [4, §4.7], [Barcelona], economics [5] [6] [7] ...

[4, §4.3] [8] discuss the relaxation of NP-hard combinatorial problems by semidefinite programming. antenna array design, structural mechanics, medical imaging, ...

Convex geometry and linear algebra are inextricably bonded...

Summarize what lies ahead...

# 2 Essential convexity theorems, definitions

There is relatively less published pertaining to *matrix*-valued convex sets and functions. We present only a few pertinent results; purposely abbreviated. We assume the reader to be comfortable with chapters 2 and 3 from [9], while familiar with chapters 4 and 5 there. The essential references are [10] [9] [11]. The reader is referred to [12] [13] [14] [15] [16] (in that order) for a more comprehensive treatment of convexity.

## 2.1 Sets

**Definition.** *Convex set.* A set $\mathcal{C}$ is convex iff for all $Y, Z \in \mathcal{C}$ and $0 \leq \mu \leq 1$,

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

◇

Under that defining constraint on $\mu$, the linear sum in (1) is called a *convex combination* of $Y$ and $Z$. If $Y$ and $Z$ are points in Euclidean 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; so are all affine sets (§3.1.1), any ray (§3.4.2), halfspace (§3.2.1), hyperplane (§3.2.2), and *subspace.*[1] Apparent from the definition, a convex set is a connected set. [18, §3.4, §3.5]

**Example.** *Orthant*: the name given to a higher-dimensional generalization of the term *quadrant* from the classical Cartesian partition of $\mathbb{R}^{\mathbf{2}}$. The orthant $\mathbb{R}^n_{i\text{-}}$ for example, identifies the region in $\mathbb{R}^n$ whose members' sole negative coordinate is their $i^{\text{th}}$ (analog to quadrant II or IV). The most common is the nonnegative orthant $\mathbb{R}^n_+$ or $\mathbb{R}^{n\times n}_+$ (I) to which membership denotes all nonnegative vector- or matrix-entries respectively. The nonpositive orthant $\mathbb{R}^n_{\text{-}}$ or $\mathbb{R}^{n\times n}_{\text{-}}$ (III) denotes all negative or zero entries. Orthant convexity is easily verified by definition (1).[2] □

[1] A nonempty subset of a vector space $\mathbb{R}^n$ is called a subspace 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 both in the subset. [5, §2.3] A subspace contains the origin, by definition, and is a convex set. Any subspace that does not constitute the whole vector space is called a *proper subspace*; for example, any hyperplane through the origin. The vector space is itself a subspace, [17, §2.1] inclusively, although not proper.

[2] We will later learn that all orthants are self-dual simplicial cones. (§3.6.2)

**Theorem.** *Intersection.* [9, §2] [11, §2] The intersection of an arbitrary collection of convex sets is convex. $\diamond$

**Theorem.** *Image, Inverse image.* [11, §3] [9, §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

$$f(\mathcal{C}) = \{f(X) \mid X\in\mathcal{C}\} \subseteq \mathbb{R}^{m\times n} \tag{2}$$

  is convex.

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

$$f^{-1}(\mathcal{F}) = \{X \mid f(X)\in\mathcal{F}\} \subseteq \mathbb{R}^{p\times k} \tag{3}$$

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

$\diamond$

Each converse of this two-part theorem is generally *not* true; *id est*, 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 that set $\mathcal{F}$ is convex. A counter-example is easy to visualize when the affine function is an orthogonal projector [19] [5]:

**Corollary.** *Projection on subspace.* [11, §3] The orthogonal projection of a convex set on a subspace is another convex set. $\diamond$

The corollary is true more generally for projection on hyperplanes. [14, §6.6] Again, the converse is not true. Shadows, for example, are umbral projections that can be convex when the object providing the shade is not.

### 2.1.1 Vectorized matrix inner product

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

$$<y\,,z> = y^T z \tag{4}$$

that is linear. 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 transformation *vectorization.* For example, the vectorization of $Y = [y_1\; y_2 \cdots y_k] \in \mathbb{R}^{p\times k}$ is [20] [21]

$$\operatorname{vec} Y \triangleq \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix} \in \mathbb{R}^{pk} \tag{5}$$

Then the vectorized-matrix inner product is the trace of the matrix inner product; for $Z \in \mathbb{R}^{p\times k}$, [9, §2] [10, §0.3.1] [22, §8] [23, §2.2]

$$<Y, Z> \triangleq \operatorname{tr}(Y^T Z) = \operatorname{vec}^T Y \operatorname{vec} Z \tag{6}$$

where

$$\operatorname{tr}(Y^T Z) = \operatorname{tr}(Z Y^T) = \operatorname{tr}(Y Z^T) = \operatorname{tr}(Z^T Y) = \mathbf{1}^T (Y \circ Z)\mathbf{1} \tag{7}$$

and where $\circ$ denotes the Hadamard product[3] of matrices [24] [25, §1.1.4].

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

$$<vw^T, \mathcal{C}_1> = v^T \mathcal{C}_1 w = \operatorname{tr}(wv^T \mathcal{C}_1) = \mathbf{1}^T \big((vw^T)\circ \mathcal{C}_1\big)\, \mathbf{1} \tag{8}$$

**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

$$\Re \triangleq v^T \mathcal{C} w = <vw^T, \mathcal{C}> \subseteq \mathbb{R} \tag{9}$$

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 $\Re$ remains an element of $\Re$. □

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 (9) that are two

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

elements of $\Re$ by definition. Now make a convex combination of those inner products; *videlicet*, for $0 \leq \mu \leq 1$,

$$\mu <vw^T, \mathcal{C}_1> \; + \; (1-\mu)<vw^T, \mathcal{C}_2> \; = \; <vw^T, \mu\,\mathcal{C}_1 + (1-\mu)\mathcal{C}_2> \tag{10}$$

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 $\Re$. Since that holds true for any two elements from $\Re$, then it must be a convex set. ♦

More generally, $vw^T$ may be replaced with any particular matrix $Z \in \mathbb{R}^{p\times k}$ while convexity of the set $<Z\,,\, \mathcal{C}> \subseteq \mathbb{R}$ persists. Further, replacing $v$ and $w$ with any particular respective matrices $V$ and $W$ of dimension compatible with $\mathcal{C}$, the set $V^T\mathcal{C}W$ is convex because it is a linear mapping of $\mathcal{C}$.

**2.1.1.1 Frobenius.** When $Z = Y$ in (6), the *Frobenius norm* is resultant;

$$\|Y\|_{\mathrm{F}}^2 \;=\; \|\operatorname{vec} Y\|_2^2 \;=\; <Y, Y> \;=\; \operatorname{tr}(Y^TY) \;=\; \sum_{i,j} Y_{ij}^2 \;=\; \sum_i \lambda(Y^TY)_i \;=\; \sum_i \sigma(Y)_i^2 \tag{11}$$

where $\lambda(Y^TY)_i$ is the $i^{\text{th}}$ eigenvalue of $Y^TY$, and $\sigma(Y)_i$ is the $i^{\text{th}}$ singular value of $Y$. When $Y$ is normal, $\sigma(Y) = |\lambda(Y)|$, thus

$$\|Y\|_{\mathrm{F}}^2 \;=\; \sum_i \lambda(Y)_i^2 \tag{12}$$

Because the metrics are equivalent

$$\|X - Y\|_{\mathrm{F}}^2 = \|\operatorname{vec} X - \operatorname{vec} Y\|_2^2 \tag{13}$$

and because vectorization (5) is a linear *bijective* map, vector space $\mathbb{R}^{p\times k}$ is *isometrically isomorphic* with $\mathbb{R}^{pk}$ in the Frobenius sense.[4]

[4] An isometric isomorphism is a linear bijective mapping (one-to-one and onto [17, App.A1.2]) that preserves distance. For example, the orthonormal operator $Q : \mathbb{R}^n \to \mathbb{R}^n$, where $Q \in \mathbb{R}^{n\times n}$ is an orthogonal matrix (§C.6), is an isometric isomorphism. Yet the isometric operator $T : \mathbb{R}^{\mathbf{2}} \to \mathbb{R}^{\mathbf{3}}$, where

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

and $\mathcal{R}(T) \triangleq \mathbb{R}^{\mathbf{3}}$, is injective but not surjective [17, §1.6].

### 2.1.2 Symmetric matrices

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

$$\mathbb{S}^M \triangleq \left\{A = A^T \in \mathbb{R}^{M\times M}\right\} \tag{14}$$

This subspace of symmetric matrices $\mathbb{S}^M$ is *isomorphic* [17, §2.8-8, §3.2-2][5] [26] 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* [19] [5] of $\mathbb{S}^M$ is $\mathbb{S}^{M\perp}$ the subspace of all *antisymmetric* matrices; *id est*, $\mathbb{S}^M \oplus \mathbb{S}^{M\perp} = \mathbb{R}^{M\times M}$. ◇

Indeed, any square matrix $A\in\mathbb{R}^{M\times M}$ can be written as the sum of its symmetric and antisymmetric parts: respectively, $A=(A+A^T)/2+(A-A^T)/2$. The symmetric part is orthogonal in $\mathbb{R}^{M^2}$ to the antisymmetric part; *videlicet*,

$$\operatorname{tr}\big((A^T+A)(A-A^T)\big) = 0 \tag{15}$$

When a matrix is symmetric in $\mathbb{S}^M$, the vectorization transformation (5) to $\mathbb{R}^{M^2}$ is identical although we may instead visualize in subspace $\mathbb{R}^{M(M+1)/2}$ which remains isomorphic but not isometric. Lack of isometry is a spatial distortion due now to a disparity in metric between $\mathbb{R}^{M^2}$ and $\mathbb{R}^{M(M+1)/2}$. To visualize in $\mathbb{R}^{M(M+1)/2}$, we must make a correction: For $Y=[Y_{ij}]\in\mathbb{S}^M$,

$$\operatorname{svec} Y \triangleq \begin{bmatrix} Y_{11} \\ \sqrt{2}Y_{12} \\ Y_{22} \\ \sqrt{2}Y_{13} \\ \sqrt{2}Y_{23} \\ Y_{33} \\ \vdots \\ Y_{MM} \end{bmatrix} \in \mathbb{R}^{M(M+1)/2} \tag{16}$$

Then because the metrics become equivalent,

$$\|X-Y\|_F^2 = \|\operatorname{svec} X - \operatorname{svec} Y\|_2^2 \tag{17}$$

[5] 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.

for $X \in \mathbb{S}^M$, and because symmetric vectorization (16) 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 Frobenius sense under the transformation svec.

#### 2.1.2.1 Hollow matrices

**Definition.** *Symmetric hollow subspace.* [27] Define a subspace of $\mathbb{S}^M$: the set of all symmetric $M \times M$ matrices having zero main-diagonal;

$$\mathbb{S}^M_\delta \triangleq \left\{A \in \mathbb{S}^M \mid \delta(A) = \mathbf{0}\right\} \tag{18}$$

where $\delta(A)$ isolates the main diagonal of $A$ (§C.5). This subspace of symmetric hollow matrices is isomorphic with subspace $\mathbb{R}^{M(M-1)/2}$. The orthogonal complement of $\mathbb{S}^M_\delta$ is $\mathbb{S}^{M\perp}_\delta$ the subspace of all antisymmetric matrices having main diagonal $\delta(A) \in \mathbb{R}^M$; *id est*, $\mathbb{S}^M_\delta \oplus \mathbb{S}^{M\perp}_\delta = \mathbb{R}^{M \times M}$. $\diamond$

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

$$A = \left(\frac{1}{2}(A + A^T) - \delta^2(A)\right) + \left(\frac{1}{2}(A - A^T) + \delta^2(A)\right) \tag{19}$$

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

$$\operatorname{tr}\left(\left(\frac{1}{2}(A + A^T) - \delta^2(A)\right)\left(\frac{1}{2}(A - A^T) + \delta^2(A)\right)\right) = 0 \tag{20}$$

$\mathbb{S}^M$ and $\mathbb{S}^M_\delta$ are convex sets.

### 2.1.3 PSD cone

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

$$\mathbb{S}^M_+ \triangleq \left\{A \in \mathbb{S}^M \mid A \succeq 0\right\} \tag{21}$$

It is a unique immutable non-polyhedral closed pointed nonempty convex cone in the subspace of symmetric matrices $\mathbb{S}^M$. The positive *definite* matrices comprise the cone interior.

$$\operatorname{int} \mathbb{S}_+^M = \left\{ A \in \mathbb{S}^M \mid A \succ 0 \right\} \tag{22}$$

◇

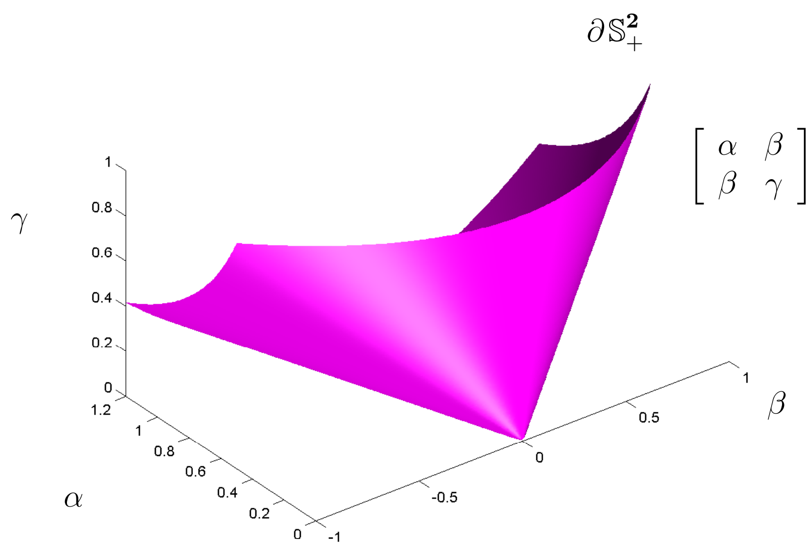


Figure 1: Truncated boundary of PSD cone in $\mathbb{S}^2$ plotted in isomorphic $\mathbb{R}^3$; courtesy, Alexandre W. d'Aspremont. Plotted is a 0-contour of the minimum eigenvalue (564). The geometry is not as simple in higher dimensions [13, §II.12], although for real matrices the PSD cone is self-dual [28, §II] (§3.6).

We call the set $\mathcal{K}$ a *convex cone* iff (§3.4.2)

$$\Gamma_1 , \Gamma_2 \in \mathcal{K} \;\Rightarrow\; \zeta\Gamma_1 + \xi\,\Gamma_2 \in \mathcal{K} \;\text{ for all }\; \zeta , \xi \geq 0 \tag{23}$$

The set of all positive semidefinite matrices forms a convex cone because any pair satisfies definition (23); [24, §7.1] *videlicet*, for all $\zeta_1 , \zeta_2 \geq 0$,

$$\begin{array}{c} \zeta_1 A_1 + \zeta_2 A_2 \succeq 0 \\ \zeta_1 A_1 + \zeta_2 A_2 \in \mathbb{S}^M \end{array} \;\Leftarrow\; \begin{array}{cc} A_1 \succeq 0\,, & A_2 \succeq 0 \\ A_1 \in \mathbb{S}^M, & A_2 \in \mathbb{S}^M \end{array} \tag{24}$$

Observe the notation $A \succeq 0$; meaning,[6] the symmetric part of $A$ (§C.2) belongs to the positive semidefinite cone in the subspace of symmetric matrices, while $A \succ 0$ denotes membership to that cone's interior. (§3.6.1.1)

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 1. When $M = 3$ the PSD cone is six-dimensional, and so on.

**2.1.3.1 PSD cone boundary.** To construct the PSD cone, we resort to the basic definition of positive semidefiniteness for $A \in \mathbb{S}^M$;[7] $A \succeq 0 \Leftrightarrow y^T A\, y \geq 0$ for all $y \in \mathbb{R}^M$. The PSD cone is formed by the intersection of an infinite number of halfspaces specified by the basic definition, hence it is closed [28, §II]; the PSD cone contains its boundary.
Reader pg.15...
To see the halfspaces, imagine for each particular $y$ the product $y^T A y$ is a linear function of the matrix entries... show for M=2...

need the following for EDM boundary arguments...

- For all $y$, [*sic*] $y^T A y = 0$ defines boundary...
- $y^T A y$ proportional to coefficient of projection on PSD cone. (Appendix)
- coefficient proportional to eigenvalue when...
- Hence 0 eigenvalue indicates $A$ on boundary.

PSD cone in Figure 1 is strictly convex. define...
In higher dimensions, that is no longer true. [29, §II.A]

All the positive semidefinite matrices having at least one 0 eigenvalue reside on the boundary of the PSD cone in any dimension. The boundary is delimited by all the supporting hyperplanes defined by that scalar inequality.

---

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

[7]Because $y^T A\, y = y^T A^T y$, $A$ is almost always assumed symmetric. [24, §7.1]

Conversely, boundary is composed of all matrices whose rank is less than full.

By the *proper-cone boundary theorem* in §3.4.3, there exist rays having base $\mathbf{0}$ through the boundary of the PSD cone of any dimension.

Prove that the direction of every ray on the boundary is an exposed direction.

Exposed directions of any convex set are a dense subset [11] of all extreme directions?

$\beta$

In Figure 1, the only matrix having two 0 eigenvalues lies at the origin.

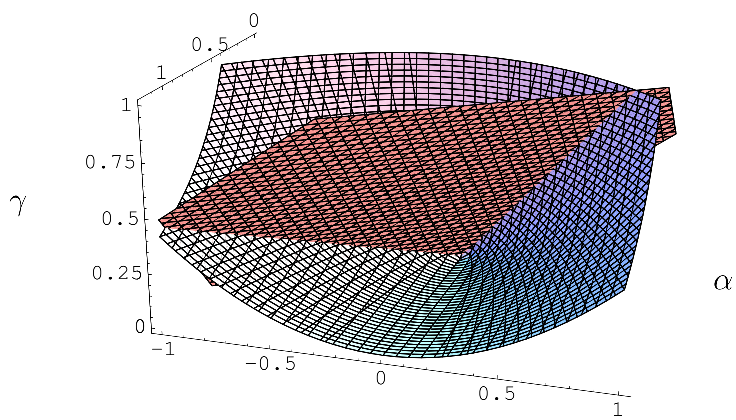


Figure 2: Truncated boundary (tiled) of PSD cone in isomorphic $\mathbb{R}^{\mathbf{3}}$ sliced by a plane through the origin. (Looking downward from behind with respect to Figure 1.) The intersection of the plane with the PSD cone contains two rays whose directions are extreme with respect to either the intersection or the PSD cone.

### extreme combination

It follows from the *extremes theorem* (§3.4.4) that any element of a convex set may be expressed as a linear combination of its extreme elements. Symmetric rank-one matrices constitute all the extreme directions of the PSD cone. [28, §III] [30, §6] For example, any (symmetric) positive semidefinite matrix can be expressed as a conic combination of symmetric rank-one matrices; that follows from diagonalization. If we limit consideration to bounded positive semidefinite matrices $A$ such that $\operatorname{tr} A = 1$, then any matrix from that set may be expressed as a *convex* combination of symmetric rank-one matrices.

#### 2.1.3.2 Polyhedral cones within

**Definition.** *Set slice.* We define a *slice* of a set $\mathcal{C}$ as the intersection of $\mathcal{C}$ with a (two-dimensional) plane. When $\mathcal{C}$ is convex, the slice remains convex by the *intersection theorem* (§2.1). $\diamond$

**slice dissection**

The PSD cone of any dimension comprises an infinite number of two-dimensional polyhedral cones revealed by *slicing* it with any plane through the origin. The extreme directions (§3.4.4) of those polyhedral cones must be extreme directions of the PSD cone. [11, §18]

Indeed, any *slice* through the origin of the PSD cone is a polyhedral cone having two extreme directions. We sketched rays corresponding to a few arbitrarily chosen slices in Figure 3. Conversely, in Figure 3, any two rays sketched are extreme directions of some slice through the origin. The rays shown emanating from the origin all lie along the boundary of the PSD cone and along the relative boundary of the corresponding polyhedral cone. Hence the extreme directions of the polyhedral cones are also extreme directions of the PSD cone, and *vice versa.*

By (23) it follows that there exist rays emanating from the origin which travel along the boundary of the PSD cone of any dimension, because each of those rays corresponds to an extreme direction of some polyhedral cone made by slicing the PSD cone using a plane through the origin.

Alternate construction of PSD cone is the convex hull of all the extreme directions and the origin, by the *extremes theorem* in §3.4.4.

**2.1.3.3 Hyperplanes hinged on PSD cone.** (23) is the inspiration for this section. From Sweep.nb,
Show that all symmetric rank-one 3x3 and 2x2 and all symmetric positive semidefinite rank-two 3x3 matrices can be described by matrix on pg.141 of Nascence notebook. Plot a three-dimensional slice of the surface of the

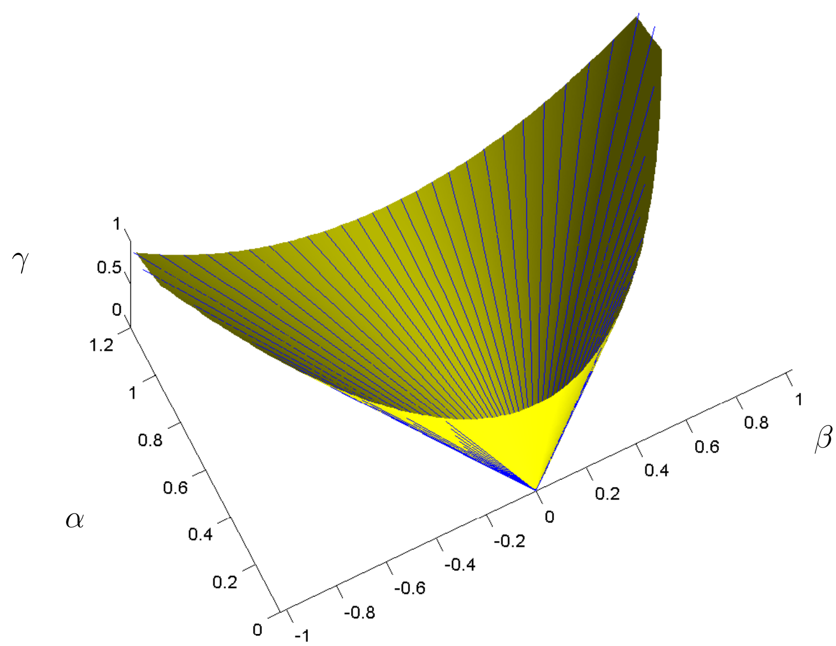


Figure 3: Truncated drawing of the PSD cone in isomorphic $\mathbb{R}^{\mathbf{3}}$ showing some arbitrary rays, lining the boundary, corresponding to extreme directions $yy^T$. (Peering over the top with respect to Figure 1.) Only in this dimension is the entire boundary constituted by extreme directions.

six-dimensional PSD cone for particular s1 and s3; it is described completely by the nullspace of the hinge equations pg.140 *ibidem*

Want to sweep rays corresponding to extreme directions of PSD cone, NOT its boundary.

Extreme directions DO NOT constitute the boundary of the PSD cone except for the 2x2 case. We know this from a fundamental definition of positive semidefiniteness $y^TAy \geq 0$; *id est*,

$$\mathbb{S}_+^m = \{A \in \mathbb{S}^m \mid <yy^T, A> \;\geq\; 0,\; y \in \mathbb{R}^m\} \tag{25}$$

defines the positive semidefinite cone; it is an intersection of halfspaces in the variable $A \in \mathbb{R}^{m(m+1)/2}$. All singular positive semidefinite matrices therefore constitute the boundary; *id est*, there are no positive definite matrices on the boundary,

$$\partial\mathbb{S}_+^m = \{A \in \mathbb{S}_+^m \mid <yy^T, A> \;=\; 0,\; y \neq \mathbf{0}\} \tag{26}$$

## 2.2 Functions

The icon for the convex function is bowl-shaped (Figure 33, p.214), whereas the concave icon is the inverted bowl. Because of this simple inverse relationship, the usage of the term *convexity* is often implicitly inclusive of *concavity* in the literature. We will distinguish the two terms wherever convenient. Despite the iconic imagery, the reader is reminded that the set of all convex, concave, quasiconvex, and quasiconcave functions contains the *monotone* [9, old§2.6.1] functions; *e.g.*, [9, old§2, exer.2.43A].

### 2.2.1 Convex functions

The vector-valued continuous function $f(X):\mathbb{R}^{p\times k}\to\mathbb{R}^M$ 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 $0\leq\mu\leq 1$,

$$f(\mu Y+(1-\mu)Z)\underset{\mathbb{R}_+^M}{\preceq}\mu f(Y)+(1-\mu)f(Z) \tag{27}$$

Since comparison of vectors here is with respect to $\mathbb{R}_+^M$ (118), the $M$-dimensional nonnegative orthant, the test prescribed by (27) is simply a comparison on $\mathbb{R}$ of each entry[8] of the vector function. The vector-valued function case is therefore a straightforward generalization of conventional convexity theory for a real function. (See [9, §3, §4] for all the details.)

When, under the same previous conditions, $f(X)$ instead satisfies

$$f(\mu Y+(1-\mu)Z)\underset{\mathbb{R}_+^M}{\prec}\mu f(Y)+(1-\mu)f(Z) \tag{28}$$

we shall say $f$ is a *strictly* convex function.

We are primarily interested in matrix-valued functions $g(X)$. We choose *symmetric* $g(X)\in\mathbb{S}^M$ because matrix-valued functions are most often compared (31) with respect to the positive semidefinite cone $\mathbb{S}_+^M$ in the subspace of symmetric matrices (§2.1.3).[9] Yet some of the following results depend

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[8] This same conclusion also follows directly from the nice theory of *generalized inequality* (§3.6.1) that states $f$ is convex if and only if $w^Tf$ is convex for each and every $w\succeq 0$. Discretization [30, §1] allows relaxation of the $w$ inequality to: each and every $w\in\{e_i\,,\ i=1\ldots M\}$; the standard basis for $\mathbb{R}^M$.

[9] 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

upon a scalar definition of positive (semi)definiteness (§C.2.2).

**Scalar-Definition.** *Convex matrix-valued function.* [9, §3]
$g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ 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 $\|w\| = 1$. ⋄

Observing for each and every real vector $w$ of unit norm, $\|w\| = 1$, [24, §7.7, prob.9]

$$w^T g(X) w \leq t \;\Leftrightarrow\; g(X) \underset{\mathbb{S}_+^M}{\preceq} tI \tag{29}$$

it then follows:

**Definition.** *Convex matrix-valued function.*
**1)** *Epigraph.* We define $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$ to be a convex function of $X$ iff its epigraph

$$\begin{aligned} \operatorname{epi} g &\triangleq \left\{(X,t) \mid X \in \operatorname{dom} g\,,\;\; w^T g(X) w \leq t\,,\;\; \|w\| = 1\right\} \subseteq \mathbb{R}^{p\times k} \times \mathbb{R} \\ &= \left\{(X,t) \mid X \in \operatorname{dom} g\,,\;\; g(X) \underset{\mathbb{S}_+^M}{\preceq} tI\,\right\} \end{aligned} \tag{30}$$

forms a convex set.
**2)** *Inequality form.* 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 $0 \leq \mu \leq 1$,

$$g(\mu Y + (1-\mu)Z) \underset{\mathbb{S}_+^M}{\preceq} \mu\, g(Y) + (1-\mu) g(Z) \tag{31}$$

Strict convexity is defined less a stroke of the pen in (31) similarly to (28). ⋄

**2.2.1.1** It is well established that a continuous real function $f : \mathbb{R}^{p\times k} \to \mathbb{R}$ is convex if and only if its epigraph $\operatorname{epi} f \subseteq \mathbb{R}^{p\times k} \times \mathbb{R}$ forms a convex set. [10] [9] [11] [15] [14] [5] Given a continuous matrix-valued function $g(X) : \mathbb{R}^{p\times k} \to \mathbb{S}^M$

---

respect to the nonnegative orthant $\mathbb{R}_+^{mk}$. Symmetric convex functions share the same benefits as symmetric matrices; *e.g.*, (569)-(571). Horn [24, §7.7] likens symmetric matrices to real numbers, and (symmetric) positive definite matrices to positive real numbers.

consequent to the *scalar-definition*, we defined the epigraph of $g(X)$ in terms of the corresponding real function $w^T g(X)w$ ; *id est*,

$$\operatorname{epi} g \;=\; \bigcap_{\|w\|=1} \operatorname{epi}\left(w^T g\, w\right) \tag{32}$$

Concisely then, the following are equivalent statements: For each and every real vector of unit norm, $\|w\|=1$,

1. $w^T g w$ is a convex real function,
2. $\operatorname{epi}\big(w^T g w\big)$ is a convex set,
3. $g$ is a convex matrix-valued function.

**Line Theorem.** [9, §3] $g(X) : \mathbb{R}^{p\times k} \rightarrow \mathbb{S}^M$ is convex in $X$ if and only if it remains convex on the intersection of any line with its domain. ⋄

Now we assume a twice differentiable function, and we drop the subscript $\mathbb{S}_+^M$ from the inequality when it is apparent.

**Definition.** *Differentiable convex matrix-valued function.*
$g(X) : \mathbb{R}^{p\times k} \rightarrow \mathbb{S}^M$ is convex in $X$ iff $\operatorname{dom} g$ is an open convex set, and its second derivative $g''(X + t\,Y) : \mathbb{R} \rightarrow \mathbb{S}^M$ 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 $t \in \mathbb{R}$ ,

$$\frac{d^2}{dt^2}\, g(X + t\,Y) \succeq 0 \tag{33}$$

Similarly, if

$$\frac{d^2}{dt^2}\, g(X + t\,Y) \succ 0 \tag{34}$$

then $g$ is strictly convex; the converse is generally false. [9, old§2.1.4][10] ⋄

[10] Quadratic forms constitute a notable exception where the strict-case converse is reliably true.

**Example.** *Matrix inverse.* The matrix-valued function $g(X)=X^{-1}$ is convex on $\operatorname{int}\mathbb{S}_+^M$. For each and every $Y\in\mathbb{S}^M$, (§F.2.1.1, §C.2.3)

$$\frac{d^2}{dt^2}\,g(X+t\,Y) \;=\; 2(X+t\,Y)^{-1}Y(X+t\,Y)^{-1}Y(X+t\,Y)^{-1} \;\succeq\; 0 \tag{35}$$

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;[11] $\operatorname{tr}X^{-1}$ is convex on that same domain. [24, §7.6, prob.2] □

**Example.** $X^2$... □

**Example.** *Matrix exponential.* The matrix-valued function $g(X)=e^X:\mathbb{S}^M\to\mathbb{S}^M$ is convex on the subspace of symmetric circulant matrices. Applying the *line theorem*, for all $t\in\mathbb{R}$ and for circulant $X,Y\in\mathbb{S}^M$ we have (§F.2.5, (566), (724), §C.2.3)

$$\frac{d^2}{dt^2}e^{X+t\,Y} \;=\; Y e^{X+t\,Y}Y\succeq 0\,,\qquad (XY)^T \;=\; XY \tag{36}$$

because circulant matrices are commutative (§12.3).

Changing the function domain to the subspace of all diagonal matrices reduces the matrix exponential to a vector-valued function (27) in an isometrically isomorphic subspace; [31, §5.3][12] known convex from the real-valued function case [9, §3]. □

There are, of course, multifarious methods to determine function convexity, [9] each of them efficient when appropriate.

### 2.2.2 Quasiconvex functions

Quasiconvex functions [9, §3] [10] [12] [14] are useful in practical problem solving because they are *unimodal* (by definition when non-monotonic); a global minimum is guaranteed to exist over the function domain or over any convex set in the function domain. In terms of *sublevel set*, their definition is elegant and analogous to the epigraph-form definition for convex functions:

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[11] $d/dt\operatorname{tr}g(X+t\,Y)=\operatorname{tr}d/dt\,g(X+t\,Y)$.

[12] The matrix exponential of a diagonal matrix exponentiates each individual diagonal entry.

**Definition.** *Quasiconvex matrix-valued function.*
**1)** *Sublevel set.* We define $g(X):\mathbb{R}^{p\times k}\to\mathbb{S}^M$ to be a quasiconvex function of matrix $X$ iff $\operatorname{dom} g$ is a convex set, and for each and every $\nu\in\mathbb{R}$ the corresponding sublevel set

$$\begin{aligned}\mathcal{L}_\nu &\triangleq \left\{X\in \operatorname{dom} g \mid w^T g(X)w \leq \nu\,,\ \|w\|=1\right\} \subseteq \mathbb{R}^{p\times k} &(37)\\ &= \{X\in \operatorname{dom} g \mid g(X) \preceq \nu I\,\} &(38)\end{aligned}$$

is convex.
**2)** *Inequality form.* $g(X):\mathbb{R}^{p\times k}\to\mathbb{S}^M$ is a quasiconvex function of matrix $X$ iff $\operatorname{dom} g$ is a convex set and for each and every $Y,Z\in\operatorname{dom} g$ and $0\leq\mu\leq 1$,

$$g(\mu Y + (1-\mu)Z) \ \preceq\ \max\{g(Y),\, g(Z)\} \tag{39}$$

◇

The sublevel set $\mathcal{L}_\nu$ of a matrix-valued function is an intersection of sublevel sets of real functions (37); similarly to the epigraph as discussed on page 15. While convex functions must have convex sublevel sets, it is not a sufficient condition for their definition as it is for quasiconvex functions.

**Example.** *Rank function.*
For $A,B\in\mathbb{R}^{m\times n}$ [24, §0.4]

$$\operatorname{rank} A + \operatorname{rank} B \ \geq\ \operatorname{rank}(A+B) \tag{40}$$

that follows from the fact [19, §3.6]

$$\dim\mathcal{R}(A) + \dim\mathcal{R}(B) \ =\ \dim\mathcal{R}(A+B) + \dim(\mathcal{R}(A)\cap\mathcal{R}(B)) \tag{41}$$

For $A,B\in\mathbb{S}^M_+$ [9, §3]

$$\operatorname{rank} A + \operatorname{rank} B \ \geq\ \operatorname{rank}(A+B) \ \geq\ \min\{\operatorname{rank} A,\, \operatorname{rank} B\} \tag{42}$$

that follows from the fact [30, §6]

$$\mathcal{N}(A+B) = \mathcal{N}(A)\cap\mathcal{N}(B)\,, \qquad A,B\in\mathbb{S}^M_+ \tag{43}$$

Rank is a quasiconcave function on $\mathbb{S}^M_+$ because the right-hand side of (42) has the concave form of (39); *id est*,

$$\operatorname{rank}(A+B) = \operatorname{rank}(\mu A + (1-\mu)B) \tag{44}$$

on the open interval $(0,1)$, which follows from the *dyadic linear independence definition* in §C.7.1. □

**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*[13] [32] [33] becomes zero, the second directional derivative is positive definite there [9, §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 $t \in \mathbb{R}$,

$$\left.\frac{d}{dt}\right|_{t=0} g(X+t\,Y) = \mathbf{0} \quad\Rightarrow\quad \left.\frac{d^2}{dt^2}\right|_{t=0} g(X+t\,Y) \succ 0 \tag{45}$$

Conversely, if $g(X)$ is quasiconvex then for each and every $X \in \operatorname{dom} g$ and *all* $Y \in \mathbb{R}^{p\times k}$,

$$\left.\frac{d}{dt}\right|_{t=0} g(X+t\,Y) = \mathbf{0} \quad\Rightarrow\quad \left.\frac{d^2}{dt^2}\right|_{t=0} g(X+t\,Y) \succeq 0 \tag{46}$$

◇

### 2.2.3 More salient properties of convex and quasiconvex functions

1. 
   - A convex (or *concave*) function is assumed continuous on the relative interior of its domain. [11, §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.
   Concavity $\Rightarrow$ quasiconcavity.

[13] By using a generalization of the Taylor series in §F.1.4, we extend the traditional definition of directional derivative so that *direction* may be indicated by a vector or a matrix.

4. The *scalar-definition* of matrix-valued function convexity and the *line theorem* (§2.2.1) translate identically to quasiconvexity (and quasiconcavity). [9, §3]

5. *Composition* $g(h(X))$ 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 $X \in \mathbb{R}^{m\times n}$. Likewise for the quasiconvex (quasiconcave) functions $g$. [10, §B.2.1]

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.

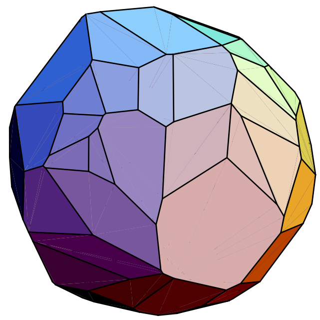

Figure 4: Convex hull of a random list of points in $\mathbb{R}^{\mathbf{3}}$. Some points from that generating list reside in the relative interior of this convex polyhedron. [34, *Convex Polyhedron, Avis-Fukuda*]

# 3 Basic 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 [13]

## 3.1 Hulls

### 3.1.1 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 $X$ ;

$$X = [x_1 \ \cdots \ x_N] \in \mathbb{R}^{n \times N} \tag{47}$$

The *affine dimension* of any list (or set) in $\mathbb{R}^n$ is the dimension of the smallest *affine set* (empty set, point, line, plane, hyperplane, subspace, $\mathbb{R}^n$) that contains it. Affine dimension is the same as the dimension of the subspace parallel to that affine set. [11, §1] [10, §A.2.1] In particular, we define the affine dimension $r$ as the dimension of the smallest affine set in Euclidean space $\mathbb{R}^n$ that contains the list $X$ of $N$ points; it is a lower bound sometimes called the *embedding dimension* [27] [35]:

$$r \triangleq \dim \operatorname{aff} X \tag{48}$$

That affine set in which the points are embedded is unique and called the *affine hull* [9, §2];

$$\mathcal{A} \overset{\Delta}{=} \operatorname{aff}\{x_\ell\,,\ \ell=1\dots N\} \;=\; \operatorname{aff} X \;=\; \{Xa \mid a^T\mathbf{1} = 1\} \;\subseteq\; \mathbb{R}^n \tag{49}$$

All affine sets are convex.

### 3.1.2 Convex hull

The *convex hull* [10, §A.1.4] [9, §2] [11] of any *bounded*[14] list (or set) of $N$ points $X\in\mathbb{R}^{n\times N}$ forms a unique closed convex polyhedron (§3.5) whose vertices constitute some subset of that list;

$$\mathcal{P} \overset{\Delta}{=} \operatorname{conv}\{x_\ell\,,\ \ell=1\dots N\} \;=\; \operatorname{conv} X \;=\; \{Xa \mid a^T\mathbf{1} = 1,\ a\succeq 0\} \;\subseteq\; \mathbb{R}^n \tag{50}$$

The *relative boundary* and *relative interior*[15] of the polyhedron constitute the convex hull $\mathcal{P}$, the smallest convex set that contains the list in $X$; *e.g.*, Figure 4. Given $\mathcal{P}$, the *generating list* $\{x_\ell\}$ is not unique.

### 3.1.3 Conic hull

In terms of a finite-length point list (or set) contained in the columns of $X\in\mathbb{R}^{n\times N}$ (47), its conic hull is expressed

$$\mathcal{K} \;=\; \operatorname{cone}\{x_\ell\,,\ \ell=1\dots N\} \;=\; \operatorname{cone} X \;=\; \{Xa \mid a\succeq 0\} \;\subseteq\; \mathbb{R}^n \tag{51}$$

The conic hull of any list forms a closed *polyhedral cone* (§3.5.1; *e.g.*, Figure 14) [10, §A.4.3]; the smallest convex cone that contains the list.

The constraints in (49), (50), and (51) respectively define an affine, convex, and conic combination of elements from the list or set.

---

[14] A set in $\mathbb{R}^n$ is bounded iff it can be contained in a Euclidean ball having finite radius. (*confer* §4.5.3)

[15] We distinguish interior from *relative* interior throughout. [12] [14] [15] The relative interior of a set $\mathcal{C}\subseteq\mathbb{R}^n$ is the interior relative to the affine hull of $\mathcal{C}$. [10, §A.2.1] (Likewise for the relative boundary.) Thus defined, it is exceedingly possible (though a bit confusing) for the interior of $\mathcal{C}$ to be empty while the relative interior is not; this happens whenever $\dim\operatorname{aff}\mathcal{C} < n$.

## 3.2 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. [11] [10] Every hyperplane partially bounds a halfspace (which are not affine).

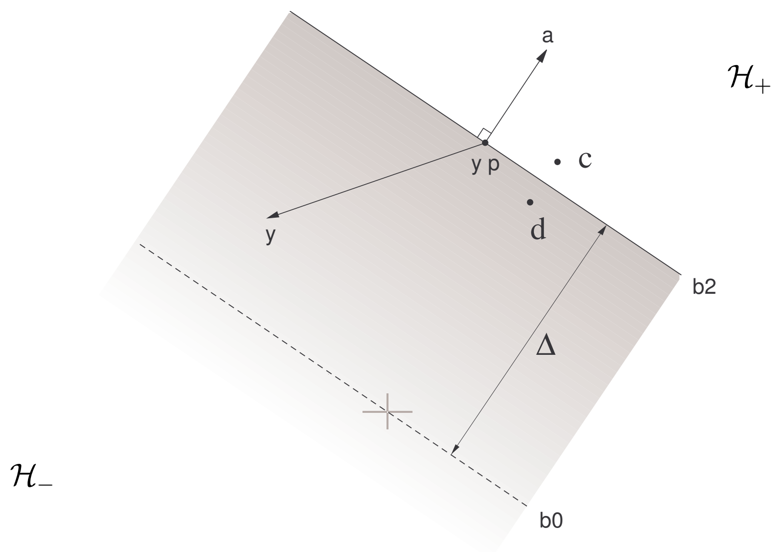


Figure 5: Hyperplane illustrated $\partial\mathcal{H}=\{y \mid a^Ty=b\}$ is a line partially bounding halfspaces $\mathcal{H}_-=\{y \mid a^Ty\leq b\}$ and $\mathcal{H}_+=\{y \mid a^Ty\geq b\}$ in $\mathbb{R}^{\mathbf{2}}$. Shaded is a rectangular piece of semi-infinite $\mathcal{H}_-$ to which vector $a$ is an outward normal; vector $a$ is inward-normal to $\mathcal{H}_+$. Normal $a$ always belongs to $\mathcal{H}_+$. In this particular instance, $\mathcal{H}_-$ contains nullspace $\mathcal{N}(a^T)=\{y \mid a^Ty=0\}$ (dashed line through origin) because $b>0$. The hyperplane, halfspace, and nullspace are each drawn truncated. Points $\mathrm{c}$ and $\mathrm{d}$ are equidistant from the hyperplane, and vector $\mathrm{c}-\mathrm{d}$ is normal to it. $\Delta$ is distance from the origin to hyperplane.

### 3.2.1 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

$$\mathcal{H}_- \;=\; \{y \mid a^Ty\leq b\} \;=\; \{y \mid a^T(y-y_o)\leq 0\} \tag{52}$$

$$\mathcal{H}_+ \;=\; \{y \mid a^T y \geq b\} \;=\; \{y \mid a^T(y - y_o) \geq 0\} \tag{53}$$

where vector $a$ is an *outward normal* to $\mathcal{H}_-$ while an *inward normal* to $\mathcal{H}_+$. Visualization is easier if we say $b = a^T y_o \in \mathbb{R}$. Then for any vector $y - y_o$ that makes an obtuse angle with normal $a$, $y$ will lie in the halfspace $\mathcal{H}_-$ on one side (shaded in Figure 5) of the hyperplane, while acute angles denote $y$ in $\mathcal{H}_+$ on the other side.

An equivalent more intuitive description of a halfspace comes about when we consider all the points in $\mathbb{R}^n$ closer to point $\mathrm{d}$ than to point $\mathrm{c}$ or equidistant, in the Euclidean sense; from Figure 5,

$$\mathcal{H}_- = \{y \mid \|y - \mathrm{d}\| \leq \|y - \mathrm{c}\|\} \tag{54}$$

This description, in terms of distance, is resolved with the halfspace description (52) by squaring both sides of the inequality in (54);

$$\mathcal{H}_- = \left\{y \mid (\mathrm{c} - \mathrm{d})^T y \leq \frac{\|\mathrm{c}\|^2 - \|\mathrm{d}\|^2}{2}\right\} \;=\; \left\{y \mid (\mathrm{c} - \mathrm{d})^T \left(y - \frac{\mathrm{c} + \mathrm{d}}{2}\right) \leq 0\right\} \tag{55}$$

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

$$\mathcal{H}_- \;=\; \{Y \in \mathbb{R}^{mn} \mid \langle A\,, Y\rangle \;\leq\; b\} \;=\; \{Y \in \mathbb{R}^{mn} \mid \langle A\,, Y - Y_o\rangle \;\leq\; 0\} \tag{56}$$

$$\mathcal{H}_+ \;=\; \{Y \in \mathbb{R}^{mn} \mid \langle A\,, Y\rangle \;\geq\; b\} \;=\; \{Y \in \mathbb{R}^{mn} \mid \langle A\,, Y - Y_o\rangle \;\geq\; 0\} \tag{57}$$

**Theorem.** *Halfspaces.* [9, §2] [11, §18] [10, §A.4.2(b)] A closed convex set in $\mathbb{R}^n$ is equivalent to the intersection of all halfspaces that contain it. $\diamond$

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

$$\bigcap_i \mathcal{H}_{i-} \;=\; \{y \mid A^T y \preceq b\} \;=\; \{y \mid A^T(y - y_o) \preceq 0\} \tag{58}$$

$$\bigcap_i \mathcal{H}_{i+} \;=\; \{y \mid A^T y \succeq b\} \;=\; \{y \mid A^T(y - y_o) \succeq 0\} \tag{59}$$

where $b$ is now a vector, and the $i^{\text{th}}$ column of $A$ is normal to a hyperplane $\partial\mathcal{H}_i$ partially bounding $\mathcal{H}_i$.

### 3.2.2 Hyperplane $\partial\mathcal{H}$ descriptions

Every hyperplane $\partial\mathcal{H}$ is parallel to an $(n-1)$-dimensional subspace; it is itself a subspace iff it contains the origin.

$$\dim \partial\mathcal{H} = n-1 \tag{60}$$

Every hyperplane can be described as the intersection of complementary halfspaces;

$$\partial\mathcal{H} = \mathcal{H}_+ \cap \mathcal{H}_- \tag{61}$$

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 5 for $\mathbb{R}^{\mathbf{2}}$;

$$\partial\mathcal{H} \overset{\Delta}{=} \{y \mid a^T y = b\} = \{y \mid a^T(y - y_o) = 0\} = \{Z\xi + y_o \mid \xi \in \mathbb{R}^{n-1}\} \subset \mathbb{R}^n \tag{62}$$

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

$$y = Z\xi + y_o \tag{63}$$

where the columns of $Z \in \mathbb{R}^{n \times n-1}$ constitute a basis for the nullspace $\mathcal{N}(a^T)$.[16]

Conversely, given any point $y_o$ in $\mathbb{R}^n$, the unique hyperplane containing it having normal $a$ is the affine set $\partial\mathcal{H}$ (62) where $b$ equals $a^T y_o$ and $\mathcal{R}(Z) = \mathcal{N}(a^T)$.

**3.2.2.1** Given the (shortest) distance $\Delta \in \mathbb{R}_+$ from the origin to a hyperplane having normal vector $a$, we find its description $\partial\mathcal{H}$ by dropping a perpendicular. The point thus found is the orthogonal projection of the origin on $\partial\mathcal{H}$ (§A.2.1.3), equal to $a\Delta/\|a\|$ if the origin is known *a priori* to belong to halfspace $\mathcal{H}_-$ (Figure 5), or to $-a\Delta/\|a\|$ if the origin belongs to halfspace $\mathcal{H}_+$; *id est*, when $\mathcal{H}_- \ni \mathbf{0}$

$$\partial\mathcal{H} = \left\{y \mid a^T(y - a\Delta/\|a\|) = 0\right\} = \left\{y \mid a^T y = \|a\|\Delta\right\} \tag{64}$$

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

$$\partial\mathcal{H} = \left\{y \mid a^T(y + a\Delta/\|a\|) = 0\right\} = \left\{y \mid a^T y = -\|a\|\Delta\right\} \tag{65}$$

[16] 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.

The knowledge of only distance $\Delta$ and normal $a$ thus introduces ambiguity.

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

$$\partial\mathcal{H} \;=\; \{Y \mid <\!A\,,Y\!> \;=\; b\} \;=\; \{Y \mid <\!A\,,Y - Y_o\!> \;=\; 0\} \subset \mathbb{R}^{mn} \tag{66}$$

Vector $a$ is normal to the hyperplane illustrated in Figure 5. In the case of matrix variables, for nonzero $A$ we have

$$A \perp \partial\mathcal{H} \text{ in } \mathbb{R}^{mn} \tag{67}$$

**3.2.2.2**

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

$$\underline{\partial\mathcal{H}}_- \;=\; \left\{y \mid a^T(y - y_o) = 0\,,\quad y_o\in\mathcal{B}\,,\quad a^T(z - y_o) \leq 0 \;\; \forall z\in\mathcal{B}\right\} \tag{68}$$

where normal $a$ and set $\mathcal{B}$ reside in opposite halfspaces. An equivalent representation is

$$\underline{\partial\mathcal{H}}_+ \;=\; \left\{y \mid a^T(y - y_o) = 0\,,\quad y_o\in\mathcal{B}\,,\quad a^T(z - y_o) \geq 0 \;\; \forall z\in\mathcal{B}\right\} \tag{69}$$

where normal $a$ and set $\mathcal{B}$ reside in the same halfspace. When the supporting hyperplane contains only a single point of $\mathcal{B}$, that hyperplane is termed *strictly* supporting, and termed *tangent* to $\mathcal{B}$ when it is unique. [11, §18, p.169] $\diamond$

Other than the fact that a supporting hyperplane intersects the boundary of some set $\mathcal{B}$, there is no difference between $\underline{\partial\mathcal{H}}_-$ or $\underline{\partial\mathcal{H}}_+$ or the generic supporting hyperplane $\underline{\partial\mathcal{H}}$ and an ordinary hyperplane $\partial\mathcal{H}$ coincident with them.

## 3.3 Subspace descriptions

There are two common forms of expression for subspaces, both coming from elementary linear algebra. From the four fundamental subspaces associated with a matrix $A\in\mathbb{R}^{m\times n}$, [19, §3.1] its rowspace and range identify one form of subspace description,

$$\mathcal{R}(A^T) \triangleq \{A^T y \mid y\in\mathbb{R}^m\} = \{x\in\mathbb{R}^n \mid A^T y = x\,,\; y\in\mathcal{R}(A)\} \tag{70}$$

$$\mathcal{R}(A) \triangleq \{Ax \mid x\in\mathbb{R}^n\} = \{y\in\mathbb{R}^m \mid Ax = y\,,\; x\in\mathcal{R}(A^T)\} \tag{71}$$

while its nullspaces identify the second common form,

$$\mathcal{N}(A) \triangleq \{x\in\mathbb{R}^n \mid Ax=\mathbf{0}\} \tag{72}$$

$$\mathcal{N}(A^T) \triangleq \{y\in\mathbb{R}^m \mid A^T y=\mathbf{0}\} \tag{73}$$

We recall that the fundamental subspaces are ordinarily related

$$\mathcal{R}(A^T) \perp \mathcal{N}(A)\,, \qquad \mathcal{N}(A^T) \perp \mathcal{R}(A) \tag{74}$$

and of dimension:

$$\dim\mathcal{R}(A^T) \;=\; \dim\mathcal{R}(A) \;=\; \operatorname{rank} A \;\leq\; \min\{m\,,n\} \tag{75}$$

$$\dim\mathcal{N}(A) = n - \operatorname{rank} A\,, \qquad \dim\mathcal{N}(A^T) = m - \operatorname{rank} A \tag{76}$$

**3.3.0.3 Hyperplane intersection.** The nullspace form (72) or (73) is the solution set to an affine equation similar to the hyperplane definition (62). Yet because matrix $A$ generally has multiple columns and rows, each respective nullspace form is actually the intersection of as many hyperplanes through the origin. (Were the vector constant nonzero, then each hyperplane would not necessarily contain the origin although the solution set would remain an intersection of hyperplanes.)

### 3.3.1 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

$$\mathcal{N}(A)\cap\mathcal{N}(B) \;=\; \mathcal{N}\left(\begin{bmatrix} A \\ B \end{bmatrix}\right) \;\triangleq\; \{x\in\mathbb{R}^n \mid \begin{bmatrix} A \\ B \end{bmatrix} x = \mathbf{0}\} \tag{77}$$

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 [25, §12.4.2]

$$\mathcal{N}(A)\cap\mathcal{N}(B) = \mathcal{R}(ZW) \tag{78}$$

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

In the particular circumstance that both $A$ and $B$ are positive semidefinite, [30, §6]

$$\mathcal{N}(A) \cap \mathcal{N}(B) = \mathcal{N}(A+B)\,, \qquad A\,,B \in \mathbb{S}^M_+ \qquad (43)$$

## 3.4 Extreme, Exposed

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

$$\mu\, x_1 + (1-\mu)x_2 \neq x_\varepsilon\,, \quad \mu \in [0,1] \tag{79}$$

◇

In other words, $x_\varepsilon$ is an extreme point of $\mathcal{C}$ iff $x_\varepsilon$ is not a point relatively interior to any line segment in $\mathcal{C}$. [15, §2.10]

**Definition.** *Face, edge.* [10, §A.2.3]

- A *face* of a convex set $\mathcal{C}$ is a convex subset $\mathcal{F} \subseteq \mathcal{C}$ such that every closed line segment $\overline{x_1 x_2}$ in $\mathcal{C}$, having a relative 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 $\mathcal{C}$ are called extreme points. The empty set and $\mathcal{C}$ itself are conventional faces of $\mathcal{C}$. [11, §18]
- All faces $\mathcal{F}$ are extreme sets by definition; *id est*, for $\mathcal{F} \subseteq \mathcal{C}$ and all $x_1\,, x_2 \in \mathcal{C} \backslash \mathcal{F}$ ,
$$\mu\, x_1 + (1-\mu)x_2 \notin \mathcal{F}\,, \quad \mu \in [0,1] \tag{80}$$
- A one-dimensional face of a convex set is called an *edge.*

◇

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

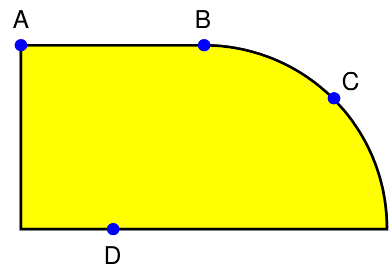


Figure 6: Closed convex set in $\mathbb{R}^{\mathbf{2}}$. Point A is exposed hence extreme, point B is extreme but not exposed, point C is exposed and extreme, point D is neither exposed nor extreme. [10, §A.2.4] [12, §3.6] Closed face $\overline{\mathrm{AB}}$ is exposed.

### 3.4.1 Exposure

**Definition.** *Exposed face, exposed point, vertex, facet.* [10, §A.2.4]

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

$$\mathcal{F} = \mathcal{C} \cap \underline{\partial\mathcal{H}} \tag{81}$$

  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 convex set $\mathcal{C} \subseteq \mathbb{R}^n$; in one-to-one correspondence with the $(n-1)$-dimensional faces.[17]

- exposed faces $\subseteq$ faces
  exposed points $\subseteq$ extreme points

$\diamond$

[17]This coincidence occurs because the dimension of the facet is the same as the dimension of the supporting hyperplane exposing it.

Exposed points constitute a *dense* subset of extreme points for some closed convex set $\mathcal{C}$; [11, §18] [36] [12, §3.6, p.115] dense in the sense [34] that closure of that subset yields the set of extreme points. For the convex set illustrated in Figure 6, point B cannot be exposed because it relatively bounds both the facet $\overline{\text{AB}}$ 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.

**3.4.1.1** Faces enjoy a transitive relationship. If $\mathcal{F}_2$ is a face (an extreme set) of $\mathcal{F}_1$ which, in turn, is a face of $\mathcal{C}$, then it is always true that $\mathcal{F}_2$ is a face of $\mathcal{C}$. [11, §18] [37, def.115/6, p.358] For example, any extreme point of $\mathcal{F}_1$ is an extreme point of $\mathcal{C}$. 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 4, for example, the 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.

The classical definition of *boundary* of a set $\mathcal{C}$ is the closure of $\mathcal{C}$ less its interior; [9, old§1.5.2]

$$\partial\mathcal{C} = \bar{\mathcal{C}} \setminus \operatorname{int}\mathcal{C} \tag{82}$$

A more suitable description is equivalent for closed convex sets:

**Definition.** *Boundary* $\partial$ *of convex set.* [10, §C.3.1] The boundary $\partial\mathcal{C}$ of a nonempty closed convex set $\mathcal{C}$ is the union of all the exposed faces of $\mathcal{C}$. ◇

A convex polyhedron, for example, in $\mathbb{R}$ has a boundary constructed from points, in $\mathbb{R}^2$ from line segments, in $\mathbb{R}^3$ from polygons, while a convex *polychoron* (a polyhedron in $\mathbb{R}^4$ [34]) has a boundary constructed from three-dimensional polyhedra.

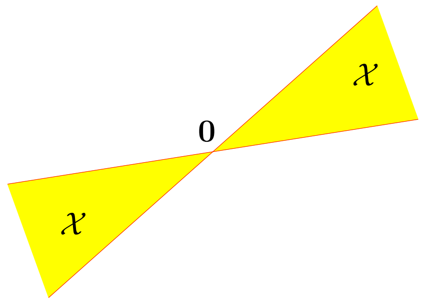


Figure 7: Two-dimensional non-convex cone drawn truncated. Boundary of this cone is itself a cone. [5, §2.4]

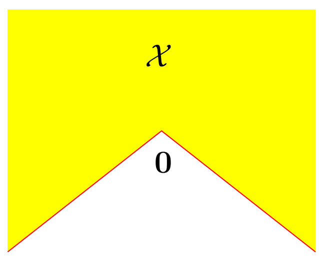


Figure 8: Truncated non-convex cone in $\mathbb{R}^{\mathbf{2}}$. Boundary is also a cone. [*ibidem*]

### 3.4.2 Convex cone

**Definition.** *Ray.* The set

$$\{\zeta\Gamma + B \mid \zeta \geq 0\,,\ \Gamma \neq \mathbf{0}\} \subset \mathbb{R}^n \tag{83}$$

defines a *halfline* 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 $\Gamma$; hence a cone. ⋄

A set $\mathcal{X}$ is called a *cone* iff

$$\Gamma \in \mathcal{X} \ \Rightarrow\ \zeta\Gamma \in \mathcal{X} \ \text{ for all } \zeta \geq 0 \tag{84}$$

An example of such a cone is the union of two opposing quadrants; *e.g.*, $\mathcal{X} = \left\{x \in \mathbb{R}^{\mathbf{2}} \mid x_1 x_2 \geq 0\right\}$. [14, §2.5] Similar examples are shown in Figure 7

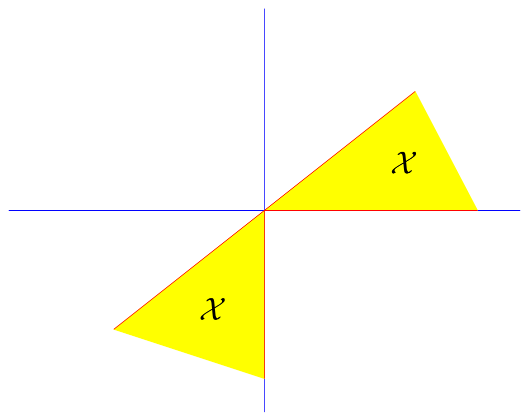


Figure 9: Truncated non-convex cone $\mathcal{X} = \{x \in \mathbb{R}^{\mathbf{2}} \mid x_1 \geq x_2 \,,\; x_1 x_2 \geq 0\}$. Boundary is also a cone. [*ibidem*]

and Figure 9. We see that cones are not necessarily convex, but are exclusively composed of rays emanating from the origin. Hence all relatively nonempty cones contain the origin and are unbounded, with the exception of the simplest cone $\{\mathbf{0}\}$.

We call the set $\mathcal{K}$ a convex cone if and only if

$$\Gamma_1 \,, \Gamma_2 \in \mathcal{K} \;\Rightarrow\; \zeta\Gamma_1 + \xi\Gamma_2 \in \mathcal{K} \;\text{ for all }\; \zeta \,, \xi \geq 0 \tag{23}$$

Obviously, $\{\mathcal{K}\} \subset \{\mathcal{X}\}$; *id est*, the set of all convex cones is a subset of all cones. The set of convex cones is a narrower but more familiar class of cone 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. The convex cone is implicitly a closed set, by definition of the halfspace in (52) and (53), possibly with empty interior.

Familiar examples of convex cones include an unbounded ice-cream cone and its interior (`a.k.a.` second-order, quadratic, or Lorentz cone [9, §...]), or the boundary and interior of any orthant formed by the Cartesian axes. Esoteric examples of convex cones include the empty set,[18] the point at the origin, any line through the origin, any ray having the origin as base such as the nonnegative real line in subspace $\mathbb{R}$, any halfspace partially bounded

[18]Inclusion of the empty set will facilitate the definition of dual cone.

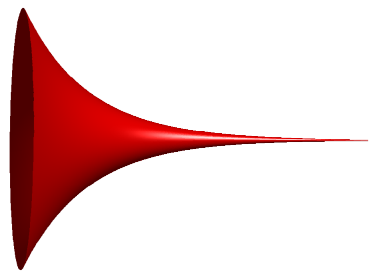

Figure 10: Not a cone; three-dimensional *flared horn* drawn truncated.

by a hyperplane through the origin, the positive semidefinite cone $\mathbb{S}_+^M$ (21) (§2.1.3), the cone of Euclidean distance matrices $\mathbb{EDM}^N$ (179) (§5), any subspace, and $\mathbb{R}^n$. More Euclidean objects are cones, it seems, than are not (*confer* Figure 7-Figure 10).

**Theorem.** *Cone intersection.* [11, §2] The intersection of an arbitrary collection of convex cones is a convex cone. $\diamond$

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

**Definition.** *Pointed convex cone.* A convex cone $\mathcal{K}$ is *pointed* if it contains no line. If the origin is an extreme point of $\mathcal{K}$ or, equivalently, if

$$\mathcal{K} \cap -\mathcal{K} = \{\mathbf{0}\} \tag{85}$$

then $\mathcal{K}$ is pointed [12, §2.10] since it is implicitly closed. $\mathcal{K}$ is *not* pointed if there exists any nonzero $\Gamma \in \mathcal{K}$ such that $-\Gamma \in \mathcal{K}$. [9, old p.22] $\diamond$

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

**Definition.** *Proper cone*: [9, §2]

- is convex
- closed
- pointed
- and has nonempty interior.

$\diamond$

Examples of proper cones are the positive semidefinite cone $\mathbb{S}_+^M$ , the cone of Euclidean distance matrices $\mathbb{EDM}^N$, the nonnegative real line in vector space $\mathbb{R}$ , and any orthant in $\mathbb{R}^n$.

### 3.4.3 Cone boundary

Every hyperplane supporting a convex cone contains the origin. [13, §II.8] [10, §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:

**Lemma.** *Cone faces.* [13, §II.8] Each exposed face of a convex cone is a convex cone. $\diamond$

**Theorem.** *Proper-cone boundary.* Suppose a nonzero point $\Gamma$ 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 $\partial\mathcal{K}$ . $\diamond$

**Proof.** By virtue of its propriety, a proper cone guarantees the existence of a strictly supporting hyperplane at the origin. [11, Cor. 11.7.3][19] 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 $\Gamma$, and the ray belongs to $\mathcal{K}$ by definition (84). By the *cone faces lemma*, every 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. That means there exists a supporting hyperplane $\underline{\partial\mathcal{H}}$ to $\mathcal{K}$ containing $\overline{\mathbf{0}\Gamma}$ . Hence the ray through $\Gamma$ belongs both

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

to $\mathcal{K}$ and to $\underline{\partial\mathcal{H}}$. $\underline{\partial\mathcal{H}}$ must therefore expose a face of $\mathcal{K}$ which contains the ray; *id est*,

$$\{\zeta\Gamma \mid \zeta \geq 0\} \subseteq \mathcal{K} \cap \underline{\partial\mathcal{H}} \subset \partial\mathcal{K} \tag{86}$$

♦

#### 3.4.4 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. [11, §18, p.162][20] An extreme direction $\Gamma_\varepsilon$ of $\mathcal{K}$ corresponds to an edge that is a ray.[21] Nonzero direction $\Gamma_\varepsilon$ in pointed $\mathcal{K}$ is extreme if and only if,

$$\zeta_1\Gamma_1 + \zeta_2\Gamma_2 \neq \Gamma_\varepsilon \quad \forall\, \zeta_1\,, \zeta_2 \geq 0\,, \quad \forall\, \Gamma_1\,, \Gamma_2 \in \mathcal{K} \backslash \{\zeta\Gamma_\varepsilon \in \mathcal{K} \mid \zeta \geq 0\} \tag{87}$$

In words, an extreme direction in a pointed 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 it. For example, the extreme directions of the positive semidefinite cone comprise the set of all symmetric rank-one matrices. [28, §III] [30, §6]

An extreme *direction* is unique, but its vector representation is not because any positive scaling of it produces another vector in the same (extreme) direction.

If (closed) convex $\mathcal{K}$ is not pointed, then it has no extreme directions and no vertex. [30, §1] Conversely, pointed convex $\mathcal{K}$ is the convex hull of its extreme directions and vertex. [11, §18, p.167] That is the practical utility of extreme direction; to facilitate construction of polyhedral sets, apparent from the *extremes theorem*:

**Theorem (Klee).** *Extremes.* [12, §3.6] [11, §18, p.166] (*confer* §3.1.2, §3.5.2) Any closed convex set containing no lines can be expressed as the convex hull of all its extreme points and directions. ◇

**3.4.4.1 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

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

[21] 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.

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 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 $i^{\text{th}}$ extreme direction by $\Gamma_i \in \mathbb{R}^n$, then the convex hull is (50)

$$\begin{aligned}\mathcal{P} &= \left\{[\mathbf{0}\;\;\Gamma_1\;\;\Gamma_2 \cdots \Gamma_N]\, a\,\zeta \mid a^T\mathbf{1} = 1,\; a \succeq 0,\; \zeta \geq 0\right\} &(88)\\ &= \left\{[\Gamma_1\;\;\Gamma_2 \cdots \Gamma_N]\, a\,\zeta \mid a^T\mathbf{1} \leq 1,\; a \succeq 0,\; \zeta \geq 0\right\} &(89)\\ &= \left\{[\Gamma_1\;\;\Gamma_2 \cdots \Gamma_N]\, b \quad \mid b \succeq 0\right\} \subset \mathbb{R}^n &(90)\end{aligned}$$

that is simply a conic hull like (51). □

### 3.4.5 Exposed direction

**Definition.** *Exposed direction, exposed point of a convex cone.* [11, §18] (*confer* §3.4.1)

- When a convex cone has a vertex, an exposed point, it resides at the origin.
- In a convex cone, an *exposed direction* is the direction of a one-dimensional exposed face that is a ray emanating from the origin.
- exposed directions $\subseteq$ extreme directions

◇

### 3.4.6 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 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 $\zeta_i \geq 0$,

$$\Gamma_i\,\zeta_i + \cdots + \Gamma_j\,\zeta_j - \Gamma_k\,\zeta_k = \mathbf{0}\,, \qquad i \neq \cdots \neq j \neq k = 1 \ldots N \qquad (91)$$

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 11,

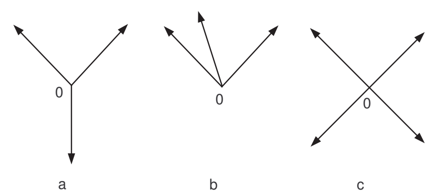


Figure 11: Vectors in $\mathbb{R}^{\mathbf{2}}$ : (a) conically independent, (b) conically dependent. Neither example exhibits linear independence.

for example. A Matlab implementation of test (91) is given in §E.1.) 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,

$$X \triangleq [\Gamma_1 \ \Gamma_2 \ \cdots \ \Gamma_N] \in \mathbb{R}^{n\times N} \tag{92}$$

and denoting by $k$ the number of conically independent generators contained in $X$, we have the most fundamental rank inequality for convex cones

$$\operatorname{rank} X \leq k \leq N \tag{93}$$

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

#### 3.4.6.1 Table: Maximum number conically independent directions

| $n$ | $\sup k$ (pointed) | $\sup k$ (not pointed) |
|---|---|---|
| 0 | 0 | 0 |
| 1 | 1 | 2 |
| 2 | 2 | 4 |
| 3 | $\infty$ | $\infty$ |
| $\vdots$ | $\vdots$ | $\vdots$ |

(a)

(b)

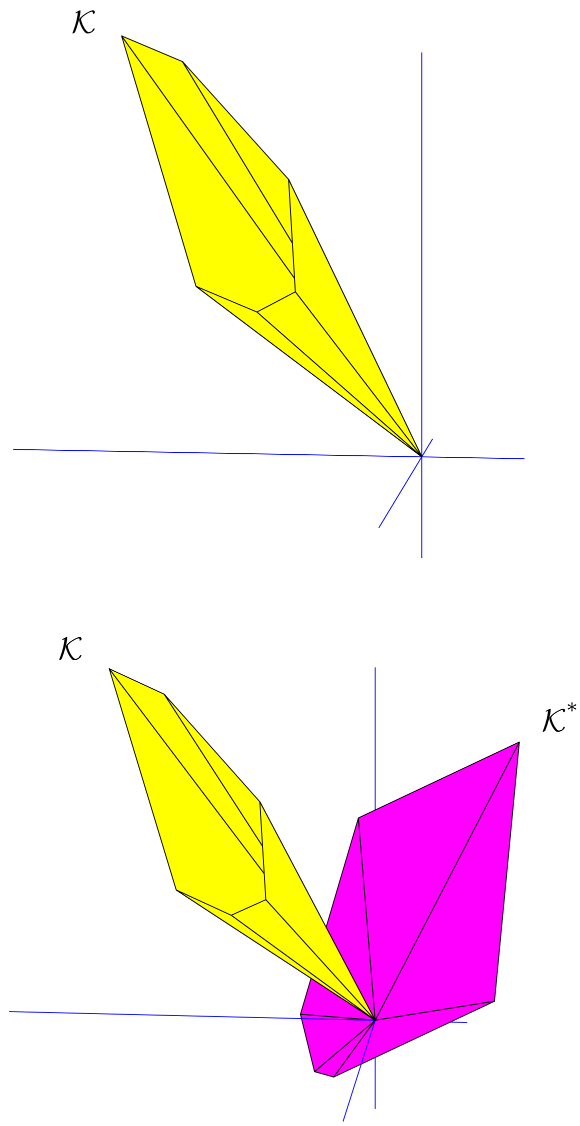


Figure 12: (a) A pointed polyhedral cone (drawn truncated) in $\mathbb{R}^{\mathbf{3}}$ having six facets. The extreme directions, corresponding to the six edges emanating from the origin, are generators for this cone; not linearly independent but they must be conically independent.
(b) The boundary of dual cone $\mathcal{K}^*$ (drawn truncated) is now added to the drawing of the same $\mathcal{K}$. $\mathcal{K}^*$ is polyhedral, proper, and has the same number of extreme directions as $\mathcal{K}$ has facets.

**3.4.6.2 Pointed convex $\mathcal{K}$ and conic independence.** The set of all extreme directions from a pointed convex cone $\mathcal{K} \subset \mathbb{R}^n$ are not necessarily linearly independent, yet they must be conically independent; (compare Figure 12(a) and Figure 14, p.44)

- extreme directions $\Rightarrow$ c.i.

Yet any collection of $n$ or fewer extreme directions from pointed 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 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 convex $\mathcal{K} \Rightarrow$ extreme directions

These results follow from the definitions (87) and (91) in conjunction with the *extremes theorem* (§3.4.4).

### 3.4.7 When extreme means exposed

For any convex polyhedral set in $\mathbb{R}^n$, the distinction between the terms "extreme" and "exposed" vanishes [12, §2.4] for faces of all dimensions except $n$; their meanings become equivalent as we saw in Figure 4 (§3.4.1.1). In other words, all faces of any polyhedral set (except the set itself) are properly exposed, and *vice versa.*

## 3.5 Convex polyhedra

**Definition.** *Convex polyhedra, halfspace description.* [9, §2]
A polyhedron is the intersection of a finite number of halfspaces and hyperplanes;

$$\mathcal{P} = \{y \mid Ay \succeq b\,,\ Cy = d\} \subseteq \mathbb{R}^n \tag{94}$$

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. $\diamond$

By the *halfspaces theorem* in §3.2.1, a polyhedron thus described[22] must be a closed convex set having possibly empty interior, a convex *polytope* [34]; *e.g.*, Figure 4. Convex polyhedra[23] are finite dimensional, comprising all affine sets (§3.1.1), polyhedral cones, line segments, rays, halfspaces, convex polygons, *solids* [37, def.104/6, p.343], polychora, *etcetera*

When $b$ and $d$ in (94) are zero, the resultant is a polyhedral cone. The set of all polyhedral cones is a subset of convex cones:

### 3.5.1 Polyhedral cone

From §3.4.2, 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* [11, §19]. We distinguish polyhedral cones in the set of all convex cones for this very reason.

**Definition.** *Polyhedral cone, halfspace description.* (*confer* (108))
A polyhedral cone is the intersection of a finite number of halfspaces and hyperplanes about the origin;

$$\begin{aligned}\mathcal{K} &= \{y \mid Ay \succeq 0\,,\ Cy = \mathbf{0}\} \ \subseteq \mathbb{R}^n && \text{(a)}\\ &= \{y \mid Ay \succeq 0\,,\ Cy \succeq 0\,,\ Cy \preceq 0\} && \text{(b)}\end{aligned} \tag{95}$$

where coefficients $A$ and $C$ generally denote matrices of finite dimension. Each row of $C$ is a vector normal to a hyperplane through 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 (§3.4.4.1), and *vice versa.* [Minkowski/Weyl] [12, §2.8]

The direction of an arbitrary ray on the relative boundary of a convex cone is not necessarily an exposed or extreme direction. For the polyhedral

[22] Rockafellar [11, §19] proposes affine sets be handled via complementary pairs of affine inequalities; *e.g.*, $Cy \succeq d$ and $Cy \preceq d$.

[23] We consider only convex polyhedra throughout, but acknowledge the existence of concave polyhedra. [34, *Kepler-Poinsot Solid*]

cone illustrated in Figure 14, 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. Because that set is polyhedral, the exposed directions are in one-to-one correspondence with the extreme directions; the directions of the edges that are rays (there are only three edges).

The most familiar example of a polyhedral cone is the boundary and interior of any quadrant (or orthant) formed by the Cartesian axes. Esoteric examples of polyhedral cones include the empty set,[24] the point at the origin, any line through the origin, any ray having the origin as base such as the nonnegative real line in subspace $\mathbb{R}$, any halfspace partially bounded by a hyperplane through the origin, any subspace, and $\mathbb{R}^n$. More examples are illustrated in Figure 12 and Figure 14.

### 3.5.2 Vertices of convex polyhedra

A vertex always lies on the relative boundary of a convex polyhedron. [37, def.115/6, p.358] In Figure 4, each vertex of the polyhedron is located at the intersection of three or more facets, and every edge belongs to precisely two facets [13, §VI.1, p.252]. In Figure 14, 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 (50). Hence we propose a universal vertex description of polyhedra in terms of that same finite-length list (47) in $X$ :

**Definition.** *Convex polyhedra, vertex description.* (*confer* 3.4.4)
Denote the truncated $a$-vector,

$$a_{i:\ell} = \begin{bmatrix} a_i \\ \vdots \\ a_\ell \end{bmatrix} \tag{96}$$

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

$$\mathcal{P} = \left\{ Xa \mid a_{1:k}^T \mathbf{1} = 1\,,\; a_{m:N} \succeq 0\,,\; \{1 \ldots k\} \cup \{m \ldots N\} = \{1 \ldots N\} \right\} \tag{97}$$

[24] For example, $C = [\emptyset]$ .

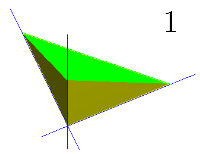


Figure 13: The unit simplex in $\mathbb{R}^3$ is a unique solid tetrahedron, but is not regular.

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

The coefficient indices in (97) may or may not be overlapping, but all the coefficients are assumed constrained. From (49), (50), and (51), we summarize how the constraints may be applied;

$$\left.\begin{array}{lcl} \text{affine sets} & \longrightarrow & a_{1:k}^T\mathbf{1} = 1 \\ \text{polyhedral cones} & \longrightarrow & a_{m:N} \succeq 0 \end{array}\right\} \longleftarrow \text{convex hull } (m \leq k) \tag{98}$$

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

$$\{a_{m:k} \mid a_{m:k}^T\mathbf{1} = 1,\ a_{m:k} \succeq 0\} \subseteq \{a_{m:k} \mid a_{1:k}^T\mathbf{1} = 1,\ a_{m:N} \succeq 0\} \tag{99}$$

Members of a generating list are not necessarily vertices of the corresponding polyhedron; certainly true for (50) and (97), some subset of list members reside in the polyhedron's relative interior. Conversely, when boundedness (50) applies, the convex hull of the vertices is a polyhedron identical to the convex hull of the generating list.

### 3.5.3 Unit simplex

A peculiar convex subset of the nonnegative orthant having halfspace description

$$\mathcal{S} \triangleq \{s \mid s \succeq 0\,,\ \mathbf{1}^T s \leq 1\} \subset \mathbb{R}_+^n \tag{100}$$

is a unique convex polyhedron called *unit simplex* (Figure 13) having nonempty interior, $n+1$ vertices, and dimension [9, §2]

$$\dim \mathcal{S} = n \tag{101}$$

The origin supplies one vertex while heads of the *standard basis* [24] [19] $\{e_i\,,\ i\!=\!1\ldots n\}$ in $\mathbb{R}^n$ constitute those remaining;[25] thus its vertex description:

$$\begin{aligned}\mathcal{S} &= \operatorname{conv}\{\mathbf{0},\ \{e_i\,,\ i\!=\!1\ldots n\}\}\\ &= \left\{[\mathbf{0}\ \ e_1\ \ e_2\ \cdots\ e_n]\,a \mid a^T\mathbf{1} = 1\,,\ a \succeq 0\right\}\end{aligned} \tag{102}$$

**Definition.** *Simplicial cone.* A polyhedral proper cone $\mathcal{K}$ in $\mathbb{R}^n$ is called *simplicial* iff $\mathcal{K}$ has exactly $n$ extreme directions; [29, §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 $\mathbb{R}^n$; one example is drawn in Figure 14.

### 3.5.4 Converting between descriptions

Conversion between halfspace/hyperplane (94) (95) and vertex descriptions (50) (97) is nontrivial, in general, [38] but the conversion is easy for simplices. [9, old§1.2] Nonetheless, we tacitly assume the two descriptions to be equivalent. [11, §19, thm.19.1] We explore some conversions in §3.6.

## 3.6 Dual cone, generalized inequality, biorthogonal expansion

For any cone $\mathcal{K}$ (convex or not), the *dual cone* [9, old§1.6.1]

$$\mathcal{K}^* = \left\{y \in \mathbb{R}^n \mid x^Ty \geq 0 \ \text{ for all } \ x \in \mathcal{K}\right\} \tag{103}$$

[25] 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 13), in $\mathbb{R}^{\mathbf{4}}$ it is the convex hull of a polychoron [34], and so on. The *unit* simplex comes from a class of general polyhedra called *simplex*, having vertex description: [7] [11] [14]

$$\{\operatorname{conv}\{v_i \in \mathbb{R}^n\} \mid \dim\operatorname{aff}\{v_i\,,\ i=0\ldots k\} = k\,,\ n \geq k\}$$

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

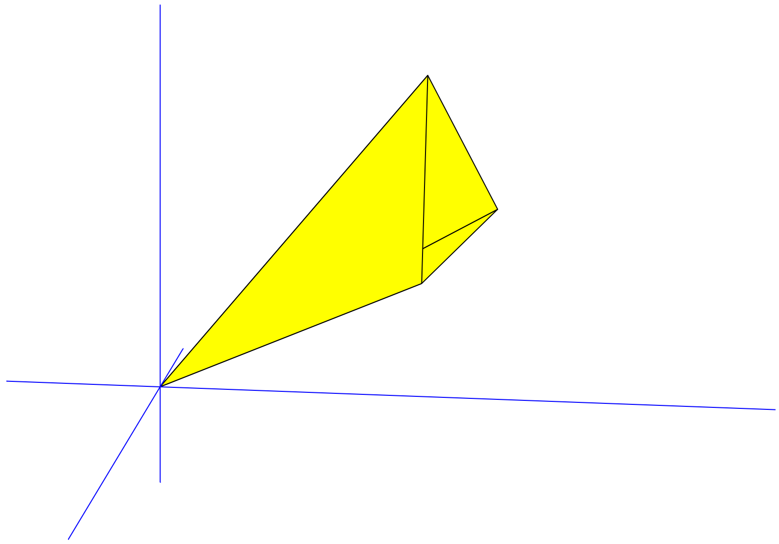

Figure 14: A simplicial cone in $\mathbb{R}^{\mathbf{3}}$ whose boundary is drawn truncated; constructed using $A \in \mathbb{R}^{\mathbf{3}\times\mathbf{3}}$ and $C = \mathbf{0}$ in (95). The extreme directions are the directions of the three edges emanating from the origin; they are conically and linearly independent for this cone.

is a unique cone[26] that is always closed and convex (regardless of $\mathcal{K}$ convexity) because it is an intersection of closed halfspaces (*halfspaces theorem*, §3.2.1). Geometrically, the dual cone $\mathcal{K}^*$ consists of all vectors $y$ inward-normal to a hyperplane supporting $\mathcal{K}$.

As defined, the 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.[27] Rockafellar formulates the dimension of $\mathcal{K}$ and $\mathcal{K}^*$. [11, §14][28]

### 3.6.1 Key properties of dual cone

- For any cone, $(-\mathcal{K})^* = -\mathcal{K}^*$
- For any cones $\mathcal{K}_1$ and $\mathcal{K}_2$, $\mathcal{K}_1 \subseteq \mathcal{K}_2 \;\Rightarrow\; \mathcal{K}_1^* \supseteq \mathcal{K}_2^*$ [12, §2.7]

[26] The dual cone is the negative of the *polar cone* defined by some authors; $\mathcal{K}^* = -\mathcal{K}^\circ$. [10] [11] [39] [13] [12]

[27] $\not\Rightarrow$ empty relative interior.

[28] His monumental work has not one drawing or picture. See [13, §II.16] for a good illustration of Rockafellar's *recession cone.*

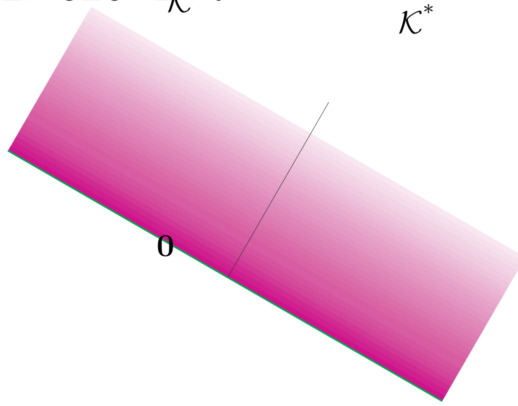


Figure 15: $\mathcal{K}$ is a halfspace about the origin in $\mathbb{R}^{\mathbf{2}}$. $\mathcal{K}^*$ is a ray base $\mathbf{0}$, hence empty in $\mathbb{R}^{\mathbf{2}}$; so $\mathcal{K}$ cannot be pointed. (Both convex cones appear truncated.)

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

$$\mathcal{K} \text{ nonempty } \Rightarrow \mathcal{K}^* \text{ pointed} \tag{104}$$

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

$$\overline{\mathcal{K}} \text{ pointed } \Rightarrow \mathcal{K}^* \text{ nonempty} \tag{105}$$

- When $\mathcal{K}$ is closed and convex, the dual of the dual cone is the original cone; $\mathcal{K}^{**} = \mathcal{K}$.

- For convex cones $\mathcal{K}_1$ and $\mathcal{K}_2$, (the dual vector sum [13, §IV.1])

$$(\mathcal{K}_1 + \mathcal{K}_2)^* = \mathcal{K}_1^* \cap \mathcal{K}_2^* \tag{106}$$

- For (closed) convex cones $\mathcal{K}_1$ and $\mathcal{K}_2$,

$$(\mathcal{K}_1 \cap \mathcal{K}_2)^* = \overline{\mathcal{K}_1^* + \mathcal{K}_2^*} \tag{107}$$

  (the closure of the vector sum of duals [13, §IV.1])

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

- $\mathcal{K}$ is polyhedral if and only if $\mathcal{K}^*$ is polyhedral. [12, §2.8]

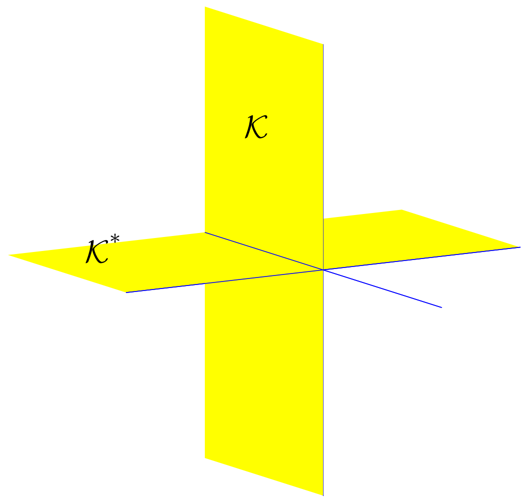


Figure 16: $\mathcal{K}$ and $\mathcal{K}^*$ are halfplanes in $\mathbb{R}^{\mathbf{3}}$. (Both convex cones appear truncated.) Cartesian coordinate axes drawn for reference.

- $\mathcal{K}$ is simplicial if and only if $\mathcal{K}^*$ is simplicial. (§3.6.3.1)

When cone $\mathcal{K}$ is a halfspace in $\mathbb{R}^n$ with $n>0$, Figure 15 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.* (§A.5.1) 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 halfplane in $\mathbb{R}^{\mathbf{3}}$ (Figure 16), it is neither pointed nor nonempty; hence, the dual cone $\mathcal{K}^*$ can be neither nonempty nor 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: $\mathbb{R}^{\mathbf{3}}_{+} + \mathbb{R}^{\mathbf{3}}_{3-}$ .

**Example.** *Vertex description/dual halfspace-description.* 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 (92), then that cone is described setting $m=1$ and $k=0$ in vertex description (97):

$$\mathcal{K} \;=\; \{Xa \mid a\succeq 0\} \;\subseteq\; \mathbb{R}^n \tag{108}$$

a conic hull, like (51), of $N$ generators. Assuming all generators are nonzero, $\mathcal{K}$ is pointed (§3.4.2) if and only if there is no $a\neq\mathbf{0}$, $a\succeq 0$ that solves

$Xa = \mathbf{0}$. [12, §2.10] This means there is at least one hyperplane, whose normal is a row of $X$, that strictly supports the nonnegative orthant in $\mathbb{R}^N$.

The halfspace description of the corresponding dual cone is equally simple: (103) (*confer* (95))

$$\begin{aligned}\mathcal{K}^* &= \left\{y \in \mathbb{R}^n \mid z^T y \geq 0 \text{ for all } z = Xa\,,\ a \succeq 0\right\}\\ &= \left\{y \in \mathbb{R}^n \mid a^T X^T y \geq 0\,,\ a \succeq 0\right\}\\ &= \left\{y \in \mathbb{R}^n \mid X^T y \succeq 0\right\}\end{aligned} \tag{109}$$

that follows from the *generalized inequality corollary* (111). 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. □

For any polyhedral cone $\mathcal{K}$, the dual cone $\mathcal{K}^*$ is also polyhedral, and $\mathcal{K}^{**} = \mathcal{K}$. [12, §2.7, §2.8] A simplicial cone $\mathcal{K}$ and its dual $\mathcal{K}^* \subset \mathbb{R}^n$ are polyhedral proper cones ($\dim \operatorname{aff} \mathcal{K} = \dim \operatorname{aff} \mathcal{K}^* = n$; *e.g.*, Figure 18, p.57), but polyhedral proper cones are not necessarily simplicial.

**Corollary.** *Generalized inequality.* [10, §A.4.2] Let $\mathcal{K}$ be a closed convex cone and $\mathcal{K}^*$ its dual, and let $x$ and $y$ belong to a vector space $\mathbb{R}^n$. Then

$$x \in \mathcal{K} \;\Leftrightarrow\; y^T x \geq 0 \text{ for all } y \in \mathcal{K}^* \tag{110}$$

which is a generalization of the fact

$$x \succeq 0 \;\Leftrightarrow\; y^T x \geq 0 \text{ for all } y \succeq 0 \tag{111}$$

where implicitly $\mathcal{K} = \mathcal{K}^* = \mathbb{R}^n_+$ the nonnegative orthant. By symmetry we also have

$$y \in \mathcal{K}^* \;\Leftrightarrow\; y^T x \geq 0 \text{ for all } x \in \mathcal{K} \tag{112}$$

When $\mathcal{K}$ is a pointed closed convex cone, the generalized inequality (110) is often written

$$x \underset{\mathcal{K}}{\succeq} 0 \;\Leftrightarrow\; y^T x \geq 0 \text{ for all } y \underset{\mathcal{K}^*}{\succeq} 0 \tag{113}$$

meaning that the coordinates for *biorthogonal expansion* of $x$ [23] can be nonnegative when $x$ belongs to $\mathcal{K}$, and must be nonnegative when $x$ belongs to simplicial $\mathcal{K}$. By symmetry

$$y \underset{\mathcal{K}^*}{\succeq} 0 \;\Leftrightarrow\; y^T x \geq 0 \;\text{ for all }\; x \underset{\mathcal{K}}{\succeq} 0 \tag{114}$$

⋄

The *generalized inequality corollary* is discretized in the following theorem [30, §1][29] that follows from (109):

**Theorem.** *Discrete generalized inequality.* Given any discrete set of generators (§3.4.4.1) 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 a vector space $\mathbb{R}^n$. Then

$$x \in \mathcal{K} \;\Leftrightarrow\; \gamma^{*T} x \geq 0 \;\text{ for all }\; \gamma^* \in \mathcal{G}(\mathcal{K}^*) \tag{115}$$

$$y \in \mathcal{K}^* \;\Leftrightarrow\; \gamma^T y \geq 0 \;\text{ for all }\; \gamma \in \mathcal{G}(\mathcal{K}) \tag{116}$$

⋄

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

$$x \succeq 0 \;\Leftrightarrow\; x \in \mathcal{K} \tag{117}$$

**3.6.1.1 Pointed, closed, convex cone.** A pointed closed convex cone $\mathcal{K}$ induces a *partial-order* [34] relation on $\mathbb{R}^n$ or $\mathbb{S}^M$ [30, §1], respectively defined by vector or matrix inequality;

$$A \preceq B \;\;\Leftrightarrow\;\; B - A \in \mathcal{K} \tag{118}$$

$$A \prec B \;\;\Leftrightarrow\;\; B - A \in \operatorname{rel\,int} \mathcal{K} \tag{119}$$

*Comparable points* [9, old§1.4.2] (Figure 17) and the minimum element of some vector- or matrix-valued set [9, old§1.6.3] are thus well defined.[30] Examples of pointed closed convex cones $\mathcal{K}$: any zero-based ray in a subspace, any two-dimensional V-shaped cone in a subspace, the Lorentz (ice-cream) cone, the proper cones: $\mathbb{S}^M_+$ in $\mathbb{S}^M$, the cone of Euclidean distance matrices $\mathbb{EDM}^N$ in $\mathbb{S}^N_\delta$, the nonnegative real line in vector space $\mathbb{R}$, any orthant in $\mathbb{R}^n$.

[29] Barker and Carlson only state the theorem for the *pointed* convex case.

[30] We say $x \in \mathcal{C}$ is the (unique) minimum element of $\mathcal{C}$ with respect to $\mathcal{K}$ if for every $y \in \mathcal{C}$ we have $x \preceq y$; equivalently, iff $\mathcal{C} \subseteq x + \mathcal{K}$.

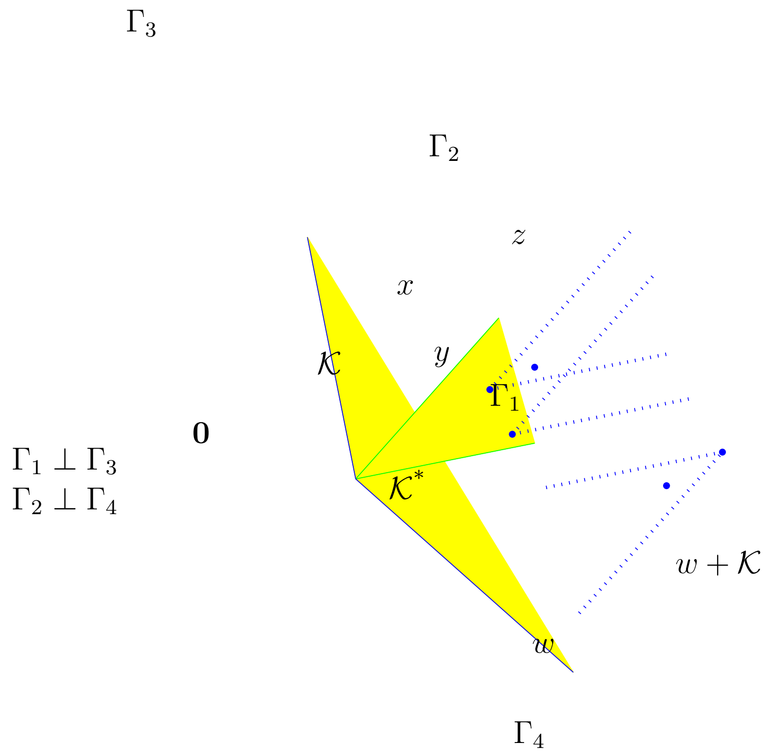


Figure 17: Simplest example in $\mathbb{R}^{\mathbf{2}}$ of biorthogonal expansion of $x$ (121). Polyhedral proper cone $\mathcal{K}$ and its dual $\mathcal{K}^*$ drawn truncated. Point $x$ comparable to point $z$ (and *vice versa*) but not to $y$; $z \succeq x \Leftrightarrow z - x \in \mathcal{K} \Leftrightarrow z - x \succeq_{\mathcal{K}} 0$ 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 $w + \mathcal{K}$. Conically independent generators $\Gamma_1$ and $\Gamma_2$ constitute extreme directions of $\mathcal{K}$ while $\Gamma_3$ and $\Gamma_4$ constitute extreme directions of $\mathcal{K}^*$.

#### 3.6.1.2 Examples of biorthogonal expansion.

**Example.** *Biorthogonal expansion, relationship to dual polyhedral cone.* The proper cone $\mathcal{K}$ illustrated in Figure 17 induces a partial-order relation on $\mathbb{R}^{\mathbf{2}}$. All points greater than $x$ with respect to $\mathcal{K}$, for example, are contained in the translated cone $x+\mathcal{K}$. The extreme directions $\Gamma_1$ and $\Gamma_2$ of $\mathcal{K}$ do not make an orthogonal set; neither do extreme directions $\Gamma_3$ and $\Gamma_4$ of dual cone $\mathcal{K}^*$; rather, we have the *biorthogonality condition*, [23]

$$\begin{gathered}\Gamma_3^T\Gamma_1 = \Gamma_4^T\Gamma_2 = 0\\ \Gamma_4^T\Gamma_1 \neq 0\,, \quad \Gamma_3^T\Gamma_2 \neq 0\end{gathered} \tag{120}$$

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

$$x \,=\, \Gamma_1\,\frac{\Gamma_4^T x}{\Gamma_4^T\Gamma_1} \,+\, \Gamma_2\,\frac{\Gamma_3^T x}{\Gamma_3^T\Gamma_2} \tag{121}$$

where $\Gamma_4^T x/(\Gamma_4^T\Gamma_1)$ is the nonnegative coefficient of *non*orthogonal projection (§A.3.1) of $x$ on $\Gamma_1$ in the direction orthogonal to $\Gamma_4$, and where $\Gamma_3^T x/(\Gamma_3^T\Gamma_2)$ is the nonnegative coefficient of nonorthogonal projection of $x$ on $\Gamma_2$ in the direction orthogonal to $\Gamma_3$. Those coefficients must be nonnegative $x\succeq_{\mathcal{K}} 0$ because $x\in\mathcal{K}$ (117) and $\mathcal{K}$ is simplicial. If we ascribe the extreme directions of $\mathcal{K}$ to the columns of a matrix $X$,

$$X \triangleq [\Gamma_1 \;\; \Gamma_2] \tag{122}$$

then we find

$$X^{\dagger T} = \begin{bmatrix}\dfrac{\Gamma_4}{\Gamma_4^T\Gamma_1} & \dfrac{\Gamma_3}{\Gamma_3^T\Gamma_2}\end{bmatrix} \tag{123}$$

Therefore,

$$x = XX^\dagger x \tag{124}$$

is the biorthogonal expansion (121) (§A.0.1), and the biorthogonality condition (120) can be expressed succinctly (§A.1.2)[31]

$$X^\dagger X = I \tag{125}$$

[31]Possibly confusing is the fact that formula $XX^\dagger x$ is simultaneously the orthogonal projection of $x$ on $\mathcal{R}(X)$ (493), and the sum of nonorthogonal projections of $x\in\mathcal{R}(X)$ on each column of full-rank $X$ skinny-or-square (§A.3.1).

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

The biorthogonality condition $X^\dagger X = I$ (125) means $\Gamma_1$ and $\Gamma_2$ are linearly independent generators of $\mathcal{K}$. (§C.7.1.1) From §3.4.6 we know that means they 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 (§3.4.4). We will address the problem of biorthogonal expansion with respect to a pointed polyhedral cone having empty interior in §3.6.3.

**Example.** *Biorthogonal expansion with respect to* $\mathbb{S}^M_+$. When the cone $\mathcal{K}$ under consideration is the positive semidefinite cone $\mathbb{S}^M_+$ (21) and $X \in \mathcal{K}$, the coordinates for biorthogonal expansion of $X$ can be its nonnegative eigenvalues (§C.2.1); *id est*, for $X \in \mathbb{S}^M_+$,

$$X \;=\; QQ^TX \;=\; \sum_{i=1}^{M} q_i\, q_i^TX \;=\; \sum_{i=1}^{M} \lambda_i\, q_i q_i^T \;\in\; \mathbb{S}^M_+ \tag{126}$$

is a biorthogonal expansion with biorthogonality condition $Q^TQ = I$ where $\lambda_i \geq 0$ is the $i^{\text{th}}$ eigenvalue of $X$, $q_i$ is the $i^{\text{th}}$ eigenvector of $X$ arranged columnar in orthogonal matrix

$$Q = [\, q_1 \;\, q_2 \cdots q_M \,] \in \mathbb{R}^{M\times M} \tag{127}$$

and $q_i q_i^T$ is the $i^{\text{th}}$ member of an orthonormal basis for $\mathbb{S}^M$ and an extreme direction of $\mathbb{S}^M_+$. The *dual positive semidefinite cone* $\mathcal{K}^*$ is defined

$$\mathbb{S}^{M*}_+ \;\stackrel{\Delta}{=}\; \{Y \in \mathbb{S}^M \mid \operatorname{tr}(X^TY) \geq 0 \;\text{ for all } X \in \mathbb{S}^M_+\} \;=\; \mathbb{S}^M_+ \tag{128}$$

The positive semidefinite cone is self-dual for real matrices [40] [28, §II] [9, old pg.30], $\mathcal{K} = \mathcal{K}^*$, and the biorthogonal expansion (126) is an orthogonal expansion. □

Whenever a pointed convex cone is *self-dual*, an associated biorthogonal expansion becomes an orthogonal expansion; *id est*, the biorthogonality condition $X^\dagger X = I$ becomes instead $X^TX = I$.

### 3.6.2 Dual of pointed polyhedral cone

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

**Example.** *Biorthogonal expansion with respect to nonpositive orthant.* Suppose $x \in \mathcal{K}$ any orthant in $\mathbb{R}^n$ (which are simplicial and self-dual). 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 for $x \in \mathbb{R}^n_-$ the biorthogonal expansion becomes an orthogonal expansion

$$x \;=\; XX^Tx \;=\; \sum_{i=1}^{n} -e_i(-e_i^Tx) \;=\; \sum_{i=1}^{n} -e_i|e_i^Tx| \;\in\; \mathbb{R}^n_- \tag{129}$$

with biorthogonality 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 (§3.4.4) of $\mathcal{K}$. $\square$

In a subspace of $\mathbb{R}^n$, now we consider a pointed polyhedral cone $\mathcal{K}$ given in terms of its extreme directions $\Gamma_i$ arranged columnar in $X$ as for the vertex description (108);

$$X = [\Gamma_1 \; \Gamma_2 \; \cdots \; \Gamma_N] \in \mathbb{R}^{n\times N} \tag{92}$$

The *extremes theorem* (§3.4.4) 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.* (*confer* (108)) Given pointed polyhedral cone $\mathcal{K}$ in a subspace of $\mathbb{R}^n$, denoting its $i^{\text{th}}$ extreme direction by $\Gamma_i \in \mathbb{R}^n$ arranged in a matrix $X$ as in (92), then that cone may be described, (50) (100)

$$\begin{aligned}
\mathcal{K} \;&=\; \left\{[\mathbf{0} \;\; X]\, a\,\zeta \mid a^T\mathbf{1} = 1,\; a \succeq 0,\; \zeta \geq 0\right\} && (130)\\
&=\; \left\{X a\,\zeta \mid a^T\mathbf{1} \leq 1,\; a \succeq 0,\; \zeta \geq 0\right\} && (131)\\
&=\; \{Xb \mid b \succeq 0\} \subset \mathbb{R}^n && (132)
\end{aligned}$$

that is simply a conic hull, like (51), of a finite number ($N$) of directions. $\diamond$

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

$$\begin{aligned}\mathcal{K}^* &= \big\{y \mid \gamma^T y \geq 0 \ \text{ for all } \gamma \in \{\Gamma_i\,,\ i=1\ldots N\} \subseteq \operatorname{rel}\partial\mathcal{K}\big\} &(133)\\ &= \big\{y \mid X^T y \succeq 0\big\} \subset \mathbb{R}^n &(134)\end{aligned}$$

Whenever the set $\{\Gamma_i\}$ constitutes generators for $\mathcal{K}$, the discretization result (109) allows relaxation of the requirement $\forall x \in \mathcal{K}$ in (103) to $\forall \gamma \in \{\Gamma_i\}$ in (133) directly;[32] *e.g.*, apply this result to Figure 17. That dual cone so defined is unique, polyhedral, identical to (103), and nonempty, but not necessarily pointed unless $\mathcal{K}$ is nonempty (§3.6.1).

**3.6.2.1 Facet normal.** We see from (134) that the conically independent generators of $\mathcal{K}$ (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. If $\mathcal{K}$ were proper, then the dual statement would also be true because $\mathcal{K}^*$ is then pointed (§3.6.1); *id est*, the extreme directions of proper $\mathcal{K}^*$ each define a hyperplane that supports $\mathcal{K}$ and exposes a facet. We may conclude that the extreme directions of proper $\mathcal{K}$ are respectively orthogonal to the facets of $\mathcal{K}^*$; likewise, the extreme directions of proper $\mathcal{K}^*$ are respectively orthogonal to the facets of $\mathcal{K}$.

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

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, convex and, of course, relatively nonempty. In this section, we consider $\mathcal{K}$ possibly having 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 $x \in \operatorname{aff}\mathcal{K}$; we seek a vertex description for $\mathcal{K}^* \cap \operatorname{aff}\mathcal{K}$ in terms of a finite set of dual generators $\{\Gamma_i^*\}$ in the same quantity[33] as the extreme directions $\{\Gamma_i\}$ arranged columnar in

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[32] We learned from (109) that *any* discrete set of generators for $\mathcal{K}$ including its extreme directions can be used to make a halfspace description of $\mathcal{K}^*$. Barker and Carlson [30, §1] call the extreme directions a *minimal generating set.*

[33] The problem of finding a complete set of generators for the ordinary dual cone $\mathcal{K}^*$ is discussed in [41]. When $\mathcal{K}$ is contained in a proper subspace of $\mathbb{R}^n$, the ordinary dual cone will have more (conic) generators in any minimal set than $\mathcal{K}$ has extreme directions.

$X\in\mathbb{R}^{n\times N}$. We assume that the quantity of extreme directions $N$ does not exceed the dimension $n$ of the host vector space because, otherwise, the expansion could not be unique; *id est*, assume $N$ linearly independent extreme directions, hence $N\leq n$. From (104), we know that $\mathcal{K}^*\cap\operatorname{aff}\mathcal{K}$ must be pointed because $\mathcal{K}$ is assumed relatively nonempty.

Suppose $x$ belongs to $\mathcal{K}\subset\mathbb{R}^n$. Then for $X$ as in (92), $x=Xa$ for some $a\succeq 0$. Vector $a$ is unique only when $\{\Gamma_i\}$ is a linearly independent set.[34] Vector $a$ 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 $B=X^\dagger\in\mathbb{R}^{N\times n}$ is suitable when $X$ is *skinny*[35]-or-square and full rank. (§A) In that case $\operatorname{rank}X=N$, and for all $c\succeq 0$ and $i=1\ldots N$,

$$a\succeq 0\;\Leftrightarrow\;X^\dagger Xa\succeq 0\;\Leftrightarrow\;a^TX^TX^{\dagger T}c\geq 0\;\Leftrightarrow\;\Gamma_i^TX^{\dagger T}c\geq 0 \tag{135}$$

The penultimate inequality follows from the *generalized inequality corollary*, while the last inequality is a consequence of that corollary's discretization (§3.6.1).[36] From (133) it follows

$$\mathcal{K}^*\cap\operatorname{aff}\mathcal{K}\;=\;\{X^{\dagger T}c\mid c\succeq 0\}\subset\mathbb{R}^n \tag{136}$$

is the vertex description for the part of $\mathcal{K}^*$ in the affine hull of $\mathcal{K}$ because $\mathcal{R}(X^{\dagger T})=\mathcal{R}(X)$ by definition of the pseudoinverse.

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

$$X^{\dagger T}\triangleq\left[\Gamma_1^*\;\Gamma_2^*\;\cdots\;\Gamma_N^*\right]\in\mathbb{R}^{n\times N} \tag{137}$$

comprises the extreme directions $\{\Gamma_i^*\}$ of the dual cone section in $\operatorname{aff}\mathcal{K}$. From the *discrete generalized inequality theorem* (§3.6.1) we derive an *affine*

[34] Conic independence alone (§3.4.6) is insufficient to guarantee uniqueness.

[35] "Skinny" meaning more rows than columns.

[36] Intuitively, any nonnegative vector $a$ is a conic combination of the standard basis $\{e_i\in\mathbb{R}^N\}$; $a\succeq 0\Leftrightarrow a_ie_i\succeq 0$ for all $i$. The last inequality in (135) 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 (135) 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.

*dual* to (133); *id est*, for $x \in \operatorname{aff} \operatorname{cone} X^{\dagger T}$,

$$x \in \mathcal{K} \;\Leftrightarrow\; \gamma^{*T} x \geq 0 \;\text{ for all }\; \gamma^* \in \left\{ \Gamma_i^* \,,\; i = 1 \ldots N \right\} \subseteq \partial\mathcal{K}^* \cap \operatorname{aff} \mathcal{K} \tag{138}$$

$$\Leftrightarrow\; X^\dagger x \succeq 0 \tag{139}$$

that leads to the halfspace description,

$$\mathcal{K} \;=\; \left\{ x \in \operatorname{aff} \operatorname{cone} X^{\dagger T} \mid X^\dagger x \succeq 0 \right\} \tag{140}$$

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 ($\operatorname{rank} X = N$), so is its pseudoinverse $X^\dagger$. (§A) 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. (§3.4.6) The section of the dual cone thus found is itself a polyhedral cone (by (95) or the *cone intersection theorem*, §3.4.2) having the same number of extreme directions as $\mathcal{K}$. These results are summarized for skinny or square $X$: Assuming pointed closed convex $\mathcal{K}$ such that

$$\operatorname{rank} X \in \mathbb{R}^{n \times N} \;=\; N \;\stackrel{\Delta}{=}\; \dim \operatorname{aff} \mathcal{K} \;=\; \dim \operatorname{aff} \operatorname{cone} X \;\leq\; n \tag{141}$$

we have

| **Cone Table 1** | $\mathcal{K}$ | $\mathcal{K} \cap \operatorname{aff} \operatorname{cone} X^{\dagger T}$ | $\mathcal{K}^*$ | $\mathcal{K}^* \cap \operatorname{aff} \operatorname{cone} X$ |
|---|---|---|---|---|
| vertex description | $X$ | | | $X^{\dagger T}$ |
| halfspace description | | $X^\dagger$ | $X^T$ | |

where

$$\operatorname{aff} \operatorname{cone} X^{\dagger T} \;=\; \operatorname{aff} \operatorname{cone} X \;=\; \operatorname{aff} \mathcal{K} \tag{142}$$

When $X$ is full rank, the unique biorthogonal expansion (124) of $x \in \mathcal{K}$ is therefore

$$x \;=\; X X^\dagger x \;=\; \sum_{i=1}^{N} \Gamma_i \, \Gamma_i^{*T} x \tag{143}$$

Further, the extreme directions of $\mathcal{K}$ and $\mathcal{K}^* \cap \operatorname{aff} \operatorname{cone} X$ 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. That is a biorthogonality condition [23, §2.2.4] [24] implying the biorthogonal expansion applies more broadly; *videlicet*, for any $x \in \operatorname{aff} \mathcal{K}$ (§A.1.2), $x$ can be expressed $x = Xb$ where $b \in \mathbb{R}^N$. Thus the expansion becomes $x = X X^\dagger X b = X b$.

**3.6.3.1 Simplicial case.** When a convex cone is simplicial (§3.5.3), Cone Table 1 simplifies because then $\operatorname{aff\,cone} X^{\dagger T} = \operatorname{aff\,cone} X = \mathbb{R}^n$ : For square $X$ and assuming simplicial $\mathcal{K}$ such that

$$\operatorname{rank} X \in \mathbb{R}^{n \times N} \;=\; N \;\triangleq\; \dim \operatorname{aff} \mathcal{K} \;=\; n \tag{144}$$

then we have

| **Cone Table 2** | $\mathcal{K}$ | $\mathcal{K}^*$ |
|---|---|---|
| vertex description | $X$ | $X^{\dagger T}$ |
| halfspace description | $X^\dagger$ | $X^T$ |

For example, vertex description (136) simplifies to

$$\mathcal{K}^* \;=\; \{X^{\dagger T} c \mid c \succeq 0\} \subset \mathbb{R}^n \tag{145}$$

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

**Example.** *The monotone nonnegative cone.* [9, §2, exer.2.33] [42, §2] Simplicial cone (§3.5.3) $\mathcal{K}_{\mathcal{M}+}$ is the cone of all nonnegative vectors having their entries sorted in nonincreasing order:

$$\begin{aligned} \mathcal{K}_{\mathcal{M}+} &\triangleq \{x \mid x_1 \geq x_2 \geq \cdots \geq x_n \geq 0\} \subseteq \mathbb{R}^n_+ \\ &= \bigcap \{x \mid (e_i - e_{i+1})^T x \geq 0,\ i = 1 \ldots n-1,\ e_n^T x \geq 0\} \\ &= \{x \mid X^\dagger x \succeq 0\} \end{aligned} \tag{146}$$

a halfspace description where $e_i$ is the $i^{\text{th}}$ standard basis vector, and where

$$X^{\dagger T} \triangleq [\,e_1 - e_2 \quad e_2 - e_3 \quad \cdots \quad e_n\,] \in \mathbb{R}^{n \times n} \tag{147}$$

(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 inequalities in their derivation.) For any $x$ and $y$, simple algebra demands

$$\begin{aligned} x^T y \;=\; \sum_{i=1}^n x_i y_i \;=\; & (x_1 - x_2) y_1 + (x_2 - x_3)(y_1 + y_2) + (x_3 - x_4)(y_1 + y_2 + y_3) + \cdots \\ & + (x_{n-1} - x_n)(y_1 + \cdots + y_{n-1}) + x_n (y_1 + \cdots + y_n) \end{aligned} \tag{148}$$

(a)

(b)

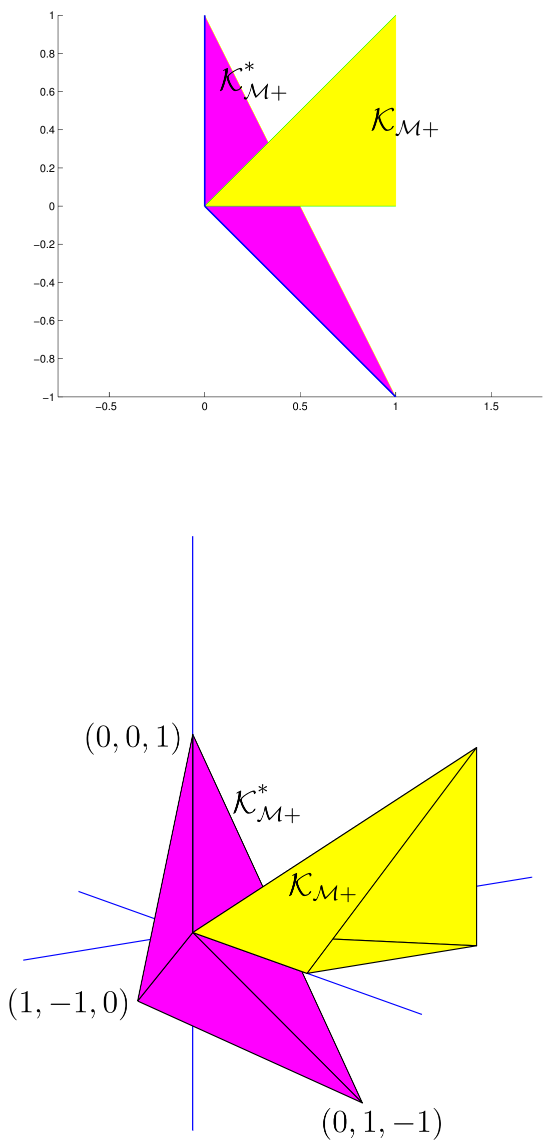


Figure 18: (a) Monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$ and its dual $\mathcal{K}^*_{\mathcal{M}+}$ (drawn truncated) in $\mathbb{R}^2$. (b) Boundaries of the monotone nonnegative cone and its dual (drawn truncated) in $\mathbb{R}^3$. The extreme directions of $\mathcal{K}^*_{\mathcal{M}+}$ are labelled with their coordinates.

Because $x_i - x_{i+1} \geq 0 \;\; \forall i$ when $x \in \mathcal{K}_{\mathcal{M}+}$ , we employ generalized inequality (114) with $\mathcal{K} = \mathbb{R}^n_+$ to find the halfspace description of the dual cone $\mathcal{K}^*_{\mathcal{M}+}$ . Then $x^T y \geq 0$ for all $X^\dagger x \succeq 0$ if and only if,

$$y_1 \geq 0\,, \quad y_1 + y_2 \geq 0\,, \quad \ldots\,, \quad y_1 + y_2 + \cdots + y_n \geq 0 \tag{149}$$

*id est*, by (103) the dual cone comprises all $y$ for which it is true:

$$y \underset{\mathcal{K}^*_{\mathcal{M}+}}{\succeq} 0 \;\Leftrightarrow\; x^T y \geq 0 \;\forall\, x \underset{\mathcal{K}_{\mathcal{M}+}}{\succeq} 0 \;\Leftrightarrow\; X^T y \succeq 0 \;\Leftrightarrow\; x^T y \geq 0 \;\forall\, X^\dagger x \succeq 0 \tag{150}$$

where

$$X = [e_1 \quad e_1 + e_2 \quad e_1 + e_2 + e_3 \quad \cdots \quad \mathbf{1}] \in \mathbb{R}^{n \times n} \tag{151}$$

Thus the halfspace description,

$$\mathcal{K}^*_{\mathcal{M}+} = \{y \underset{\mathcal{K}^*_{\mathcal{M}+}}{\succeq} 0\} = \{y \mid \sum_{i=1}^{k} y_i \geq 0\,,\; k = 1 \ldots n\} = \{y \mid X^T y \succeq 0\} \subset \mathbb{R}^n \tag{152}$$

The monotone nonnegative cone and its dual are simplicial, illustrated for two Euclidean spaces in Figure 18.

From §3.6.2.1, 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 (152). Hence the vertex description for $\mathcal{K}_{\mathcal{M}+}$ employs the columns of $X$ in agreement with Cone Table 2 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 (146). So the vertex description for $\mathcal{K}^*_{\mathcal{M}+}$ employs the columns of $X^{\dagger T}$. □

#### 3.6.3.2 Halfspace description with equality constraints, pointed $\mathcal{K}$

Consider again pointed polyhedral $\mathcal{K}$ whose subspace membership is explicit; *id est*, we are given the ordinary halfspace description,

$$\mathcal{K} = \{x \mid Ax \succeq 0\,,\; Cx = \mathbf{0}\} \subset \mathbb{R}^n \tag{95a}$$

where $A \in \mathbb{R}^{m \times n}$, $C \in \mathbb{R}^{p \times n}$, and $C$ is assumed nonzero. This can be equivalently written in terms of nullspace of $C$ and vector $\xi$ :

$$\mathcal{K} = \{Z\xi \in \mathbb{R}^n \mid AZ\xi \succeq 0\} \tag{153}$$

where $\mathcal{R}(Z) \stackrel{\Delta}{=} \mathcal{N}(C)$ and $Z \in \mathbb{R}^{n \times n-\operatorname{rank} C}$. Assuming (141) is satisfied

$$\operatorname{rank} X \;=\; \operatorname{rank}(AZ)^{\dagger} \in \mathbb{R}^{n-\operatorname{rank} C \times m} \;=\; m-\ell \;=\; \dim \operatorname{aff} \mathcal{K} \;\leq\; n-\operatorname{rank} C \tag{154}$$

where $\ell$ is the number of conically dependent rows in $AZ$ (§3.4.6) that must be removed before proceeding. Then the results in Cone Table 1 or 2 apply to $\hat{X} \stackrel{\Delta}{=} (\hat{A}Z)^{\dagger} \in \mathbb{R}^{n-\operatorname{rank} C \times m-\ell}$ where $\hat{A} \in \mathbb{R}^{m-\ell \times n}$. So, we have the vertex description

$$\mathcal{K} = \{Z(\hat{A}Z)^{\dagger} b \mid b \succeq 0\} \tag{155}$$

From this we get the halfspace description (109) of the dual cone,

$$\mathcal{K}^{*} = \{y \in \mathbb{R}^{n} \mid (Z^{T}\hat{A}^{T})^{\dagger} Z^{T} y \succeq 0\} \tag{156}$$

and a vertex description, (467)

$$\mathcal{K}^{*} \cap \operatorname{aff} \mathcal{K} = \{Z^{\dagger T}(\hat{A}Z)^{T} c \mid c \succeq 0\} \tag{157}$$

**3.6.3.3** In the circumstance (154) is false, we may instead try

$$\begin{aligned}\mathcal{K} &= \{x \mid Ax \succeq 0\,,\; Cx \succeq 0\,,\; Cx \preceq 0\} \qquad \text{(95b)}\\ &= \{x \mid \begin{bmatrix} A \\ C \\ -C \end{bmatrix} x \succeq 0\}\end{aligned}$$

and (assuming (141) is satisfied) hope that

$$\operatorname{rank} X^{\dagger} \;=\; \operatorname{rank} \begin{bmatrix} A \\ C \\ -C \end{bmatrix} \in \mathbb{R}^{m+2p \times n} \;=\; m+2p-\ell \;=\; \dim \operatorname{aff} \mathcal{K} \;\leq\; n-\operatorname{rank} C \tag{158}$$

As before, $\ell$ conically dependent rows must be removed from $X^{\dagger}$ before proceeding. Then the results in Cone Table 1 or 2 apply to

$$\hat{X} \;\stackrel{\Delta}{=}\; \begin{bmatrix} \hat{A} \\ \hat{C} \\ -\hat{C} \end{bmatrix}^{\dagger} \in \mathbb{R}^{n \times m+2p-\ell} \tag{159}$$

### 3.6.4 Dual of proper $\mathcal{K}$ not simplicial, $X$ fat full-rank

Having found formula (145) 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 $\mathcal{K} = \bigcup \mathcal{K}_i$ . (That proposition presupposes, of course, that we know how to perform the simplicial decomposition efficiently.) The existence of multiple simplicial parts means the biorthogonal expansion of $x \in \mathcal{K}$ like (143) 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[37] (§3.4.6) of $\mathcal{K}$ 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.* [12, §2.7] Suppose proper cone $\mathcal{K} \subset \mathbb{R}^n$ equals the union of $M$ simplicial cones $\mathcal{K}_i$ whose extreme directions are all coincident with those of $\mathcal{K}$ . Then proper dual cone $\mathcal{K}^*$ is the intersection of $M$ dual simplicial cones $\mathcal{K}_i^*$ ; *id est*,

$$\mathcal{K} = \bigcup_{i=1}^{M} \mathcal{K}_i \quad \Rightarrow \quad \mathcal{K}^* = \bigcap_{i=1}^{M} \mathcal{K}_i^* \tag{160}$$

$\diamond$

**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,

$$\mathcal{K}_i = \{X_i\, c \mid c \succeq 0\} \tag{161}$$

Now suppose,

$$\mathcal{K} \;=\; \bigcup_{i=1}^{M} \mathcal{K}_i \;=\; \bigcup_{i=1}^{M} \{X_i\, c \mid c \succeq 0\} \tag{162}$$

[37] We can always eliminate conically dependent columns from $X$ to construct $\mathcal{K}$ or to determine $\mathcal{K}^*$. (§E.1)

The union of all $\mathcal{K}_i$ can be equivalently expressed

$$\mathcal{K} \;=\; \left\{ [X_1 \; X_2 \; \cdots \; X_M] \begin{bmatrix} a \\ b \\ \vdots \\ c \end{bmatrix} \;\mid\; a, b, \ldots, c \succeq 0 \right\} \tag{163}$$

Because extreme directions of the simplices $\mathcal{K}_i$ are extreme directions of $\mathcal{K}$ by assumption, then by the *extremes theorem*, (§3.4.4)

$$\mathcal{K} \;=\; \{\, [X_1 \; X_2 \; \cdots \; X_M]\, d \mid d \succeq 0 \,\} \tag{164}$$

Defining $X \triangleq [X_1\, X_2 \cdots X_M]$ (with any redundant columns optionally removed from $X$), then $\mathcal{K}^*$ can be expressed, (134) (Cone Table 2)

$$\mathcal{K}^* \;=\; \{y \mid X^T y \succeq 0\} \;=\; \bigcap_{i=1}^{M} \{y \mid X_i^T y \succeq 0\} \;=\; \bigcap_{i=1}^{M} \mathcal{K}_i^* \tag{165}$$

♦

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 proper cone $\mathcal{K}$, the extreme directions of the dual cone $\mathcal{K}^*$ are respectively orthogonal to the facets of $\mathcal{K}$. (§3.6.2.1) 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 2,

$$\mathcal{K}^* \;=\; \bigcap_{i=1}^{M} \mathcal{K}_i^* \;=\; \bigcap_{i=1}^{M} \{X_i^{\dagger T} c \mid c \succeq 0\} \tag{166}$$

The set of extreme directions 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 (134):

$$\left\{\Gamma_1^*,\, \Gamma_2^* \ldots \Gamma_N^*\right\} \;=\; \text{c.i.}\left\{X_i^{\dagger T}(:,j),\; i=1\ldots M,\; j=1\ldots n \mid X_i^{\dagger}(j,:)\Gamma_\ell \geq 0,\; \ell=1\ldots N\right\} \tag{167}$$

where c.i. denotes the selection of only the conically independent vectors from the argument set, and argument $(:, j)$ denotes the $j^{\text{th}}$ column while $(j, :)$ denotes the $j^{\text{th}}$ row. Figure 12(b) (p.38) shows a cone and its dual found via this formulation.

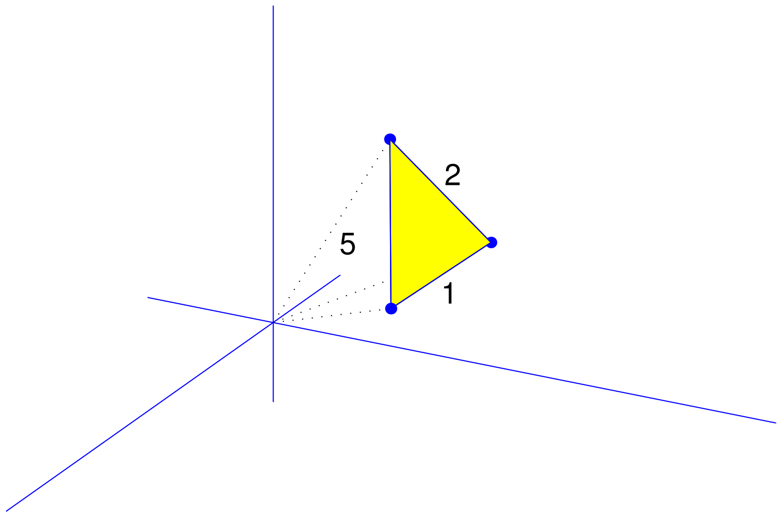


Figure 19: Convex hull of three points ($N = 3$) is shaded in $\mathbb{R}^{\mathbf{3}}$ ($n = 3$). Dotted lines are imagined vectors to points.

# 4 Euclidean Distance Matrix

[38] Euclidean space $\mathbb{R}^n$ is a finite-dimensional real vector space having an inner product defined on it, hence a metric as well. [17, §3.1] A Euclidean distance matrix, an EDM in $\mathbb{R}_+^{N\times N}$, is an exhaustive table of distance-squared $d_{ij}$ 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-squared:

$$d_{ij} \;=\; \|x_i - x_j\|_2^2 \;\triangleq\; <x_i - x_j\,,\, x_i - x_j> \tag{168}$$

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 $N{=}3$ :

$$D \;=\; [d_{ij}] \;=\; \begin{bmatrix} d_{11} & d_{12} & d_{13} \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{bmatrix} = \begin{bmatrix} 0 & d_{12} & d_{13} \\ d_{12} & 0 & d_{23} \\ d_{13} & d_{23} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 5 \\ 1 & 0 & 4 \\ 5 & 4 & 0 \end{bmatrix} \tag{169}$$

$D$ has $N^2$ entries but only $N(N-1)/2$ pieces of information. In Figure 19 we show three points in $\mathbb{R}^{\mathbf{3}}$ that can be arranged in a list to correspond to $D$ in (169). Such a list is not unique because any rotation, reflection, or offset (§4.4) of the points in Figure 19 would produce the same EDM $D$.

## 4.1 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: [17, §1.1] [18, §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 $\mathbb{R}^n$ (§4.3). Then all entries of an EDM must be in concord with the axioms: specifically, each entry must be nonnegative,[39] the main diagonal must be zero,[40] and an EDM must be symmetric. The fourth axiom provides upper and lower bounds for each entry; loose bounds when $N>3$. Axiom 4 is more generally true when there are no restrictions on indices $i,j,k$, but furnishes no new information.

## 4.2 There exists a fifth Euclidean requirement

The four axioms of the Euclidean metric provide insufficient information to reconstruct a *convex polyhedron*, more complex than a triangle, from incomplete distance information. [43, §2] Yet any list of points or the vertices of any polyhedron must conform to the axioms.

**Example.** *Triangle.* Consider the EDM in (169), but missing one of its entries:

$$D = \begin{bmatrix} 0 & 1 & d_{13} \\ 1 & 0 & 4 \\ d_{31} & 4 & 0 \end{bmatrix} \tag{170}$$

[39] Implicit from the terminology, $\sqrt{d_{ij}} \geq 0 \Leftrightarrow d_{ij} \geq 0$ is always assumed.
[40] What we call zero self-distance, Marsden calls *nondegeneracy*. [18, §1.6]

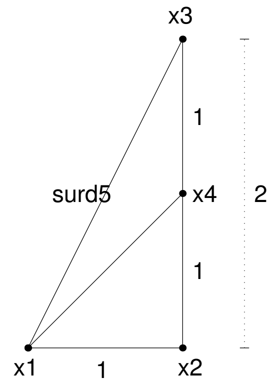


Figure 20: Four axioms of the Euclidean metric are not a recipe for reconstruction of this polyhedron.

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 zero, while axiom 3 makes $\sqrt{d_{31}}=\sqrt{d_{13}}$. The fourth axiom tells us

$$1 \leq \sqrt{d_{13}} \leq 3 \tag{171}$$

Indeed, described over that closed interval $[1,3]$ is a family of triangular polyhedra whose angle at vertex $x_2$ varies from 0 to $\pi$ radians. So, yes we can determine the unknown entries of $D$ ; but they are not unique, nor should they be for this example. □

**Example.** *Small completion problem*, I. Now consider the polyhedron in Figure 20 formed from an unknown list of four points $\{x_1, x_2, x_3, x_4\}$. The corresponding EDM less one critical piece of information, $d_{14}$ , is given by

$$D = \begin{bmatrix} 0 & 1 & 5 & d_{14} \\ 1 & 0 & 4 & 1 \\ 5 & 4 & 0 & 1 \\ d_{14} & 1 & 1 & 0 \end{bmatrix} \tag{172}$$

From axiom 4 we may write a few inequalities for the two triangles common to $d_{14}$ ; we find

$$\sqrt{5}-1 \;\leq\; \sqrt{d_{14}} \;\leq\; 2 \tag{173}$$

We cannot further narrow those loose bounds on $\sqrt{d_{14}}$ using only the four axioms (§D.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 example the triangle inequality axiom does *not* yield an interval for $\sqrt{d_{14}}$ over which a family of convex polyhedra can be reconstructed. $\square$

We will return to this simple example to illustrate more elegant methods of solution in §4.7.3, §4.9.4.1, and §D.1.1.

### 4.2.1 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 reconstruct 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 (§3.1.2). Here is the fifth requirement:

**Axiom. Fifth Euclidean requirement.** *Angle inequality.* [44, §3.1] (*confer* §4.9.2.1) 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

$$\begin{array}{c} \cos(\theta_{ik\ell}+\theta_{\ell kj}) \;\leq\; \cos\theta_{ikj} \;\leq\; \cos(\theta_{ik\ell}-\theta_{\ell kj}) \\ 0 \leq \theta_{ik\ell}\,, \theta_{\ell kj}\,, \theta_{ikj} \leq \pi \end{array} \tag{174}$$

where $\theta_{ikj} = \theta_{jki}$ is the angle between vectors at vertex $x_k$ (184), must be satisfied at each point $x_k$ regardless of affine dimension. $\diamond$

We will explore this in §4.9. One of our early objectives is to determine matrix criteria that subsume all the Euclidean axioms and further requirements. Looking ahead, we will find [45] (*confer* (334), (250))

$$\left.\begin{array}{r} -z^T D z \geq 0 \\ \mathbf{1}^T z = 0 \\ (\|z\| = 1) \\ D \in \mathbb{S}_\delta^N \end{array}\right. \;\Leftrightarrow\; D \in \mathbb{EDM}^N \tag{175}$$

where the proper cone of Euclidean distance matrices $\mathbb{EDM}^N \subseteq \mathbb{S}_\delta^N$ is defined in (179), (188), and (195). Having found axiom-equivalent matrix criteria, we will see there is a bridge from convex polyhedra to EDMs in §4.7.[41]

We digress to review some invaluable concepts and to link the axioms to matrix criteria.

## 4.3 EDM definition

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

$$X = [x_1 \ \cdots \ x_N] \in \mathbb{R}^{n\times N} \tag{47}$$

When matrix $D = [d_{ij}]$ is an EDM, its entries must be related to those points constituting the list by the Euclidean distance-squared:

$$\begin{aligned} d_{ij} &= \|x_i - x_j\|^2 \;=\; (x_i - x_j)^T(x_i - x_j) \;=\; \|x_i\|^2 + \|x_j\|^2 - 2x_i^T x_j \\ &= \begin{bmatrix} x_i^T & x_j^T \end{bmatrix} \begin{bmatrix} I & -I \\ -I & I \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} \end{aligned} \tag{176}$$

Thus each entry $d_{ij}$ is a convex (§2.2.1) quadratic function of $\begin{bmatrix} x_i \\ x_j \end{bmatrix} \in \mathbb{R}^{2n}$. [9, §3] [11, §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;

$$\mathbf{0} \in \mathbb{EDM}^N \subseteq \mathbb{S}_\delta^N \cap \mathbb{R}_+^{N\times N} \subset \mathbb{S}^N \tag{177}$$

where $\mathbb{S}_\delta^N$ is the subspace of symmetric hollow matrices (§2.1.2.1). An EDM $D$ must be expressible as a function of some list in $X$ ; *id est*, it must have the form

$$\mathcal{D}(X) \;=\; \delta(X^TX)\mathbf{1}^T + \mathbf{1}\delta(X^TX)^T - 2X^TX \;\in \mathbb{EDM}^N \tag{178}$$

$$\mathbb{EDM}^N = \left\{\mathcal{D}(X) \mid X \in \mathbb{R}^{n\times N}\right\} \tag{179}$$

where the main diagonal of $A \in \mathbb{R}^{N\times N}$ is denoted (§C.5)

$$\delta(A) \in \mathbb{R}^N \tag{180}$$

[41] From an EDM, a generating list (§3.1.2, §3.5.2) for a polyhedron can be found (§4.8) correct to within an offset, rotation, and reflection (§4.4).

and the Gram matrix is [5, §3.6]

$$X^TX = \begin{bmatrix} \|x_1\|^2 & x_1^Tx_2 & x_1^Tx_3 & \cdots & x_1^Tx_N \\ x_2^Tx_1 & \|x_2\|^2 & x_2^Tx_3 & \cdots & x_2^Tx_N \\ x_3^Tx_1 & x_3^Tx_2 & \|x_3\|^2 & \ddots & x_3^Tx_N \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ x_N^Tx_1 & x_N^Tx_2 & x_N^Tx_3 & \cdots & \|x_N\|^2 \end{bmatrix} \in \mathbb{S}^N \tag{181}$$

Conversely, $\mathcal{D}(X)$ in (178) will make an EDM for any $X\in\mathbb{R}^{n\times N}$, but $\mathcal{D}(X)$ is not a convex function of $X$ (§4.10). $\mathcal{D}(X)$ is a matrix definition of EDM and so conforms to the Euclidean axioms:

Nonnegativity of EDM entries (axiom 1, §4.1) is obvious from the distance-squared definition (176), and so assumed to hold for any $D$ expressible in the form $\mathcal{D}(X)$ in (178).

When we say $D$ is an EDM, reading from (178), it implicitly means the main diagonal must be zero (axiom 2, self-distance) and $D$ must be symmetric (axiom 3); $\delta(D)=\mathbf{0}$ and $D^T=D$ or, equivalently, $D\in\mathbb{S}_\delta^N$ are necessary matrix criteria.

The mapping $\mathcal{D}(X)$ is homogeneous in the sense, for $\zeta\in\mathbb{R}$,

$$\sqrt{\mathcal{D}(\zeta X)} = |\zeta|\sqrt{\mathcal{D}(X)} \tag{182}$$

where the square root is entry-wise.

### 4.3.1 Inner-product form EDM definition

Equivalent to (176) is [46, §1-7] [19, §3.2]

$$\begin{aligned} d_{ij} &= d_{ik} + d_{kj} - 2\sqrt{d_{ik}d_{kj}}\cos\theta_{ikj} \\ &= \begin{bmatrix} \sqrt{d_{ik}} & \sqrt{d_{kj}} \end{bmatrix} \begin{bmatrix} 1 & -e^{\imath\theta_{ikj}} \\ -e^{-\imath\theta_{ikj}} & 1 \end{bmatrix} \begin{bmatrix} \sqrt{d_{ik}} \\ \sqrt{d_{kj}} \end{bmatrix} \end{aligned} \tag{183}$$

called the *law of cosines*, where $\imath \triangleq \sqrt{-1}$, $i,k,j$ are positive integers, and $\theta_{ikj}$ is the angle at vertex $x_k$ formed by vectors $x_i - x_k$ and $x_j - x_k$;

$$\cos\theta_{ikj} = \frac{\frac{1}{2}(d_{ik}+d_{kj}-d_{ij})}{\sqrt{d_{ik}d_{kj}}} = \frac{(x_i-x_k)^T(x_j-x_k)}{\|x_i-x_k\|\,\|x_j-x_k\|} \tag{184}$$

where the numerator forms an inner product of vectors. Distance squared $d_{ij}\left(\begin{bmatrix}\sqrt{d_{ik}}\\ \sqrt{d_{kj}}\end{bmatrix}\right)$ is a convex (§2.2.1) quadratic function on $\mathbb{R}^{\mathbf{2}}_+$ whereas $d_{ij}(\theta_{ikj})$ is a *quasi*convex function (§2.2.2) [9, §3] minimized over domain $-\pi \leq \theta_{ikj} \leq \pi$ when $\theta_{ikj}=0$, we have the *Pythagorean theorem* when $\theta_{ikj}=\pm\pi/2$, and $d_{ij}(\theta_{ikj})$ is maximized when $\theta_{ikj}=\pm\pi$ ;

$$\begin{array}{ll} d_{ij} = \left(\sqrt{d_{ik}} + \sqrt{d_{kj}}\,\right)^2, & \theta_{ikj} = \pm\pi \\ d_{ij} = d_{ik} + d_{kj}\,, & \theta_{ikj} = \pm\frac{\pi}{2} \\ d_{ij} = \left(\sqrt{d_{ik}} - \sqrt{d_{kj}}\,\right)^2, & \theta_{ikj} = \;\; 0 \end{array} \tag{185}$$

so

$$|\sqrt{d_{ik}} - \sqrt{d_{kj}}\,| \;\leq\; \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}} + \sqrt{d_{kj}} \tag{186}$$

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 (183) for $k=1$:

$$\mathcal{D}(\Theta) \triangleq \begin{bmatrix} 0 \\ \delta(\Theta^T\Theta) \end{bmatrix}\mathbf{1}^T + \mathbf{1}\begin{bmatrix}0 & \delta(\Theta^T\Theta)^T\end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Theta^T\Theta \end{bmatrix} \in \mathbb{EDM}^N \tag{187}$$

$$\mathbb{EDM}^N = \left\{\mathcal{D}(\Theta) \mid \Theta \in \mathbb{R}^{n\times N-1}\right\} \tag{188}$$

for which all Euclidean axioms hold, and where

$$\Theta^T\Theta = \begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214} & \cdots & \sqrt{d_{12}d_{1N}}\cos\theta_{21N} \\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & \cdots & \sqrt{d_{13}d_{1N}}\cos\theta_{31N} \\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14} & \ddots & \sqrt{d_{14}d_{1N}}\cos\theta_{41N} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \sqrt{d_{12}d_{1N}}\cos\theta_{21N} & \sqrt{d_{13}d_{1N}}\cos\theta_{31N} & \sqrt{d_{14}d_{1N}}\cos\theta_{41N} & \cdots & d_{1N} \end{bmatrix}$$

$$\in \mathbb{S}^{N-1} \tag{189}$$

The entries of $\Theta^T\Theta$ result from inner products as in (184); *id est*,

$$\Theta = [x_2 - x_1 \quad x_3 - x_1 \quad \cdots \quad x_N - x_1] \in \mathbb{R}^{n\times N-1} \tag{190}$$

Like $\mathcal{D}(X)$ (178), $\mathcal{D}(\Theta)$ will make an EDM for any $\Theta\in\mathbb{R}^{n\times N-1}$, it is neither a convex function of $\Theta$ (§4.10.1), and it is homogeneous in the sense (182).

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, angles in $\Theta^T\Theta$ are between all vector pairs having vertex $x_1$. Yet picking arbitrary $\theta_{i1j}$ to fill $\Theta^T\Theta$ will not necessarily make an EDM; $\Theta^T\Theta$ must be positive semidefinite.

$$\Theta^T\Theta \;=\; \delta(\sqrt{d}\,)\,\Omega\,\delta(\sqrt{d}\,) \;\stackrel{\Delta}{=}$$
$$\begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \begin{bmatrix} 1 & \cos\theta_{213} & \cdots & \cos\theta_{21N} \\ \cos\theta_{213} & 1 & \ddots & \cos\theta_{31N} \\ \vdots & \ddots & \ddots & \vdots \\ \cos\theta_{21N} & \cos\theta_{31N} & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \tag{191}$$

Since $\Theta^T\Theta$ is positive semidefinite for any $\Omega\succeq 0$ (§C.2.3), $\mathcal{D}(\Theta)$ defines an EDM for any positive semidefinite *angle matrix* [9, §8]

$$\Omega \;\stackrel{\Delta}{=}\; [\cos\theta_{i1j}\;,\; i,j=2\ldots N] \in \mathbb{S}^{N-1} \tag{192}$$

and any nonnegative distance vector

$$\sqrt{d} \;\stackrel{\Delta}{=}\; [\sqrt{d_{1j}}\;,\; j=2\ldots N] \in \mathbb{R}^{N-1} \tag{193}$$

The decomposition (191) and the *angle matrix inequality* $\Omega\succeq 0$ lead to a different expression of the inner-product form EDM definition (187) that is perhaps more appropriate for applications such as stellar cartography:

$$\mathcal{D}(\Omega\,,d) \;\stackrel{\Delta}{=}\; \begin{bmatrix} 0 \\ d \end{bmatrix}\mathbf{1}^T + \mathbf{1}\begin{bmatrix} 0 & d^T \end{bmatrix} - 2\,\delta\!\left(\begin{bmatrix} 0 \\ \sqrt{d} \end{bmatrix}\right)\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Omega \end{bmatrix}\delta\!\left(\begin{bmatrix} 0 \\ \sqrt{d} \end{bmatrix}\right) \;\in\; \mathbb{EDM}^N \tag{194}$$

$$\mathbb{EDM}^N = \left\{\mathcal{D}(\Omega\,,d) \mid \Omega\succeq 0,\; \sqrt{d}\succeq 0\right\} \tag{195}$$

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[42] with respect to EDM $D$.

[42] 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 $x_\ell$ in a length-$N$ list by increasing angle of vector $x_\ell - x_1$ with respect to $x_2 - x_1$, $\theta_{i1j}$ 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, $O(N)$.

## 4.4 Rotation, reflection, offset invariance

When $D$ is an EDM, there exist an infinite number of corresponding $N$-point lists $X$ (47) in Euclidean space. All those lists are related by isometric transformation: rotation, reflection, and offset (*translation* or shift).

### 4.4.1 Offset

Any offset common among all the points $x_\ell$ in a list will be cancelled in the formation of each $d_{ij}$. Proof follows directly from (176). Knowing that offset $\alpha$ in advance, we may remove it from the list in $X$ by subtracting $\alpha\mathbf{1}^T$. Then it stands to reason by definition (178) of an EDM, for any offset $\alpha\in\mathbb{R}^n$,

$$\mathcal{D}(X-\alpha\mathbf{1}^T)=\mathcal{D}(X) \tag{196}$$

In words, inter-point distances are unaffected by translation; EDM $D$ is *offset invariant*. When $\alpha=x_1$ in particular,

$$\mathcal{D}(X-x_1\mathbf{1}^T) \;=\; \mathcal{D}(X-Xe_1\mathbf{1}^T) \;=\; \mathcal{D}\big(X\big[\,\mathbf{0}\quad\sqrt{2}V_{\mathcal{N}}\,\big]\big) \;=\; \mathcal{D}(X) \tag{197}$$

where

$$e_1 \triangleq \begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix} \tag{198}$$

and where we introduce the full-rank skinny matrix (§C.9.3)

$$V_{\mathcal{N}} \;\triangleq\; \frac{1}{\sqrt{2}}\begin{bmatrix}-1&-1&\cdots&-1\\1&&&0\\&1&&\\&&\ddots&\\0&&&1\end{bmatrix} \;=\; \frac{1}{\sqrt{2}}\begin{bmatrix}-\mathbf{1}^T\\I\end{bmatrix}\in\mathbb{R}^{N\times N-1} \tag{199}$$

($\mathcal{N}(V_{\mathcal{N}})=\mathbf{0}$) having range

$$\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^T),\quad \mathcal{N}(\mathbf{1}^T)\perp\mathcal{R}(\mathbf{1})\,;\quad V_{\mathcal{N}}^T\mathbf{1}=\mathbf{0} \tag{200}$$

For the inner-product form EDM definition $\mathcal{D}(\Theta)$ and $\alpha\in\mathbb{R}^n$, it generally holds

$$\mathcal{D}(\Theta-\alpha\mathbf{1}^T)\neq\mathcal{D}(\Theta) \tag{201}$$

But because (190)

$$\Theta = X\sqrt{2}V_{\mathcal{N}} \tag{202}$$

and

$$\mathcal{D}(X - x_1\mathbf{1}^T) \;=\; \mathcal{D}\big(X[\,\mathbf{0}\quad \sqrt{2}V_{\mathcal{N}}\,]\big) \;=\; \mathcal{D}\big([\,\mathbf{0}\quad \Theta\,]\big) \;=\; \mathcal{D}(X) \tag{203}$$

we have offset invariance in the following sense:

$$\mathcal{D}\big([\,-\alpha \quad \Theta - \alpha\mathbf{1}^T\,]\big) \;=\; \mathcal{D}\big([\,\mathbf{0}\quad \Theta\,]\big) \tag{204}$$

### 4.4.2 Rotation/Reflection

Rotation of the list in $X\in\mathbb{R}^{n\times N}$ about some arbitrary point $\alpha\in\mathbb{R}^n$, or reflection through some affine set containing $\alpha$ is accomplished via $QX-\alpha\mathbf{1}^T$, where $Q$ is an orthogonal matrix (§C.6).

We rightfully expect

$$\mathcal{D}(QX - \alpha\mathbf{1}^T) = \mathcal{D}\big(Q(X - \alpha\mathbf{1}^T)\big) = \mathcal{D}(QX) = \mathcal{D}(X) \tag{205}$$

Because $\mathcal{D}(X)$ is offset 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 (205) follows directly from (178).

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 (178), it appears that any matrix $Q_o$ such that

$$X^TQ_o^TQ_o\,X = X^TX \tag{206}$$

will have the property

$$\mathcal{D}(Q_oX) = \mathcal{D}(X) \tag{207}$$

An example is skinny $Q_o\in\mathbb{R}^{m\times n}$ $(m>n)$ having orthonormal columns.

Likewise, $\mathcal{D}(\Theta)$ (187) is rotation/reflection invariant;

$$\mathcal{D}(Q\Theta) = \mathcal{D}(\Theta) \tag{208}$$

so (206) and (207) would similarly apply.

### 4.4.3 Invariance conclusion

In the construction of an EDM, absolute rotation, reflection, or offset information is lost. Reconstruction of point position, the list in $X$, can be guaranteed correct only in the affine dimension $r$; *id est*, in relative position.

## 4.5 Embedding in the affine hull

The affine hull $\mathcal{A}$ (49) of a point list $\{x_\ell\}$, arranged columnar in $X \in \mathbb{R}^{n\times N}$ (47), is identical to the affine hull of that polyhedron $\mathcal{P}$ (50) formed from all convex combinations of the $x_\ell$; [9, §2] [11, §17]

$$\mathcal{A} = \operatorname{aff} X = \operatorname{aff} \mathcal{P} \tag{209}$$

Comparing definitions (49) and (50), it becomes obvious that the $x_\ell$ and their convex hull $\mathcal{P}$ are embedded in their unique affine hull $\mathcal{A}$;

$$\mathcal{A} \supseteq \mathcal{P} \supseteq \{x_\ell\} \tag{210}$$

Recall that affine dimension $r$ is a lower bound on embedding, equal to the dimension of the subspace parallel to that affine set $\mathcal{A}$ in which the points are embedded. (§3.1.1) We define the dimension of the convex hull $\mathcal{P}$ to be the same as the dimension $r$ of the affine hull $\mathcal{A}$ [11, §2], but $r$ is not necessarily equal to the rank of $X$ (231). For the particular example illustrated in Figure 19, $\mathcal{P}$ is the triangle plus its relative interior while its three vertices constitute the entire list in $X$. 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 19, then the affine hull would instead be the unique line passing through them; $r$ would become 1 while the rank would then be 2.

### 4.5.1 Determining affine dimension

Knowledge of affine dimension $r$ is important because we lose any absolute offset component common to all the generating $x_\ell$ in $\mathbb{R}^n$ when reconstructing convex polyhedra given only distance information. (§4.4.1) 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,

$$X - \alpha\mathbf{1}^T \tag{211}$$

translating $\mathcal{A}$ to the origin:

$$\mathcal{A} - \alpha \;=\; \operatorname{aff}(X - \alpha\mathbf{1}^T) \;=\; \operatorname{aff}(X) - \alpha \tag{212}$$

$$\mathcal{P} - \alpha \;=\; \operatorname{conv}(X - \alpha\mathbf{1}^T) \;=\; \operatorname{conv}(X) - \alpha \tag{213}$$

which follow from their definitions. Because (209) and (210) translate,

$$\mathbb{R}^n \;\supseteq\; \mathcal{A} - \alpha \;=\; \operatorname{aff}(X - \alpha\mathbf{1}^T) \;=\; \operatorname{aff}(\mathcal{P} - \alpha) \;\supseteq\; \mathcal{P} - \alpha \;\supseteq\; \{x_\ell - \alpha\} \tag{214}$$

where from the previous relations it is easily shown

$$\operatorname{aff}(\mathcal{P} - \alpha) = \operatorname{aff}(\mathcal{P}) - \alpha \tag{215}$$

Translating $\mathcal{A}$ neither changes its dimension nor the dimension of the embedded polyhedron $\mathcal{P}$; (48)

$$r \;\stackrel{\Delta}{=}\; \dim \mathcal{A} \;=\; \dim(\mathcal{A} - \alpha) \;\stackrel{\Delta}{=}\; \dim(\mathcal{P} - \alpha) \;=\; \dim \mathcal{P} \tag{216}$$

For any $\alpha \in \mathbb{R}^n$, (212)-(216) remain true. [11, pg.4, pg.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 (214), and whose dimension is more easily calculated.

**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*,

$$X - x_1\mathbf{1}^T \;=\; X - Xe_1\mathbf{1}^T \;=\; X(I - e_1\mathbf{1}^T) \;=\; X\begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} \in \mathbb{R}^{n\times N} \tag{217}$$

where $V_{\mathcal{N}}$ is defined in (199), and $e_1$ in (198). Applying (214) to (217),

$$\mathbb{R}^n \;\supseteq\; \mathcal{R}(XV_{\mathcal{N}}) \;=\; \mathcal{A} - x_1 \;=\; \operatorname{aff}(X - x_1\mathbf{1}^T) \;=\; \operatorname{aff}(\mathcal{P} - x_1) \;\supseteq\; \mathcal{P} - x_1 \;\ni\; \mathbf{0} \tag{218}$$

where $XV_{\mathcal{N}} \in \mathbb{R}^{n\times N-1}$. Hence

$$r = \dim \mathcal{R}(XV_{\mathcal{N}}) \tag{219}$$

$\square$

**Example.** *Translating geometric center to origin.* We might choose to shift the geometric center of a length-$N$ point list $\{x_\ell\}$ to the origin; [27] [47]

$$\alpha \;=\; \alpha_g \;\triangleq\; Xb_g \;\triangleq\; \frac{1}{N}X\mathbf{1} \in \mathcal{P} \subseteq \mathcal{A} \tag{220}$$

If we were to associate a point-mass $m_\ell$ with each of the points $x_\ell$ 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. [32] 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 $b_g \succeq 0$. As in the earlier example, (217)

$$X - \alpha_g\mathbf{1}^T \;=\; X - \frac{1}{N}X\mathbf{1}\mathbf{1}^T \;=\; X(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T) \;\triangleq\; XV \in \mathbb{R}^{n\times N} \tag{221}$$

where properties of the auxiliary matrix $V$ are found in §C.9. Since shifting the geometric center to the origin translates the affine hull to the origin as well, then it must also be true (*confer* (219)) that

$$r \;=\; \dim \mathcal{R}(XV) \tag{222}$$

$\square$

For any matrix whose range is $\mathcal{N}(\mathbf{1}^T)$, we share the same result as in the examples; *e.g.*,

$$r \;=\; \dim \mathcal{R}(XV_{\mathcal{N}}^{\dagger T}) \tag{223}$$

because $\mathcal{R}(XV) = \{Xz \mid z \in \mathcal{N}(\mathbf{1}^T)\}$ and $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{R}(V_{\mathcal{N}}^{\dagger T})$ (§A). These *auxiliary matrices* (§C.9.3) are more closely related;

$$V = V_{\mathcal{N}} V_{\mathcal{N}}^{\dagger} \tag{224}$$

### 4.5.2 Affine dimension $r$ *versus* rank

Now, suppose $D$ is an EDM as in (178) and we pre-multiply by $-V_{\mathcal{N}}^T$ and post-multiply by $V_{\mathcal{N}}$ . Then because $V_{\mathcal{N}}^T\mathbf{1} = \mathbf{0}$ (200),

$$-\,V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \in \mathbb{S}^{N-1} \tag{225}$$

Similarly pre- and post-multiplying by $V$,

$$-\,VDV \;=\; 2VX^TXV \in \mathbb{S}^N \tag{226}$$

because $V\mathbf{1}=\mathbf{0}$ (627). Likewise, multiplying the inner-product form EDM definition (187),

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \Theta^T\Theta \in \mathbb{S}^{N-1} \tag{227}$$

For any matrix $A$, $\operatorname{rank} A^TA = \operatorname{rank} A = \operatorname{rank} A^T$. [24, §0.4][43] Hence

$$\operatorname{rank} VDV \;=\; \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \operatorname{rank} XV \;=\; \operatorname{rank} XV_{\mathcal{N}} \;=\; \operatorname{rank}\Theta \;=\; r \tag{228}$$

By conservation of dimension, (§C.4)

$$r + \dim\mathcal{N}(V_{\mathcal{N}}^T D V_{\mathcal{N}}) \;=\; N-1 \tag{229}$$

$$r + \dim\mathcal{N}(VDV) \;=\; N \tag{230}$$

The general fact[44]

$$r \leq \min\{n, N-1\} \tag{231}$$

is evident from (217) but can be visualized in the example illustrated in Figure 19. There we imagine a vector from the origin to each point in the list. Those three vectors are linearly independent in $\mathbb{R}^{\mathbf{3}}$, 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.

### 4.5.3 Summary

We collect expressions for the affine dimension: for $X\in\mathbb{R}^{n\times N}$,

$$\begin{array}{rcl} r & \overset{\Delta}{=} & \dim(\mathcal{P}-\alpha) \;=\; \dim\mathcal{P} \;=\; \dim\operatorname{conv} X \\ & = & \dim(\mathcal{A}-\alpha) \;=\; \dim\mathcal{A} \;=\; \dim\operatorname{aff} X \\ & = & \operatorname{rank}(X - x_1\mathbf{1}^T) \;=\; \operatorname{rank}(X-\alpha_g\mathbf{1}^T) \\ & = & \operatorname{rank} XV_{\mathcal{N}} \;=\; \operatorname{rank} XV \;=\; \operatorname{rank} XV_{\mathcal{N}}^{\dagger T} \\ & = & \left.\begin{array}{l} \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \;=\; \operatorname{rank} VDV \;=\; \operatorname{rank} V_{\mathcal{N}}^{\dagger} D V_{\mathcal{N}} \\ = \operatorname{rank}\Theta \\ = \operatorname{rank}\Lambda \quad (265) \end{array}\right\} D\in\mathbb{EDM}^N \end{array} \tag{232}$$

---

[43] For $A\in\mathbb{R}^{m\times n}$, $\mathcal{N}(A^TA)=\mathcal{N}(A)$. [19, §3.3]

[44] $\operatorname{rank} X \leq \min\{n, N\}$

**Theorem.** *EDM rank versus affine dimension* $r$. [47, §3] [48, §3] For $D \in \mathbb{EDM}^N$,

1. $r = \operatorname{rank}(D) - 1 \;\Leftrightarrow\; \mathbf{1}^T D^\dagger \mathbf{1} \neq 0$
   Points constituting a generating list for the corresponding polyhedron lie on the boundary of a *circumhypersphere* having

$$\text{diameter} \;=\; \sqrt{2}\left(\mathbf{1}^T D^\dagger \mathbf{1}\right)^{-1/2} \tag{233}$$

2. $r = \operatorname{rank}(D) - 2 \;\Leftrightarrow\; \mathbf{1}^T D^\dagger \mathbf{1} = 0$
   There can be no circumhypersphere whose boundary contains a generating list for the corresponding polyhedron.

$\diamond$

$$\operatorname{rank}(D) - 2 \;\leq\; r \;\leq\; \min\{n, N-1\} \tag{234}$$

## 4.6 Euclidean metric *versus* matrix criteria

### 4.6.1 Nonnegativity axiom 1

When $D$ is an EDM (178), then it is apparent from (225) that

$$2V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \;=\; -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \tag{235}$$

because for any $A$, $A^T A \succeq 0$. [45] We claim that nonnegativity of the $d_{ij}$ is enforced primarily by the matrix inequality (235); *id est*,

$$\left.\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ \delta(D) = \mathbf{0} \\ D^T = D \end{array}\right\} \Rightarrow\; d_{ij} \geq 0,\; i \neq j \tag{236}$$

(The matrix criterion to enforce strict positivity differs by a stroke of the pen. (239))

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[45] 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, $A^T A \succ 0$.

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. [25, §4.2] Given $D\in\mathbb{S}^N_\delta$ ,

$$-V_{\mathcal{N}}^TDV_{\mathcal{N}} =$$

$$\begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) & \frac{1}{2}(d_{1,i+1}+d_{1,j+1}-d_{i+1,j+1}) & \cdots & \frac{1}{2}(d_{12}+d_{1N}-d_{2N}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} & \frac{1}{2}(d_{1,i+1}+d_{1,j+1}-d_{i+1,j+1}) & \cdots & \frac{1}{2}(d_{13}+d_{1N}-d_{3N}) \\ \frac{1}{2}(d_{1,j+1}+d_{1,i+1}-d_{j+1,i+1}) & \frac{1}{2}(d_{1,j+1}+d_{1,i+1}-d_{j+1,i+1}) & d_{1,i+1} & \ddots & \frac{1}{2}(d_{14}+d_{1N}-d_{4N}) \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{1}{2}(d_{12}+d_{1N}-d_{2N}) & \frac{1}{2}(d_{13}+d_{1N}-d_{3N}) & \frac{1}{2}(d_{14}+d_{1N}-d_{4N}) & \cdots & d_{1N} \end{bmatrix}$$

$$\in\mathbb{S}^{N-1} \tag{237}$$

where row,column indices $i,j\in\{1\ldots N-1\}$. [45] It follows that

$$\left.\begin{aligned} -V_{\mathcal{N}}^TDV_{\mathcal{N}} \succeq 0 \\ \delta(D)=\mathbf{0} \\ D^T=D \end{aligned}\right\} \Rightarrow\ \delta(-V_{\mathcal{N}}^TDV_{\mathcal{N}}) = \begin{bmatrix} d_{12} \\ d_{13} \\ \vdots \\ d_{1N} \end{bmatrix} \succeq 0 \tag{238}$$

Multiplication of $V_{\mathcal{N}}$ by any permutation matrix $\Xi$ 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*, $\mathcal{R}(\Xi_rV_{\mathcal{N}})=\mathcal{R}(V_{\mathcal{N}}\Xi_c)=\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^T)$. Hence, $-V_{\mathcal{N}}^TDV_{\mathcal{N}}\succeq 0 \Leftrightarrow -V_{\mathcal{N}}^T\Xi_r^TD\Xi_rV_{\mathcal{N}}\succeq 0$ $(\Leftrightarrow -\Xi_c^TV_{\mathcal{N}}^TDV_{\mathcal{N}}\Xi_c\succeq 0)$. Various permutation matrices[46] will sift the remaining $d_{ij}$ similarly to (238) thereby proving their nonnegativity. Hence $-V_{\mathcal{N}}^TDV_{\mathcal{N}}\succeq 0$ is a sufficient test of the first axiom (§4.1) of the Euclidean metric, nonnegativity. ♦

**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 zero. By similar argument, the

[46] The rule of thumb is: If $\Xi_r(i,1)=1$, then $\delta(-V_{\mathcal{N}}^T\Xi_r^TD\Xi_rV_{\mathcal{N}})\in\mathbb{R}^{N-1}$ is some permutation of the $i^{\text{th}}$ row or column of $D$ excepting the 0 entry from the main diagonal.

strict matrix inequality is a sufficient test of strict positivity of the Euclidean distance-squared;

$$\left.\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \\ \delta(D) = \mathbf{0} \\ D^T = D \end{array}\right\} \Rightarrow \; d_{ij} > 0 ,\;\; i \neq j \tag{239}$$

### 4.6.2 Triangle inequality axiom 4

In light of Kreyszig's observation [17, §1.1, prob.15] that axioms 2 through 4 of the Euclidean metric (§4.1) together imply axiom 1, the nonnegativity criterion (236) 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*,

$$\left.\begin{array}{r} \delta(D) = \mathbf{0} \\ D^T = D \\ -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \end{array}\right\} \Rightarrow \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}} + \sqrt{d_{kj}} \,,\;\; i \neq j \neq k \tag{240}$$

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 $2\times 2$ submatrix from (237));

$$T \triangleq \left[\begin{array}{cc} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} \end{array}\right] \tag{241}$$

$T$ must be positive (semi)definite whenever $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ is. (§C.2.4) Now we have,

$$\begin{array}{c} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \;\Rightarrow\; T \succeq 0 \;\Leftrightarrow\; \sigma_1 \geq \sigma_2 \geq 0 \\ -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \;\Rightarrow\; T \succ 0 \;\Leftrightarrow\; \sigma_1 > \sigma_2 > 0 \end{array} \tag{242}$$

where $\sigma_1$ and $\sigma_2$ are the eigenvalues of $T$, real due only to symmetry of $T$:

$$\begin{array}{l} \sigma_1 = \frac{1}{2}\left(d_{12} + d_{13} + \sqrt{d_{23}^2 - 2(d_{12}+d_{13})d_{23} + 2(d_{12}^2 + d_{13}^2)}\right) \in \mathbb{R} \\ \sigma_2 = \frac{1}{2}\left(d_{12} + d_{13} - \sqrt{d_{23}^2 - 2(d_{12}+d_{13})d_{23} + 2(d_{12}^2 + d_{13}^2)}\right) \in \mathbb{R} \end{array} \tag{243}$$

Nonnegativity of eigenvalue $\sigma_1$ is guaranteed by only the nonnegativity of the $d_{ij}$ which in turn is guaranteed by the matrix inequality (236). The inequality between the eigenvalues in (242) follows from only the realness of the $d_{ij}$. Since $\sigma_1$ always exceeds or equals $\sigma_2$, conditions for the positive (semi)definiteness of submatrix $T$ can be completely determined by examining $\sigma_2$, 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*,

$$\begin{aligned} T\succeq 0 \quad&\Leftrightarrow\quad \det T=\sigma_1\sigma_2\geq 0\,,\quad d_{12}\,,d_{13}\geq 0\\ &\Leftrightarrow\\ &\sigma_2\geq 0 \\ &\Leftrightarrow\\ |\sqrt{d_{12}}-\sqrt{d_{23}}\,| \;&\leq\; \sqrt{d_{13}} \;\leq\; \sqrt{d_{12}}+\sqrt{d_{23}} \qquad\text{(a)}\end{aligned}\tag{244}$$

Triangle inequality (244a) (*confer* (186) (248)), in terms of three entries from $D$, is equivalent to §4.1 axiom 4

$$\begin{array}{l}\sqrt{d_{13}}\leq\sqrt{d_{12}}+\sqrt{d_{23}}\\ \sqrt{d_{23}}\leq\sqrt{d_{12}}+\sqrt{d_{13}}\\ \sqrt{d_{12}}\leq\sqrt{d_{13}}+\sqrt{d_{23}}\end{array}\tag{245}$$

for the corresponding points $x_1, x_2, x_3$ from some length-$N$ list.[47]

**4.6.2.1 Comment.** Given $D$ whose dimension $N$ equals or exceeds 3, there are $N!/(3!(N-3)!)$ distinct triangle inequalities in total like (186) 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, (244a) which came from $T$ (241). Yet we claim if $-V_{\mathcal{N}}^T D V_{\mathcal{N}}\succeq 0$ then all triangle inequalities will be satisfied simultaneously;

$$|\sqrt{d_{ik}}-\sqrt{d_{kj}}\,| \;\leq\; \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}}+\sqrt{d_{kj}}\,,\quad i<k<j \tag{246}$$

(There are no more.) To verify our claim, we must show that the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}}\succeq 0$ is a sufficient test of all the triangle inequalities; more efficient, we add, for larger $N$.

[47]Accounting for symmetry axiom 3 (§4.1), axiom 4 demands three inequalities be satisfied per one of type (244a). The first of those inequalities in (245) is self evident from (244a), while the two remaining follow from the left-hand side of (244a) and the fact for scalars, $|a|\leq b \Leftrightarrow a\leq b$ and $-a\leq b$.

**shore**

The columns of $\Xi_r V_{\mathcal{N}} \Xi_c$ hold a basis for $\mathcal{N}(\mathbf{1}^T)$ when $\Xi_r$ and $\Xi_c$ 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*, $\mathcal{R}(\Xi_r V_{\mathcal{N}} \Xi_c) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$ (200). 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,[48] the leading principal submatrix $T_\Xi \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$ 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 (237)-(244)). 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 (§4.1) of the Euclidean metric, triangle inequality. ♦

**strict triangle inequality**

Without exception, all the inequalities in (244) and (245) can be made strict while their corresponding implications remain true. The then strict inequality (244a) or (245) may be interpreted as a *strict triangle inequality* under which collinear arrangement of points is not allowed. [37, §24/6, pg.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*,

$$\left.\begin{array}{r} \delta(D) = \mathbf{0} \\ D^T = D \\ -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \end{array}\right\} \Rightarrow \sqrt{d_{ij}} < \sqrt{d_{ik}} + \sqrt{d_{kj}}\,,\ i \neq j \neq k \qquad (247)$$

### 4.6.3 Affine dimension reduction in two dimensions

The leading principal $2\times 2$ submatrix $T$ of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ has largest eigenvalue $\sigma_1$ (243) which is a convex function of $D$.[49] $\sigma_1$ can never be zero unless

[48] 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 $\Xi_c = I$.

[49] The maximum eigenvalue of any symmetric matrix is always a convex function of its entries, while the minimum eigenvalue is always concave. [9, §3] In our particular case,

$d_{12}=d_{13}=d_{23}=0$. $\sigma_1$ can never be negative so long as the $d_{ij}$ are nonnegative. The remaining eigenvalue $\sigma_2$ is a concave function of $D$ that becomes zero only at the upper and lower bounds of inequality (244a) and its equivalent forms: (*confer* (246))

$$\begin{array}{rcccll}
|\sqrt{d_{12}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{13}} & \leq & \sqrt{d_{12}}+\sqrt{d_{23}} & \quad\text{(a)}\\
 & & \Leftrightarrow & & & \\
|\sqrt{d_{12}}-\sqrt{d_{13}}\,| & \leq & \sqrt{d_{23}} & \leq & \sqrt{d_{12}}+\sqrt{d_{13}} & \quad\text{(b)}\\
 & & \Leftrightarrow & & & \\
|\sqrt{d_{13}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{12}} & \leq & \sqrt{d_{13}}+\sqrt{d_{23}} & \quad\text{(c)}
\end{array} \tag{248}$$

In between those bounds, $\sigma_2$ is strictly positive; otherwise, it would be negative but prevented by the condition $T\succeq 0$.

When $\sigma_2$ becomes zero, it means that triangle $\triangle_{123}$ has collapsed to a line segment; a potential reduction in affine dimension $r$. (*confer* §6.3.3, §4.9.4) The same logic is valid for any principal $2\times2$ submatrix of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$, hence applicable to other triangles.

## 4.7 Bridge: Convex polyhedra to EDMs

The criteria for the existence of an EDM include, by definition (178) (187), the axioms imposed upon its entries $d_{ij}$ by the Euclidean metric. From §4.6.1 and §4.6.2, 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* §4.1)

$$\begin{array}{l}
\sqrt{d_{ij}}\geq 0,\;\; i\neq j\\
\sqrt{d_{ij}}=0,\;\; i=j\\
\sqrt{d_{ij}}=\sqrt{d_{ji}}\\
\sqrt{d_{ij}}\;\leq\;\sqrt{d_{ik}}+\sqrt{d_{kj}}\;,\;\; i\neq j\neq k
\end{array}
\quad\Leftarrow\quad
\begin{array}{r}
-V_{\mathcal{N}}^T D V_{\mathcal{N}}\succeq 0\\
\delta(D)=\mathbf{0}\\
D^T=D
\end{array}
\quad\Leftarrow\quad D\in\mathbb{EDM}^N \tag{249}$$

In words, the Euclidean axioms are necessary conditions for $D$ to be a distance matrix. At this moment, we have no converse for (249). As of concern

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say $\underline{d}\triangleq\begin{bmatrix}d_{12}\\d_{13}\\d_{23}\end{bmatrix}\in\mathbb{R}^{\mathbf{3}}$. Then the Hessian (642) $\nabla^2\sigma_1(\underline{d})\succeq 0$ 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 zero.

in §4.2, we have yet to establish the metric requirements beyond the four Euclidean axioms that would allow $D$ to be identified as an EDM, or would 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[50] for all $N>0$ (§D); *id est*,

$$\begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D\in\mathbb{S}_\delta^N \end{array} \quad\Leftrightarrow\quad D\in\mathbb{EDM}^N \tag{250}$$

or since $-V_{\mathcal{N}}^T D V_{\mathcal{N}} = \Theta^T\Theta$ (227), for angle matrix $\Omega$ and distance vector $\sqrt{d}$ as in (191) and EDM definition (194),

$$\begin{array}{r} \Omega\succeq 0 \\ \sqrt{d}\succeq 0 \end{array} \quad\Leftrightarrow\quad D=\mathcal{D}(\Omega\,,d)\in\mathbb{EDM}^N \tag{251}$$

From (200) we know $\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^T)$, so (250) is the same as (175). In fact, any matrix $V$ in place of $V_{\mathcal{N}}$ will satisfy (250) if $\mathcal{R}(V)=\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^T)$.

### 4.7.1 Geometric criterion

We derive matrix criteria for $D$ to be an EDM, validating (250) using simple geometry: distance to the polyhedron formed by the convex hull of a list of points (47) in Euclidean space $\mathbb{R}^n$.

**EDM assertion.** $D$ is a Euclidean distance matrix if and only if $D\in\mathbb{S}_\delta^N$ and distances-squared from the origin

$$\{\|p(y)\|^2 = -y^T V_{\mathcal{N}}^T D V_{\mathcal{N}}\, y \mid y\in\mathcal{S}-\beta\} \tag{252}$$

correspond to points $p$ in some closed convex polyhedron

$$\mathcal{P}-\alpha \;=\; \{p(y) \mid y\in\mathcal{S}-\beta\} \tag{253}$$

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 function $p(y)$

[50] In 1935, Schoenberg [45] first extolled expansion (237) (predicated on symmetry and zero self-distance) showing 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 [43, §3] remarks how it is surprising that such a fundamental property of Euclidean geometry was obtained so late.

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 (100) in $\mathbb{R}^{N-1}$ has an equivalent representation:

$$\mathcal{S} = \{s \in \mathbb{R}^{N-1} \mid \sqrt{2}V_{\mathcal{N}}\, s \succeq -e_1\} \tag{254}$$

where $e_1$ is as in (198). 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 $\mathcal{P}$;

$$\begin{array}{rcl} p \;:\; \mathbb{R}^{N-1} & \to & \mathbb{R}^n \\ p\left(\left\{\begin{array}{c} -\beta \\ e_1-\beta \\ e_2-\beta \\ \vdots \\ e_{N-1}-\beta \end{array}\right\}\right) & = & \left\{\begin{array}{c} x_1-\alpha \\ x_2-\alpha \\ x_3-\alpha \\ \vdots \\ x_N-\alpha \end{array}\right\} \end{array} \tag{255}$$

**4.7.1.1 Proof.** *EDM assertion.*
$\Longrightarrow$ We demonstrate that if $D$ is an EDM, then each distance-squared $\|p(y)\|^2$ described by (252) 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 $\mathbb{R}^n$; $D = \mathcal{D}(X)$ for $X \in \mathbb{R}^{n\times N}$ as in (178). Since $D$ is offset invariant (§4.4.1), we may shift the affine hull $\mathcal{A}$ of those unknown points to the origin as in (211). Then take any point $p$ in their convex hull (50);

$$\mathcal{P}-\alpha = \{p = (X - Xb\,\mathbf{1}^T)a \mid a^T\mathbf{1} = 1,\ a \succeq 0\} \tag{256}$$

where $\alpha = Xb \in \mathcal{A} \Leftrightarrow b^T\mathbf{1} = 1$. Solutions to $a^T\mathbf{1} = 1$ are:[51]

$$a = e_1 + \sqrt{2}V_{\mathcal{N}}\, s \tag{257}$$

[51] 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, $a = e_1$.

where $s\in\mathbb{R}^{N-1}$ and $e_1$ is as in (198). Similarly, $b=e_1+\sqrt{2}V_{\mathcal{N}}\beta$ .

$$\begin{aligned}\mathcal{P}-\alpha &= \{p=X(I-(e_1+\sqrt{2}V_{\mathcal{N}}\beta)\mathbf{1}^T)(e_1+\sqrt{2}V_{\mathcal{N}}\,s)\mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\}\\ &= \{p=X\sqrt{2}V_{\mathcal{N}}(s-\beta)\mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\}\end{aligned}\tag{258}$$

that describes the domain of $p(s)$ as the unit simplex $\mathcal{S}$ ;

$$\mathcal{S}=\{s\mid \sqrt{2}V_{\mathcal{N}}\,s\succeq -e_1\}\subset\mathbb{R}^{N-1}_+\tag{259}$$

Making the substitution $y\leftarrow s-\beta$ ,

$$\mathcal{P}-\alpha \;=\; \{p=X\sqrt{2}V_{\mathcal{N}}\,y\mid y\in\mathcal{S}-\beta\}\tag{260}$$

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 $\mathcal{P}-\alpha$ (214) and the origin (when $\alpha\in\mathcal{A}$), and because $\mathcal{A}$ has dimension $r$ by definition (216). Now, any distance-squared from the origin to the polyhedron $\mathcal{P}-\alpha$ can be formulated

$$\{p^Tp \;=\; \|p\|^2 \;=\; 2y^TV_{\mathcal{N}}^TX^TXV_{\mathcal{N}}\,y\mid y\in\mathcal{S}-\beta\}\tag{261}$$

Applying (225) to (261) we get (252).

$\Longleftarrow$ To validate the *EDM assertion* in the reverse direction, we show that if each distance-squared $\|p(y)\|^2$ (252) 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

$$p(\mathcal{S}-\beta)=\mathcal{P}-\alpha\tag{262}$$

because $\mathcal{A}-\alpha=\operatorname{aff}(\mathcal{P}-\alpha)\supseteq\mathcal{P}-\alpha$ (214). So, outside the domain $\mathcal{S}-\beta$ of linear function $p(y)$, the simplex complement $\backslash\mathcal{S}-\beta\subset\mathbb{R}^{N-1}$ must contain the domain of the distance-squared $\|p(y)\|^2=p(y)^Tp(y)$ to the 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;[52]

$$-\,V_{\mathcal{N}}^TDV_{\mathcal{N}}\;\triangleq\;\Phi^T\Phi\tag{263}$$

[52] The antisymmetric part $\left(-V_{\mathcal{N}}^TDV_{\mathcal{N}}-(-V_{\mathcal{N}}^TDV_{\mathcal{N}})^T\right)/2$ 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 $y^TAy\geq 0$. [24, §7.1]

where[53] $\Phi \in \mathbb{R}^{m\times N-1}$ 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 (§3.5.2). Equivalent to (252) are

$$\{p^T p \mid p \in \mathcal{P} - \alpha\} \;=\; \{p^T p = y^T \Phi^T \Phi\, y \mid y \in \mathcal{S} - \beta\} \tag{264}$$

Because $p \in \mathcal{P} - \alpha$ may be found by factoring (264), the list $\Phi$ is found by factoring (263). A unique EDM can be constructed from that list using the inner-product form definition $\mathcal{D}(\Theta)|_{\Theta=\Phi}$ (187). That EDM will be identical to $D$ if $\delta(D)=\mathbf{0}$, by injectivity of $\mathcal{D}$ (305). ♦

### 4.7.2 Necessity and sufficiency

From (235) 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 §4.7.1, the connection between convex polyhedra and EDMs was pronounced by the *EDM assertion*; the matrix inequality together with $D \in \mathbb{S}_\delta^N$ became a sufficient test when the *EDM assertion* demanded that every convex polyhedron have a corresponding EDM. For all $N>0$ (§D), the matrix criteria in (250), (251), and (175) for the existence of an EDM are therefore necessary and sufficient and subsume all the Euclidean requirements.

### 4.7.3 Example revisited

Now we apply the necessary and sufficient EDM criteria (250) to an earlier problem.

**Example.** *Small completion problem*, II. Continuing the example on page 65 that pertains to Figure 20 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 (172) 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 21. We observe a unique value of $d_{14}$ satisfying (250) 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 (§4.6.3), we calculate its second partial derivative with respect to $d_{14}$ evaluated at 2 and find $-1/3$. We conclude

[53] $A^T = A \succeq 0 \;\Leftrightarrow\; A = R^T R$ for some real matrix $R$. [19, §6.3]

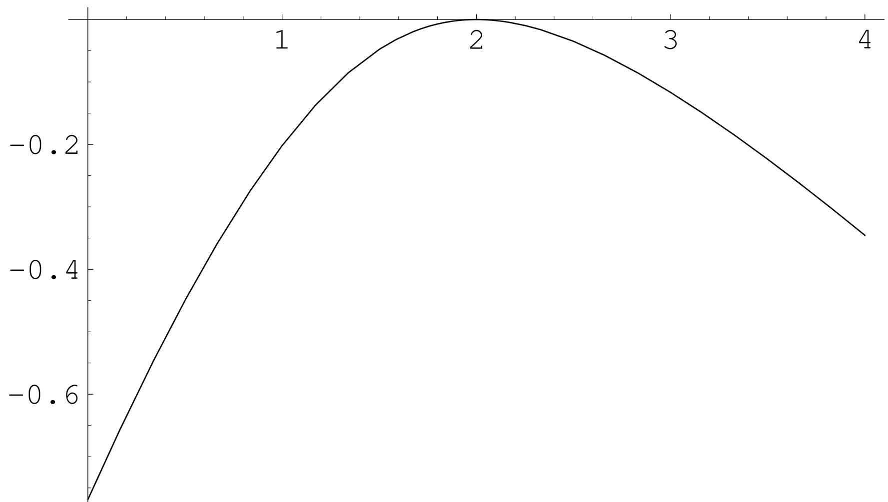


Figure 21: Minimum eigenvalue of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ , positive semidefinite for only one value of $d_{14}$ ; 2.

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 (246), 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 $N-2$. (§4.5.2) □

## 4.8 List reconstruction

At the stage of reconstruction, $D \in \mathbb{EDM}^N$ and we wish to find a generating list (§3.1.2) for $\mathcal{P} - \alpha$ by factoring positive semidefinite $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ (263) as suggested in §4.7.1.1. One way to factor (263) is via *diagonalization* of symmetric matrices; [19, §5.6] [24] (§C.2)

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \triangleq Q \Lambda Q^T \tag{265}$$

$$Q \Lambda Q^T \succeq 0 \;\Leftrightarrow\; \Lambda \succeq 0 \tag{266}$$

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 (225);

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} = 2 V_{\mathcal{N}}^T X^T X V_{\mathcal{N}} \triangleq Q \sqrt{\Lambda}\, Q_o^T Q_o \sqrt{\Lambda}\, Q^T \tag{267}$$

where $\sqrt{\Lambda}\,Q_o^TQ_o\sqrt{\Lambda} \triangleq \Lambda = \sqrt{\Lambda}\sqrt{\Lambda}$, and where $Q_o \in \mathbb{R}^{n\times N-1}$ is unknown as is its dimension $n$. Rotation/reflection is accounted for by $Q_o$ yet only its first $r$ columns are necessarily orthonormal.[54] Assuming $y \in \mathcal{S}$ then $p = X\sqrt{2}V_{\mathcal{N}}\,y = Q_o\sqrt{\Lambda}\,Q^Ty$ in $\mathbb{R}^n$ belongs to the polyhedron $\mathcal{P} - x_1$ whose generating list constitutes the columns of (217)

$$\begin{bmatrix}\mathbf{0} & X\sqrt{2}V_{\mathcal{N}}\end{bmatrix} = \begin{bmatrix}\mathbf{0} & Q_o\sqrt{\Lambda}\,Q^T\end{bmatrix} \in \mathbb{R}^{n\times N} \tag{268}$$

The simplest choice of $Q_o$ has $n$ set to $N-1$; *id est*, $Q_o = I$. Each member of the generating list then has $N-1-r$ zeros in its higher dimensional coordinates because $r \leq N-1$. (231) To truncate those zeros, choose $n$ to be

$$\operatorname{rank} V_{\mathcal{N}}^TDV_{\mathcal{N}} = \operatorname{rank} Q_o\sqrt{\Lambda}\,Q^T = \operatorname{rank}\Lambda = r \tag{269}$$

which is the smallest $n$ possible because $XV_{\mathcal{N}}$ has rank $r \leq n$ (228).[55] In that case, the simplest choice for $Q_o$ is $[I \;\; \mathbf{0}]$ having dimensions $r\times N-1$.

We may wish to verify the list (268) found from the diagonalization of $-V_{\mathcal{N}}^TDV_{\mathcal{N}}$. Because of offset and rotation/reflection invariance (§4.4), EDM $D$ can be uniquely constructed from that list by calculating: (178)

$$\mathcal{D}(X) = \mathcal{D}(X[\mathbf{0} \;\; \sqrt{2}V_{\mathcal{N}}]) = \mathcal{D}(Q_o[\mathbf{0} \;\; \sqrt{\Lambda}\,Q^T]) = \mathcal{D}([\mathbf{0} \;\; \sqrt{\Lambda}\,Q^T]) \tag{270}$$

Alternately, we may perform reconstruction using instead the auxiliary matrix $V$; (§C.9.1) re-dimensioning $Q, \Lambda \in \mathbb{R}^{N\times N}$ and $Q_o \in \mathbb{R}^{n\times N}$, (226)

$$-VDV = 2VX^TXV \triangleq Q\sqrt{\Lambda}\,Q_o^TQ_o\sqrt{\Lambda}\,Q^T \tag{271}$$

where the generating list now constitutes (*confer* (268))

$$XV = \frac{1}{\sqrt{2}}\,Q_o\sqrt{\Lambda}\,Q^T \in \mathbb{R}^{n\times N} \tag{272}$$

---

[54] $Q_o$ is not necessarily an orthogonal matrix. $Q_o$ is constrained such that only its first $r$ columns are necessarily orthonormal because there are only $r$ nonzero eigenvalues in $\Lambda$ when $V_{\mathcal{N}}^TDV_{\mathcal{N}}$ has rank $r$ (§4.5.2). The remaining columns of $Q_o$ are arbitrary.

[55] If we write $Q^T = \begin{bmatrix} q_1^T \\ \vdots \\ q_{N-1}^T \end{bmatrix}$ as row-wise eigenvectors, $\Lambda = \begin{bmatrix} \lambda_1 & & & & \mathbf{0} \\ & \ddots & & & \\ & & \lambda_r & & \\ & & & 0 & \\ \mathbf{0} & & & & \ddots \;\; 0 \end{bmatrix}$ in terms of eigenvalues, and $Q_o = \begin{bmatrix} q_{o_1} \cdots q_{o_{N-1}} \end{bmatrix}$ as column vectors, then $Q_o\sqrt{\Lambda}\,Q^T = \sum\limits_{i=1}^{r}\sqrt{\lambda_i}\,q_{o_i}q_i^T$ is a sum of $r$ linearly independent rank-one matrices (§C.7.1). Hence the summation has rank $r$.

and where

$$\mathcal{D}(X) \;=\; \mathcal{D}(XV) \;=\; \mathcal{D}(\frac{1}{\sqrt{2}}\,Q_o\sqrt{\Lambda}\,Q^T) \;=\; \mathcal{D}(\sqrt{\Lambda}\,Q^T)\frac{1}{2} \tag{273}$$

### 4.8.1 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 reconstruction from 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:

$$\begin{aligned}\phi &\stackrel{\Delta}{=} \pi/2 - \text{latitude}\\ \theta &\stackrel{\Delta}{=} \text{longitude}\\ x &= \sin(\phi)\cos(\theta)\\ y &= \sin(\phi)\sin(\theta)\\ z &= \cos(\phi)\end{aligned} \tag{274}$$

We used less than 50% of the available map data to calculate the EDM $D$ from $N = 2536$ points. The original (decimated) data and its reconstruction are shown in Figure 22(a)-(d). The Matlab code is in §E.2. The eigenvalues computed for (265) are

$$\lambda(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \{100.5\,,\ 77.26\,,\ 1.242\,,\ 0\,,\ 0\,,\ 0\,,\ \ldots\} \tag{275}$$

The 0 eigenvalues have numerical error on the order of `4E-14`; meaning, the EDM data indicates three dimensions $(r = 3)$ are required for reconstruction to within nearly machine precision.

#### 4.8.1.1 Ordinal multidimensional scaling.

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:

$$D \;=\; [d_{ij}] \;=\; \begin{bmatrix} 0 & d_{12} & d_{13}\\ d_{12} & 0 & d_{23}\\ d_{13} & d_{23} & 0 \end{bmatrix} \in \mathbb{S}_\delta^{\mathbf{3}} \tag{169}$$

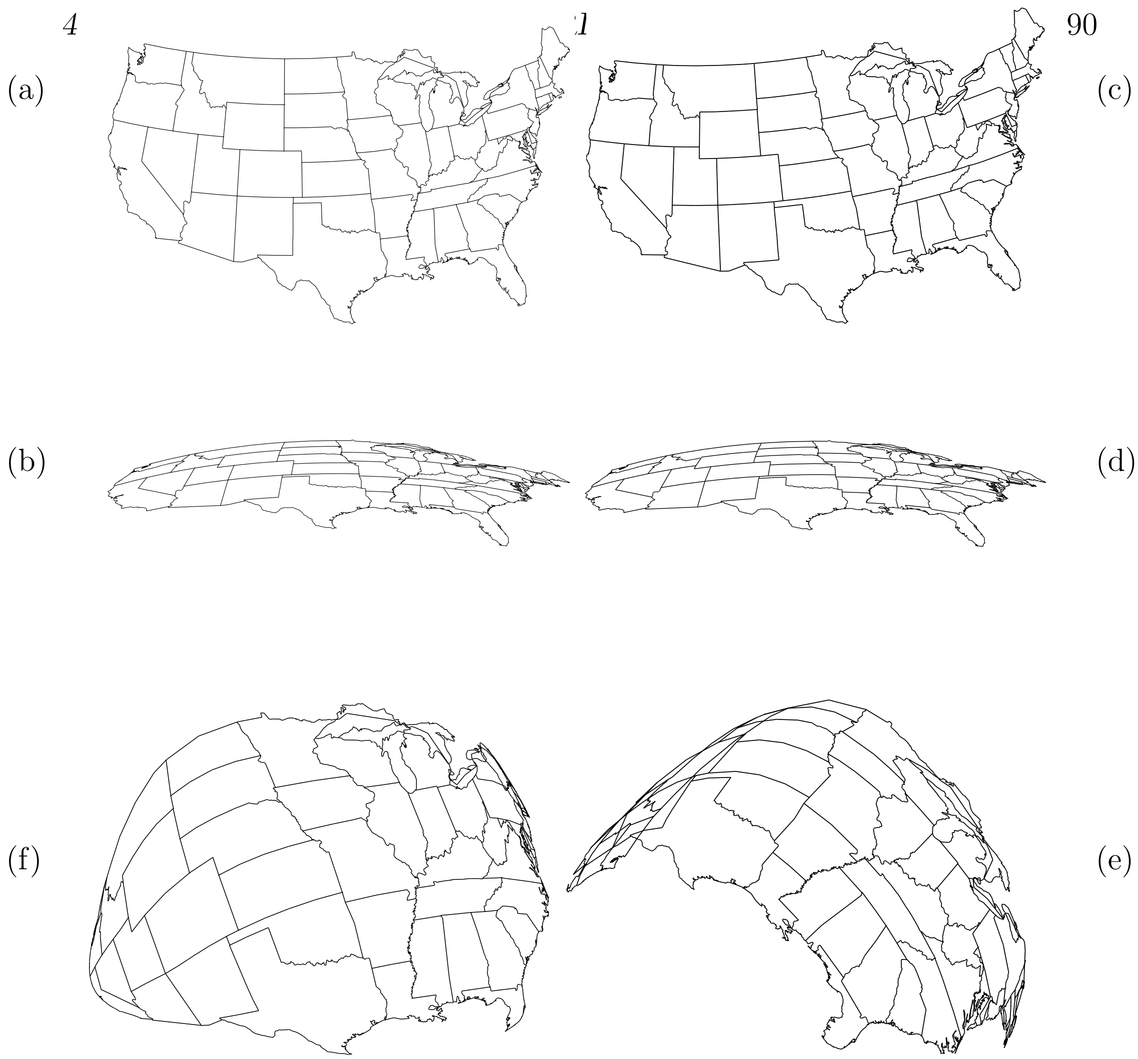


Figure 22: Map of United States of America showing some state boundaries and the Great Lakes. All plots made using 2536 connected points. Any difference in scale is an artifact of plotting routine.
(a) shows original map made from decimated (latitude, longitude) data.
(b) shows original map data rotated to highlight curvature of Earth.
(c) Map reconstructed from the EDM.
(d) Same reconstructed map illustrating curvature with reflection error.
(e)(f) Two views of one reconstruction by ordinal multidimensional scaling with no sort constraint in (282).

but the comparative data is available:

$$d_{12} \leq d_{23} \leq d_{13} \tag{276}$$

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 sorting

$$\Xi\,\underline{d} \;=\; \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} d_{12} \\ d_{13} \\ d_{23} \end{bmatrix} \;=\; \begin{bmatrix} d_{12} \\ d_{23} \\ d_{13} \end{bmatrix} \in \mathcal{K}_{+\mathcal{M}} \tag{277}$$

where $\mathcal{K}_{+\mathcal{M}}$ is the monotone nonnegative cone (§3.6.3.1, with reversed indices),

$$\mathcal{K}_{+\mathcal{M}} \triangleq \{z \mid 0 \leq z_1 \leq z_2 \leq \cdots \leq z_m\} \subseteq \mathbb{R}^m_+ \tag{278}$$

where $m \triangleq N(N-1)/2 = 3$ for the present example. From the sorted vectorization (277) we make the *sort-index matrix*

$$O = \begin{bmatrix} 0 & 1^2 & 3^2 \\ 1^2 & 0 & 2^2 \\ 3^2 & 2^2 & 0 \end{bmatrix} \tag{279}$$

where, for $j \neq i$,

$$O_{ij} = k^2 \mid D_{ij} = \big(\Xi\,\underline{d}\big)_k \tag{280}$$

When EDM data is replaced like this with indices of a nondecreasing sorting, a process of reconstruction that leaves comparative distance information intact is called *ordinal multidimensional scaling.* Beyond rotation, reflection, and offset error, (§4.4) list reconstruction by ordinal multidimensional scaling is subject to error in absolute scale (dilation) and relative point position. Yet Borg and Groenen argue [49, §2.2] that reconstruction from comparative distance information for a large number of points is as highly constrained as reconstruction from an EDM.

Suppose we make $O$ for the map of the USA and then substitute $O$ in place of EDM $D$ in the reconstruction process (§4.8). Whereas EDM $D$ returned only three significant eigenvalues (275), the sort-index matrix $O$ is not an EDM with corresponding affine dimension 3 and returns many more. The eigenvalues, calculated with numerical error on the order of `9E-7`, are plotted in Figure 23:

$$\lambda(-V_{\mathcal{N}}^T O V_{\mathcal{N}}) = \{443.1\,,\ 235.3\,,\ 93.92\,,\ 23.29\,,\ 8.602\,,\ 4.755\,,\ 4.113\,,\ 0.8406\,,\ 0.3498\,,\ 0.3171\,,\ \ldots\} \tag{281}$$

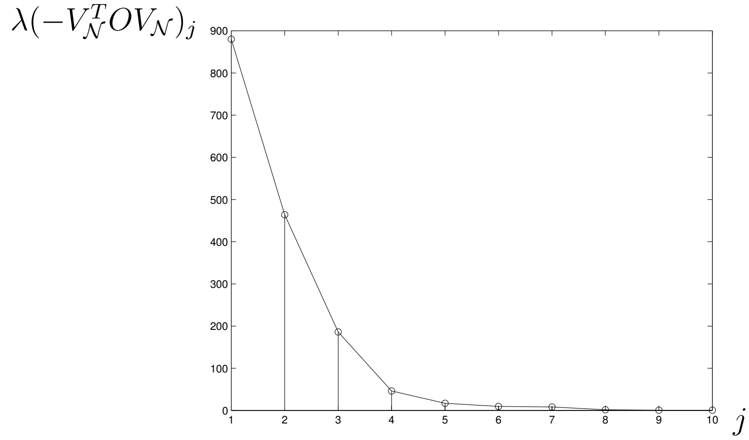


Figure 23: Largest ten eigenvalues of $-V_{\mathcal{N}}^T O V_{\mathcal{N}}$ for map of USA, sorted by nonincreasing value. In the code (§E.2.2), we normalize $O$ by $(N(N-1)/2)^2$ for numerical reasons.

The extra eigenvalues indicate that affine dimension corresponding to $O$ exceeds 3. To realize the map, we must reduce that dimensionality and find an EDM $D$ closest to $O$ in some sense (a problem explored more generally in §6) while maintaining the known comparative distance relationship; *e.g.*,

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-O)V_{\mathcal{N}}\|_{\mathrm{F}}\\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq 3\\ & \Xi\,\underline{d} \in \mathcal{K}_{+\mathcal{M}}\\ & D \in \mathbb{EDM}^N\end{array} \tag{282}$$

where $\Xi$ is a permutation matrix expressing the known sorting action on

$$\underline{d} \triangleq \begin{bmatrix} d_{12}\\ d_{13}\\ d_{23}\\ d_{14}\\ \vdots\\ d_{N-1,N}\end{bmatrix} \tag{283}$$

The analytical solution to this problem, less the sort constraint $\Xi\,\underline{d}\in\mathcal{K}_{+\mathcal{M}}$ , is known [42] (§6.2): only the three largest nonnegative eigenvalues in (281) need be retained to make (268); the rest are discarded. The reconstruction from the EDM $D$ found in this manner is plotted in Figure 22(e)(f) from which it is made clear that inclusion of the sort constraint is necessary for ordinal multidimensional scaling. Ignoring the sort constraint, obviously, violates it...

## 4.9 Fifth Euclidean requirement

We continue now with the question raised in §4.2 regarding the necessity for at least one requirement more than the four axioms of the Euclidean metric (§4.1) to reconstruct a convex polyhedron or a generating list for it from incomplete distance information. There we saw that the Euclidean axioms are necessary for $D$ to be an EDM in the case $N=3$, but become insufficient when the number of points $N$ exceeds 3 (regardless of affine dimension).

### 4.9.1 Recapitulate

In the particular case $N = 3$, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ (241) and $D \in \mathbb{S}_\delta^{\mathbf{3}}$ are the necessary and sufficient conditions for $D$ to be an EDM. From (244), the triangle inequality is then the only Euclidean constraint on the bounds of the necessarily nonnegative $d_{ij}$, and those bounds are *tight*.[56] 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 $i, j \in \{1,2,3\}$,

$$\begin{array}{l}\sqrt{d_{ij}} \geq 0,\ i \neq j \\ \sqrt{d_{ij}} = 0,\ i = j \\ \sqrt{d_{ij}} = \sqrt{d_{ji}} \\ \sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}\,,\ i \neq j \neq k \end{array} \quad \Leftrightarrow \quad \begin{array}{r} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_\delta^{\mathbf{3}} \end{array} \quad \Leftrightarrow \quad D \in \mathbb{EDM}^{\mathbf{3}} \tag{284}$$

Yet the four axioms become insufficient when $N > 3$.

### 4.9.2 Derivation

Correspondence between the triangle inequality and the EDM was developed in §4.6.2 where a triangle inequality (244a) was revealed within the leading principal $2 \times 2$ 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 (186) corresponds to any one of the

[56]The term *tight* with reference to an inequality means equality is achievable.

$(N-1)!/(2!(N-1-2)!)$ principal $2\times 2$ submatrices.[57] Assuming $D\in\mathbb{S}^{\mathbf{4}}_\delta$ and $-V_{\mathcal{N}}^T D V_{\mathcal{N}}\in\mathbb{S}^{\mathbf{3}}$, then by the *positive (semi)definite principal submatrices theorem* (§C.2.4) it is sufficient to show that all $d_{ij}$ are nonnegative, all triangle inequalities are satisfied, and $\det(-V_{\mathcal{N}}^T D V_{\mathcal{N}})$ 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.

#### 4.9.2.1 Nonnegative determinant

By (227) when $D\in\mathbb{EDM}^{\mathbf{4}}$, $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ is equal to the inner product (189),

$$\Theta^T\Theta = \begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214} \\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314} \\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14} \end{bmatrix} \tag{285}$$

Because Euclidean space is an inner-product space, the more concise inner-product form of the determinant is admitted;

$$\det(\Theta^T\Theta) = -d_{12}d_{13}d_{14}\big(\cos^2\theta_{213}+\cos^2\theta_{214}+\cos^2\theta_{314} - 2\cos\theta_{213}\cos\theta_{214}\cos\theta_{314} - 1\big) \tag{286}$$

The determinant is nonnegative if and only if

$$\begin{array}{c} \cos\theta_{214}\cos\theta_{314} - \sqrt{\sin^2\theta_{214}\sin^2\theta_{314}} \;\le\; \cos\theta_{213} \;\le\; \cos\theta_{214}\cos\theta_{314} + \sqrt{\sin^2\theta_{214}\sin^2\theta_{314}} \\ \Leftrightarrow \\ \cos\theta_{213}\cos\theta_{314} - \sqrt{\sin^2\theta_{213}\sin^2\theta_{314}} \;\le\; \cos\theta_{214} \;\le\; \cos\theta_{213}\cos\theta_{314} + \sqrt{\sin^2\theta_{213}\sin^2\theta_{314}} \\ \Leftrightarrow \\ \cos\theta_{213}\cos\theta_{214} - \sqrt{\sin^2\theta_{213}\sin^2\theta_{214}} \;\le\; \cos\theta_{314} \;\le\; \cos\theta_{213}\cos\theta_{214} + \sqrt{\sin^2\theta_{213}\sin^2\theta_{214}} \end{array} \tag{287}$$

which simplifies, for $0\le\theta_{i1\ell}\,,\theta_{\ell1j}\,,\theta_{i1j}\le\pi$ and all $i\neq j\neq\ell\in\{2,3,4\}$, to

$$\cos(\theta_{i1\ell}+\theta_{\ell1j}) \;\le\; \cos\theta_{i1j} \;\le\; \cos(\theta_{i1\ell}-\theta_{\ell1j}) \tag{288}$$

Analogously to triangle inequality (248), the determinant is zero upon equality on either side of (288) which is tight. Inequality (288) can be equivalently

[57] There are fewer principal $2\times2$ 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* §4.6.2.1)

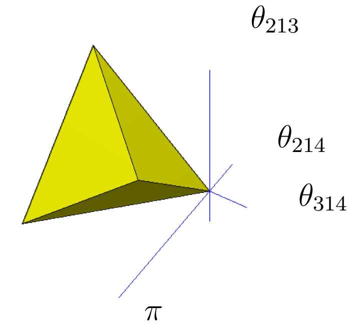


Figure 24: The angle-inequality tetrahedron (290) bounding $\mathbb{EDM}^4$ is regular; drawn in entirety. Each angle $\theta$ (184) must belong to the solid to be realizable.

written linearly as a "triangle inequality", but between angles [50, §1.4]:

$$\begin{aligned} |\theta_{i1\ell} - \theta_{\ell 1j}| \;\leq\; \theta_{i1j} \;\leq\; \theta_{i1\ell} + \theta_{\ell 1j} \\ \theta_{i1\ell} + \theta_{\ell 1j} + \theta_{i1j} \;\leq\; 2\pi \\ 0 \leq \theta_{i1\ell}\,, \theta_{\ell 1j}\,, \theta_{i1j} \leq \pi \end{aligned} \tag{289}$$

Generalizing this:

**Axiom. Fifth Euclidean requirement - restatement.** [44, §3.1] (*confer* §4.2.1) *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

$$\begin{aligned} |\theta_{ik\ell} - \theta_{\ell kj}| \;\leq\; \theta_{ikj} \;\leq\; \theta_{ik\ell} + \theta_{\ell kj} \qquad & (a) \\ \theta_{ik\ell} + \theta_{\ell kj} + \theta_{ikj} \;\leq\; 2\pi \qquad & (b) \\ 0 \leq \theta_{ik\ell}\,, \theta_{\ell kj}\,, \theta_{ikj} \leq \pi \qquad & (c) \end{aligned} \tag{290}$$

where $\theta_{ikj} = \theta_{jki}$ is the angle between vectors at vertex $x_k$ as defined in (184), must be satisfied at each point $x_k$ regardless of affine dimension. ⋄

Because point labelling is arbitrary, the fifth Euclidean requirement, *angle inequality*, must apply to each of the $N$ points as though each were in turn labelled $x_1$; hence the new index $k$ in (290). Just as the triangle inequality is the ultimate test for reconstruction of only three points, the *angle* inequality is the ultimate test for only four. For four distinct points, the triangle inequality remains a necessary although penultimate test;

$$\begin{array}{l}\text{Four Euclidean axioms (§4.1).}\\ \text{Angle inequality (174) or (290).}\end{array} \;\Leftrightarrow\; \begin{array}{r}-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0\\ D \in \mathbb{S}_\delta^{\mathbf{4}}\end{array} \;\Leftrightarrow\; D = \mathcal{D}(\Theta) \in \mathbb{EDM}^{\mathbf{4}} \tag{291}$$

The angle inequality, for this case, is illustrated in Figure 24.

#### 4.9.2.2 Beyond the fifth requirement

When the number of points $N$ exceeds 4, the four Euclidean axioms and the angle inequality together become insufficient conditions for reconstruction. In other words, the Euclidean axioms and angle inequality remain necessary Euclidean requirements but become a sufficient test of only the positive semidefiniteness of all the principal $3\times3$ submatrices in $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$. The 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 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 §C.2.4) to the sixth and last Euclidean requirement, and so on.

Yet for all values of $N$, only assuming nonnegative $d_{ij}$, the angle matrix inequality in (251) is necessary and sufficient for reconstruction; (§4.3.1)

$$\begin{array}{l}\text{Euclidean axiom 1 (§4.1).}\\ \text{Angle matrix inequality } \Omega \succeq 0 \text{ (191).}\end{array} \;\Leftrightarrow\; \begin{array}{r}-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0\\ D \in \mathbb{S}_\delta^N\end{array} \;\Leftrightarrow\; D = \mathcal{D}(\Omega\,, d) \in \mathbb{EDM}^N \tag{292}$$

Like matrix criteria (175), (250), and (251), the angle matrix inequality and nonnegativity axiom subsume all the Euclidean axioms and further requirements.

### 4.9.3 Path not followed

An alternate and intuitively appealing way to augment the Euclidean axioms is to recognize, in the case $N = 4$, that the three-dimensional analog to triangle & distance is tetrahedron & facet-area, while in the case $N = 5$, the four-dimensional analog to triangle & distance is polychoron & facet-volume, *ad infinitum.*

#### 4.9.3.1 $N = 4$

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: $A_1, A_2, A_3, A_4$. Then analogous to axiom 4, we may write a tight[58] area inequality for the facets

$$\sqrt{A_i} \leq \sqrt{A_j} + \sqrt{A_k} + \sqrt{A_\ell}, \quad i \neq j \neq k \neq \ell \in \{1,2,3,4\} \tag{293}$$

which is a generalized "triangle" inequality [17, §1.1] that follows from

$$\sqrt{A_i} = \sqrt{A_j}\cos\phi_{ij} + \sqrt{A_k}\cos\phi_{ik} + \sqrt{A_\ell}\cos\phi_{i\ell} \tag{294}$$

[51] [34, *Law of Cosines*] where $\phi_{ij}$ is the *dihedral* angle at the common edge between triangular facets $i$ and $j$.

Conveniently, the area-squared of the $i^{\text{th}}$ triangular facet has a formula in terms of $D_i \in \mathbb{EDM}^{N-1}$, the EDM corresponding to that particular facet; from the *Cayley-Menger determinant* for simplices, for $i \in \{1 \ldots N\}$, [34] [52] [43, §4]

$$\begin{aligned} A_i &= \frac{(-1)^{N-1}}{2^{N-2}(N-2)!^2} \det \begin{bmatrix} 0 & \mathbf{1}^T \\ \mathbf{1} & D_i \end{bmatrix} && (295) \\ &= \frac{(-1)^N}{2^{N-2}(N-2)!^2} \det D_i \left(\mathbf{1}^T D_i^{-1} \mathbf{1}\right) && (296) \\ &= \frac{(-1)^N}{2^{N-2}(N-2)!^2} \mathbf{1}^T C_i^T \mathbf{1} && (297) \end{aligned}$$

where $D_i$ is the $i^{\text{th}}$ principal $(N-1) \times (N-1)$ submatrix[59] of $D \in \mathbb{EDM}^N$ (the EDM corresponding to the whole tetrahedron), and $C_i$ is the matrix of *cofactors*[60] [19, §4] corresponding to $D_i$. The number of principal $3 \times 3$ 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 (293) are conditions necessary for $D$ to be an EDM.

[58]The upper bound is met when all angles in (294) are simultaneously zero; that occurs, for example, if one point is relatively interior to the convex hull of the three remaining.

[59]Every principal submatrix of an EDM remains an EDM. [44, §4.1]

[60]Hence $A_i$ is a linear function of the entries of $D_i$; even when $D_i$ is singular.

#### 4.9.3.2 $N = 5$

Moving to the next level, we might encounter a Euclidean object called polychoron, a polyhedron in four dimensions.[61] This polychoron has five $N!/(4!(N-4)!)$ facets, each of them a general tetrahedron whose *volume*-squared $A_i$ is calculated using the same formula; (295) where $D$ is the EDM corresponding to the polychoron, and $D_i$ is the EDM corresponding to the $i^{\text{th}}$ facet (the principal $4\times 4$ submatrix corresponding to the $i^{\text{th}}$ tetrahedron). The analog to triangle & distance is now polychoron & facet-volume. We could then write another generalized "triangle" inequality like (293) but in terms of facet volume;

$$\sqrt{A_i} \leq \sqrt{A_j} + \sqrt{A_k} + \sqrt{A_\ell} + \sqrt{A_m}\,, \quad i \neq j \neq k \neq \ell \neq m \in \{1 \ldots 5\} \tag{298}$$

Now, for $N = 5$, the triangle (distance) inequality (§4.1) and the area inequality (293) and the volume inequality (298) are conditions necessary for $D$ to be an EDM; we do not prove their sufficiency in conjunction with the remaining three axioms.

### 4.9.4 Affine dimension reduction in three dimensions

The determinant of any $M\times M$ matrix is equal to the product of its $M$ eigenvalues. [19, §5.1] When $N=4$ and $\det(\Theta^T\Theta)$ is zero, that means one or more eigenvalues of $\Theta^T\Theta \in \mathbb{R}^{\mathbf{3}\times\mathbf{3}}$ are zero. The determinant will go to zero whenever equality is attained on either side of (174), (290a), or (290b), 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 zero eigenvalues (§4.5.2).

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 (174) or (290a) or (290b). (*confer* §6.3.3, §4.6.3)

**4.9.4.1 Exemplum redux.** We now apply the fifth Euclidean requirement to an earlier problem:

[61] The simplest polychoron is called a pentatope [34]; a regular simplex hence convex. (A *pentahedron* is a three-dimensional object having five vertices.)

**Example.** *Small completion problem*, III. Returning again to the example on page 65 that pertains to Figure 20 where $N=4$ (*confer* §4.7.3), $d_{14}$ is ascertainable from the fifth Euclidean requirement. Because all distances in (172) are known except $\sqrt{d_{14}}$, $\cos\theta_{123}=0$ and $\theta_{324}=0$ result from identity (184). Applying (174),

$$\begin{array}{rcccl} \cos(\theta_{123}+\theta_{324}) & \leq & \cos\theta_{124} & \leq & \cos(\theta_{123}-\theta_{324}) \\ 0 & \leq & \cos\theta_{124} & \leq & 0 \end{array} \tag{299}$$

It follows from (184) that $d_{14}$ can only be 2. Because equality is attained in (299), the affine dimension $r$ cannot exceed $N-2$, as explained. $\square$

## 4.10 $-V_{\mathcal{N}}^T\mathcal{D}(X)V_{\mathcal{N}}$ convexity

In §4.3 we saw that the EDM entries $d_{ij}\left(\begin{bmatrix} x_i \\ x_j \end{bmatrix}\right)$ are convex quadratic functions. Yet $-\mathcal{D}(X)$ (178) is not a quasiconvex function of matrix $X\in\mathbb{R}^{n\times N}$ because the second directional derivative (§2.2.2)

$$-\left.\frac{d^2}{dt^2}\right|_{t=0}\mathcal{D}(X+t\,Y) = 2\left(-\delta(Y^TY)\mathbf{1}^T - \mathbf{1}\delta(Y^TY)^T + 2\,Y^TY\right) \tag{300}$$

is *indefinite* for *any* $Y\in\mathbb{R}^{n\times N}$ since its main diagonal is zero. [25, §4.2.8] [24, §7.1, prob.2] Hence $-\mathcal{D}(X)$ can neither be convex in $X$.

The outcome is different when instead we consider

$$-V_{\mathcal{N}}^T\mathcal{D}(X)V_{\mathcal{N}} = 2V_{\mathcal{N}}^TX^TXV_{\mathcal{N}} \tag{301}$$

where $V_{\mathcal{N}}$ is defined in (199). Matrix-valued function (301) meets the criterion for convexity in §2.2.1.1 over its domain that is all of $\mathbb{R}^{n\times N}$; *videlicet*, for any $Y\in\mathbb{R}^{n\times N}$,

$$-\frac{d^2}{dt^2}V_{\mathcal{N}}^T\mathcal{D}(X+t\,Y)V_{\mathcal{N}} = 4V_{\mathcal{N}}^TY^TYV_{\mathcal{N}} \succeq 0 \tag{302}$$

Quadratic matrix function $-V_{\mathcal{N}}^T\mathcal{D}(X)V_{\mathcal{N}}$ is therefore convex in $X$ achieving its minimum, with respect to the positive semidefinite cone (§3.6.1.1), at $X=\mathbf{0}$. When the penultimate number of points exceeds the dimension of the space $n<N-1$, strict convexity of the quadratic (301) becomes impossible because (302) could not then be positive definite.

### 4.10.1 Inner-product form convexity

In §4.3.1 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 $\theta_{ikj}$. Here the situation for the inner-product form $\mathcal{D}(\Theta)$ (187) of the EDM definition is identical to that in §4.10: $-\mathcal{D}(\Theta)$ is not a quasiconvex function of $\Theta$ by the same reasoning, and

$$-V_{\mathcal{N}}^T\mathcal{D}(\Theta)V_{\mathcal{N}} = \Theta^T\Theta \tag{303}$$

is a convex quadratic function of $\Theta$ on the domain $\mathbb{R}^{n\times N-1}$ achieving its minimum at $\Theta = 0$.

## 4.11 Injectivity of $\mathcal{D}$

The EDM definitions $\mathcal{D}(X)$ (178) and $\mathcal{D}(\Theta)$ (187) are many-to-one maps (§4.4) onto the same range; the EDM cone (§5): independent of dimension $n$,

$$\begin{aligned}\mathbb{EDM}^N &= \left\{\mathcal{D}(X) : \mathbb{R}^{n\times N} \rightarrow \mathbb{S}_\delta^N \mid X\in\mathbb{R}^{n\times N}\right\}\\ &= \left\{\mathcal{D}(\Theta) : \mathbb{R}^{n\times N-1} \rightarrow \mathbb{S}_\delta^N \mid \Theta\in\mathbb{R}^{n\times N-1}\right\}\end{aligned} \tag{304}$$

Substituting (303) back into the inner-product form EDM definition (187), $\mathcal{D}(\Theta)$ may be decomposed:

$$\mathcal{D} = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^T\mathcal{D}V_{\mathcal{N}}\big)\end{bmatrix}\mathbf{1}^T + \mathbf{1}\begin{bmatrix}0 & \delta\big(-V_{\mathcal{N}}^T\mathcal{D}V_{\mathcal{N}}\big)^T\end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & -V_{\mathcal{N}}^T\mathcal{D}V_{\mathcal{N}}\end{bmatrix} \tag{305}$$

This $\mathcal{D}$ is an injective (one-to-one) map of the EDM cone onto itself. Yet when the domain of (305) is instead $\mathbb{S}_\delta^N$, $\mathcal{D}$ becomes an injective map onto that same space $\mathbb{S}_\delta^N$. Proof follows directly from the fact that linear function $\mathcal{D}$ on $\mathbb{S}_\delta^N$ has no nullspace. [53, §A.1]

## 4.12 $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ concavity

Purposefully pedantic, now consider the linear function $g : \mathbb{S}^N \rightarrow \mathbb{S}^{N-1}$,

$$g(D) = -V_{\mathcal{N}}^T D V_{\mathcal{N}} \tag{306}$$

having $\operatorname{dom} g = \mathbb{S}_\delta^N$ and *superlevel sets* (*confer* (38))

$$\mathcal{L}_\nu = \{D\in\mathbb{S}_\delta^N \mid -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq \nu I\} \tag{307}$$

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 $\nu \in \mathbb{R}$ ,

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq \nu I \quad \Leftrightarrow \quad -V_{\mathcal{N}}^T(D - \nu V_{\mathcal{N}}^{\dagger T} V_{\mathcal{N}}^{\dagger})V_{\mathcal{N}} \succeq 0 \tag{308}$$

Then because all the superlevel sets $\mathcal{L}_\nu$ are convex, $g$ must be quasiconcave (§2.2.2) in $D$ on its domain, and because $g$ is concave,[62] all its superlevel sets must be convex (§2.2.3, no.3).

### 4.12.1 Monotonicity

The difference $D_2 - D_1$ belongs to the EDM cone iff $-V_{\mathcal{N}}^T(D_2 - D_1)V_{\mathcal{N}} \succeq 0$ by (250);[63] *id est*,

$$D_1 \underset{\mathbb{EDM}^N}{\preceq} D_2 \quad \Leftrightarrow \quad \left\{ \begin{array}{c} -V_{\mathcal{N}}^T D_1 V_{\mathcal{N}} \underset{\mathbb{S}_+^{N-1}}{\preceq} -V_{\mathcal{N}}^T D_2 V_{\mathcal{N}} \\ \\ D_2 - D_1 \in \mathbb{S}_\delta^N \end{array} \right. \tag{309}$$

This correspondence between the EDM cone and the positive semidefinite cone connotes monotonicity of $g$ (306); in particular, $g(D)$ is nondecreasing on domain $\mathbb{S}_\delta^N$.

## 4.13 EDM-entry compositions

Results of Schoenberg from 1938 can be used to show that certain nonlinear compositions of individual EDM entries yield more EDMs; Laurent [44, §2.3] claims, in particular,

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; 1 - e^{-\alpha D} \triangleq [1 - e^{-\alpha d_{ij}}] \in \mathbb{EDM}^N \quad \forall \alpha > 0 \tag{310}$$

Schoenberg's results suggest that certain finite positive roots of EDM entries produce another EDM; [54, §6, thm.5] [17, §2.8-8] specifically,

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; D^{1/\alpha} \triangleq [d_{ij}^{1/\alpha}] \in \mathbb{EDM}^N \quad \forall \alpha > 1 \tag{311}$$

The special case $\alpha = 2$ (absolute distance) will be of interest in §6.3.1.

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[62] Any linear function must, of course, be simultaneously concave and convex. (The *sub*level sets of $g$ are simply translations of the negative EDM cone).

[63] From (175), any matrix $V$ in place of $V_{\mathcal{N}}$ will satisfy (309) if $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$.

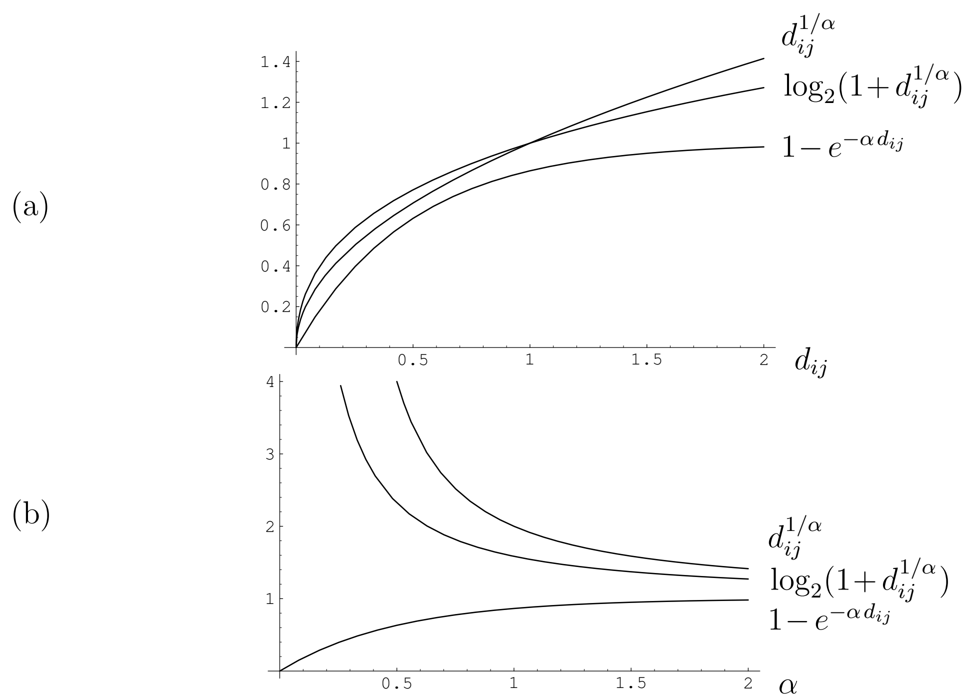



Figure 25: Some entry-wise EDM compositions: (a) $\alpha=2$. Concave nondecreasing in $d_{ij}$. (b) Trajectory convergence in $\alpha$ for $d_{ij}=2$.

Assuming that points constituting a corresponding list $X$ are distinct (239) and because $D \in \mathbb{S}_\delta^N$, then it follows:

$$\lim_{\alpha\to\infty} D^{1/\alpha} \;=\; \lim_{\alpha\to\infty} 1 - e^{-\alpha D} \;=\; -E \triangleq \mathbf{1}\mathbf{1}^T - I \tag{312}$$

Negative elementary matrix $-E$ (§C.8) is interior to the EDM cone (§5.1) and terminal to the respective trajectories (310) and (311) as functions of $\alpha$. Both trajectories never leave the EDM cone; in engineering terms, the EDM cone is an *invariant set* [55] to either trajectory. Further, if $D$ is not an EDM but for some particular $\alpha_o$ it becomes an EDM, then for all greater values of $\alpha$ 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 25 illustrates its concavity in $d_{ij}$ along with the composition functions (310) and (311).

## 4.14 EDM indefiniteness

Any *symmetric* positive semidefinite matrix having a zero entry on its main diagonal must be zero along the entire row and column to which that zero belongs. [25, §4.2.8] [24, §7.1, prob.2] In other words, when $D \in \mathbb{EDM}^N$, there can be no positive nor negative semidefinite EDM except the zero matrix because $\mathbb{EDM}^N \subseteq \mathbb{S}_\delta^N$ (177) and

$$\mathbb{S}_\delta^N \cap \mathbb{S}_+^N = \mathbf{0} \tag{313}$$

the zero matrix. So, there can be no factorization $D = A^TA$ nor $-D = A^TA$. [19, §6.3] Hence the eigenvalues of an EDM are neither all nonnegative nor all nonpositive; an EDM is indefinite and possibly invertible.

### 4.14.1 EDM eigenvalues

For any symmetric $-D$, we can find its rank and characterize its eigenvalues by *congruence transformation*: [19, §6.3]

$$-\begin{bmatrix} V_{\mathcal{N}}^T \\ \frac{1}{\sqrt{2}}\mathbf{1}^T \end{bmatrix} D \begin{bmatrix} V_{\mathcal{N}} & \dfrac{1}{\sqrt{2}}\mathbf{1} \end{bmatrix} \;=\; -\begin{bmatrix} V_{\mathcal{N}}^T D V_{\mathcal{N}} & \frac{1}{\sqrt{2}} V_{\mathcal{N}}^T D\mathbf{1} \\ \frac{1}{\sqrt{2}}\mathbf{1}^T D V_{\mathcal{N}} & \frac{1}{2}\mathbf{1}^T D\mathbf{1} \end{bmatrix} \tag{314}$$

Because $\begin{bmatrix} V_{\mathcal{N}} & \frac{1}{\sqrt{2}}\mathbf{1} \end{bmatrix} \in \mathbb{R}^{N\times N}$ has full rank,

$$\operatorname{rank} D \;=\; \operatorname{rank} \begin{bmatrix} V_{\mathcal{N}}^T \\ \frac{1}{\sqrt{2}}\mathbf{1}^T \end{bmatrix} D \begin{bmatrix} V_{\mathcal{N}} & \dfrac{1}{\sqrt{2}}\mathbf{1} \end{bmatrix} \tag{315}$$

The congruence (314) has the same number of positive, zero, and negative eigenvalues as $-D$. Further, if we denote the eigenvalues of $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$ by $\sigma_i$ , $i=1\ldots N-1$, the eigenvalues of the congruence by $\zeta_i$ , $i=1\ldots N$, and we arrange each respective set of eigenvalues in nonincreasing order, then by theory of *interlacing eigenvalues for bordered symmetric matrices*, [24, §4.3]

$$\zeta_N \le \sigma_{N-1} \le \zeta_{N-1} \le \sigma_{N-2} \le \cdots \le \sigma_2 \le \zeta_2 \le \sigma_1 \le \zeta_1 \tag{316}$$

When $D \in \mathbb{EDM}^N$, $\sigma_i \ge 0$ for all $i$ [24, §7.2] 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; $\zeta_i \ge 0$, $i=1\ldots N-1$. The remaining eigenvalue $\zeta_N$ cannot be nonnegative because then $-D$ would be positive semidefinite, an impossibility; so $\zeta_N < 0$. (*confer* [48, thm.3.1]) By congruence, nontrivial $-D$ must therefore have one and only one negative eigenvalue;

$$\left\{ \begin{array}{l} \lambda(-D)_i \;\ge\; 0\,, \quad i=1\ldots N-1 \\ \sum\limits_{i=1}^{N} \lambda(-D)_i = 0 \end{array} \right. \tag{317}$$

where the $\lambda(-D)_i$ are its eigenvalues whose sum must be zero only because $\operatorname{tr} D = 0$. [19, §5.1]

#### 4.14.2 Spectral cone

Negative EDM eigenvalues $\lambda(-D)$ belong to the particular orthant in $\mathbb{R}^N$ having the $N^{\text{th}}$ coordinate as the sole negative coordinate;

$$\mathbb{R}^N_{N-} \;\stackrel{\Delta}{=}\; \operatorname{cone}\{e_1\ ,\ e_2\ ,\ \cdots\ e_{N-1}\ ,\ -e_N\} \tag{318}$$

The eigenvalue constraints (317) define a spectral pointed polyhedral cone $\mathcal{K}_\lambda$ for $-\mathbb{EDM}^N$:

$$\begin{aligned} \mathcal{K}_\lambda &= \{\lambda \in \mathbb{R}^N \mid \lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_{N-1} \ge 0 \ge \lambda_N\,,\ \mathbf{1}^T\lambda = 0\} \\ &= \mathbb{R}^N_{N-} \cap \partial\mathcal{H} \end{aligned} \tag{319}$$

where

$$\partial\mathcal{H} = \{\lambda \mid \mathbf{1}^T\lambda = 0\} \tag{320}$$

is a hyperplane through the origin. Defining

$$A \triangleq \begin{bmatrix} e_1^T \\ e_2^T \\ \vdots \\ e_{N-1}^T \end{bmatrix} \in \mathbb{R}^{N-1\times N} \tag{321}$$

we are given the halfspace description:

$$\mathcal{K}_\lambda \triangleq \{\lambda \in \mathbb{R}^N \mid A\lambda \succeq 0\,,\ \mathbf{1}^T\lambda = 0\} \tag{322}$$

Because the solution set for $\mathbf{1}^T\lambda = 0$ is equivalent to $\{\lambda \mid \mathbf{1}^T\lambda \geq 0\,,\ \mathbf{1}^T\lambda \leq 0\}$, we have the equivalent halfspace description for the spectral cone:

$$\mathcal{K}_\lambda = \left\{\lambda \in \mathbb{R}^N \mid \begin{bmatrix} A \\ \mathbf{1}^T \\ -\mathbf{1}^T \end{bmatrix}\lambda \succeq 0\right\} \tag{323}$$

and from (155) the vertex description

$$\mathcal{K}_\lambda = \left\{V_{\mathcal{N}}(AV_{\mathcal{N}})^\dagger b \mid b \succeq 0\right\} \tag{324}$$

each providing the succinct EDM matrix criterion,

$$D \in \mathbb{EDM}^N \Leftrightarrow \left\{\begin{array}{l} \lambda(-D) \in \mathcal{K}_\lambda \\ D \in \mathbb{S}^N_\delta \end{array}\right. \tag{325}$$

The vertex description of the dual spectral cone is (107)

$$\mathcal{K}_\lambda^* = \overline{\mathbb{R}^{N*}_{N-} + \partial\mathcal{H}^*} = \left\{\begin{bmatrix} A^T & \mathbf{1} & -\mathbf{1}\end{bmatrix} a \mid a \succeq 0\right\} \subseteq \mathbb{R}^N \tag{326}$$

because any orthant is self-dual, because the dual of any subspace is its orthogonal complement, and because $-e_N$ is conically dependent on the remaining generators;

$$\begin{aligned} \mathbb{R}^{N*}_{N-} &= \left\{\begin{bmatrix} A^T & -e_N\end{bmatrix} a \mid a \succeq 0\right\} \\ \partial\mathcal{H}^* &= \{[\mathbf{1} \quad -\mathbf{1}]\, a \mid a \succeq 0\} \end{aligned} \tag{327}$$

From (156) we have the halfspace description,

$$\mathcal{K}_\lambda^* = \{y \in \mathbb{R}^N \mid (V_{\mathcal{N}}^T A^T)^\dagger V_{\mathcal{N}}^T y \succeq 0\} \tag{328}$$

The dual cone $\mathcal{K}_\lambda^*$ is closed, convex, nonempty, but not pointed because $\mathcal{K}_\lambda$ is empty.

## 4.15 Theorem of the alternative

**Theorem.** *EDM alternative.* [47, §1]
Given $D \in \mathbb{S}^N_\delta$,

$$D \notin \mathbb{EDM}^N \;\Leftrightarrow\; \exists\, z \;\text{ such that }\; \begin{cases} \mathbf{1}^T z = 1 \\ Dz = \mathbf{0} \end{cases} \tag{329}$$

$\diamond$

In words, either $\mathcal{N}(D)$ intersects hyperplane $\{z \mid \mathbf{1}^T z = 1\}$, or $D$ is an EDM; the alternatives are incompatible.

# 5 EDM cone

The set of all EDMs of dimension $N\times N$ forms a closed convex cone $\mathbb{EDM}^N$ in $\mathbb{S}^N_\delta$ because any pair of EDMs (250) satisfies definition (23); *videlicet*, for all $\zeta_1\,,\zeta_2\geq 0$,

$$\begin{array}{c}\zeta_1\,V_{\mathcal{N}}^TD_1V_{\mathcal{N}}+\zeta_2\,V_{\mathcal{N}}^TD_2V_{\mathcal{N}}\succeq 0\\ \zeta_1\,D_1+\zeta_2\,D_2\in\mathbb{S}^N_\delta\end{array}\;\Leftarrow\;\begin{array}{c}V_{\mathcal{N}}^TD_1V_{\mathcal{N}}\succeq 0\,,\quad V_{\mathcal{N}}^TD_2V_{\mathcal{N}}\succeq 0\\ D_1\in\mathbb{S}^N_\delta\,,\quad D_2\in\mathbb{S}^N_\delta\end{array} \tag{330}$$

where $V_{\mathcal{N}}$ was defined in (199). From §4.14, we know that the EDM cone does not intersect the positive semidefinite (PSD) cone except at the origin, their only vertex; there can be no positive nor negative semidefinite EDM. (*confer* (313))

$$\mathbb{EDM}^N\cap\mathbb{S}^N_+ \,=\, \mathbf{0} \tag{331}$$

Even so, the two cones can be related; we revise (250) to emphasize the correspondence between the EDM cone and the PSD cone: for $D\in\mathbb{S}^N_\delta$, (§C.2.3)

$$-\,VDV\in\mathbb{S}^N_+ \;\Leftrightarrow\; D\in\mathbb{EDM}^N \tag{332}$$

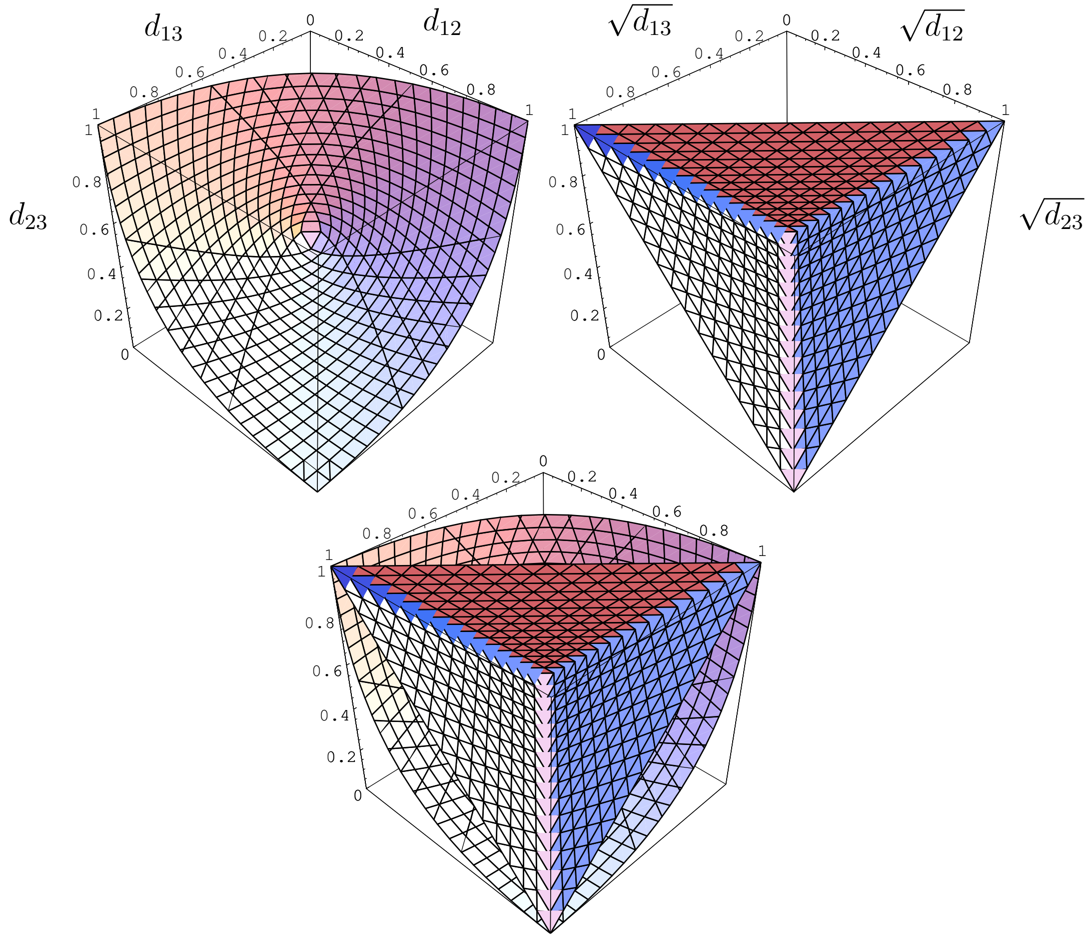
where $V=V_{\mathcal{N}}V_{\mathcal{N}}^\dagger$ ((224), §C.9.3).

**Definition.** *Cone of Euclidean distance matrices.* (*confer* (304)) In the subspace of symmetric hollow matrices $\mathbb{S}^N_\delta$ (18), the set of all Euclidean distance matrices $\mathbb{EDM}^N$ forms a unique immutable proper cone (§3.4.2) called the EDM cone. For $N>0$ (§D),

$$\mathbb{EDM}^N = \left\{D\in\mathbb{S}^N_\delta \mid -VDV\in\mathbb{S}^N_+\right\} \tag{333}$$

$\diamond$

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 27. In the case $N=3$, the Euclidean axioms are necessary and sufficient for reconstructing triangles; (284). Hence the triangle inequality (axiom 4) describes three halfspaces (245) whose intersection makes a polyhedral cone of $\sqrt{d_{ij}}$ in $\mathbb{R}^{\mathbf{3}}$; an isomorphic subspace representation of $\mathbb{EDM}^{\mathbf{3}}$ in the natural coordinates illustrated in Figure 26(b).

(a) 


(b)

(c)

Figure 26: Boundary (tiled) of the cone of Euclidean distance matrices $\mathbb{EDM}^{\mathbf{3}}$ drawn truncated in isomorphic subspace $\mathbb{R}^{\mathbf{3}}$. View is from inside looking toward origin. (Imagine it continuing out of the page.)
(a) EDM cone drawn in the usual distance-squared coordinates $d_{ij}$. It is an ice-cream (second-order) cone whose axis of revolution is the ray in direction $\mathbf{1}$. Unlike the positive semidefinite cone, the EDM cone is not self-dual; the dual EDM cone for this example belongs to isomorphic $\mathbb{R}^{\mathbf{6}}$.
(b) EDM cone drawn in natural coordinates $\sqrt{d_{ij}}$ (in absolute distance) remains convex; the intersection of three halfspaces (245) whose boundaries each contain the origin. The cone geometry becomes complicated (nonpolyhedral) in higher dimension [35, §3] but remains convex in either coordinate system. (§6.3.1)
(c) The two coordinate systems artificially superimposed. The coordinate transformation from $d_{ij}$ to $\sqrt{d_{ij}}$ is a topological contraction.

## 5.1 Boundary of EDM cone

Revising the fundamental matrix criterion for membership to the EDM cone (175),

$$\left.\begin{array}{r} -\operatorname{tr}(zz^T D) \geq 0 \\ \mathbf{1}\mathbf{1}^T zz^T = \mathbf{0} \\ (\|z\| = 1) \\ D \in \mathbb{S}^N_\delta \end{array}\right. \;\Leftrightarrow\; D \in \mathbb{EDM}^N \tag{334}$$

because $\mathcal{N}(\mathbf{1}\mathbf{1}^T) = \mathcal{N}(\mathbf{1}^T)$ and $\mathcal{R}(zz^T) = \mathcal{R}(z)$. When $D \in \mathbb{EDM}^N$, correspondence (334) means $-z^T D z$ is proportional to a nonnegative coefficient of orthogonal projection (§A.3.4) of $-D$ in isomorphic $\mathbb{R}^{N^2}$ on the vectorized range of each and every symmetric normalized[64] dyad (§C.7) in the nullspace of $\mathbf{1}\mathbf{1}^T$ ; *id est*, on (§2.1.1)[65]

$$\operatorname{vec}\left\{zz^T \mid z \in \mathcal{N}(\mathbf{1}\mathbf{1}^T) = \mathcal{R}(V)\right\} \subset \operatorname{vec} \partial\mathbb{S}^N_+ \tag{335}$$

The set of all symmetric rank-one matrices $\{zz^T \mid z \in \mathbb{R}^N\}$ constitute the extreme directions of the positive semidefinite cone (§2.1.3.1), hence lie on its boundary. Yet only symmetric rank-one matrices in $\mathcal{R}(V)$ are involved with the test (334), thus only a portion of the PSD cone boundary is observed.

In the particularly simple case $D \in \mathbb{EDM}^{\mathbf{2}} = \{d_{12} \geq 0\}$, for example, there is only one extreme direction involved (illustrated in Figure 27):

$$zz^T = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{336}$$

The convex cone of EDMs is non-polyhedral in $d_{ij}$ for $N > 2$ [*sic*] because, as Hayden and Wells assert [35, §2], there is a one-to-one correspondence (332) with symmetric hollow matrices positive semidefinite on $\mathcal{N}(\mathbf{1}^T)$; *e.g.*, Figure 26(a). To show that correspondence more clearly, we follow EDM definition (178),

$$\mathcal{D}(B) \;=\; \delta(B)\mathbf{1}^T + \mathbf{1}\delta(B)^T - 2B \;\in \mathbb{EDM}^N \tag{337}$$

[64] The particular norm and norm-constant are arbitrary. The normalization constraint may be removed from (334) and (175); then the constraints remaining become more than what is necessary. (§C.2.2, §C.1)

[65] The vectorized range of the dyads (335) cannot be isomorphic with subspace $\mathcal{R}(V)$ because operator $T(z) = \operatorname{vec}(zz^T)$ is nonlinear. [17, §2.8-8] Hence, orthogonal projection on the vectorized subspace cannot be orthogonal on $\mathcal{R}(V)$.

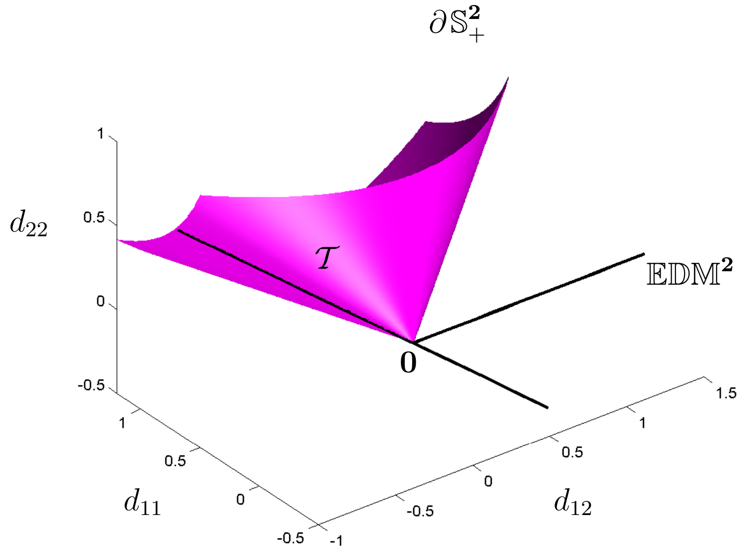



Figure 27: Truncated boundary of positive semidefinite cone $\mathbb{S}^2_+$ in isomorphic $\mathbb{R}^3$. Truncated cone of Euclidean distance matrices $\mathbb{EDM}^2$ in isomorphic subspace $\mathbb{R}$. Relative boundary of EDM cone is constituted solely by matrix $\mathbf{0}$. Half-line $\mathcal{T}=\{\text{vec}(zz^T) \mid z\in\mathcal{N}(\mathbf{1}\mathbf{1}^T)\} = \{t\,[1\ -1\ \ 1]^T \mid t\in\mathbb{R}_+\}$ on PSD cone boundary depicts vectorized range of that single symmetric normalized dyad (336) in the nullspace of $\mathbf{1}\mathbf{1}^T \in \mathbb{R}^{2\times 2}$ on which orthogonal projection of $-D$ in $\mathbb{R}^{2^2}$ (§A.3.4) must be positive semidefinite if $D$ is to belong to $\mathbb{EDM}^2$. Dual EDM cone is halfspace in $\mathbb{R}^3$ having inward-normal $\mathbb{EDM}^2$. (§3.6)

Then the EDM cone may be expressed,

$$\mathbb{EDM}^N = \left\{\mathcal{D}(B) \mid B \in \mathbb{S}_+^N\right\} \tag{338}$$

where this $\mathcal{D}$ is a linear operator, injective because it has no nullspace [53, §A.1] on domain $\mathbb{S}^N$. (*confer* §4.11) Hayden and Wells' assertion can be equivalently stated,

$$\begin{aligned} \mathcal{D}(\mathbb{S}_+^N) &= \mathbb{EDM}^N \\ -V^T\, \mathbb{EDM}^N V &= \mathbb{S}_+^N \end{aligned} \tag{339}$$

because $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$. They further claim:

1. Symmetric hollow matrices positive definite on $\mathcal{N}(\mathbf{1}^T)$ correspond to points interior to the EDM cone.

2. Symmetric hollow matrices positive semidefinite on $\mathcal{N}(\mathbf{1}^T)$ (having at least one 0 eigenvalue) correspond to points on the boundary of the EDM cone.

3. Each symmetric hollow matrix rank-one on $\mathcal{N}(\mathbf{1}^T)$ corresponds to an extreme direction of the EDM cone.

### 5.1.1 Polyhedral bounds

Albeit angles $\theta_{ikj}$ (184) 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 have the partial bound illustrated in Figure 27, while for $N = 3$ we have the partial bounds in Figure 26(b). In the case $N = 4$, angle inequality (290) together with the four Euclidean axioms are necessary and sufficient to reconstruct tetrahedra. (291) The angle inequality provides a regular tetrahedron in $\mathbb{R}^{\mathbf{3}}$ [*sic*] bounding angles $\theta_{ikj}$ at vertex $x_k$ belonging to $\mathbb{EDM}^{\mathbf{4}}$ (Figure 24). (Still, the axiom-4 triangle inequalities corresponding to each principal $3\times 3$ 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 26(b).)

Yet if we were to employ the procedure outlined in §4.9.3 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; $N > 4$.

# 6 Closest EDM

A problem common to various sciences (geodesy, economics, genetics, psychology, biochemistry, astronomy) [35, in cit.] 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 $1 \leq r \leq N-1$ (§3.1.1, §4.5.2) is predetermined, $\rho$. In [56] [57], for example, Trosset applies distance geometry (250) to an important problem in computational chemistry called *molecular conformation* [58] where $H$ represents measurements of interatomic distance. That commonality among the sciences is unified by a new field of mathematics called *multidimensional scaling* [59]; a term formalized by de Leeuw and Heiser in 1982 [60] [42] denoting the reconstruction of a list $X$ in Euclidean space from inter-point distance information.

### three prevalent problems

There are three prevalent statements of the closest-EDM problem in the literature, the multiplicity due primarily to concessions (for hard problems) and indecision characterized by vacillation between the distance-squared variable $d_{ij}$ *versus* absolute distance $\sqrt{d_{ij}}$ or $\Delta_{ij}$; they are, (340)(a), (c), and (d):

$$
\begin{array}{lllllll}
 & \underset{D}{\text{minimize}} & \|-V(D-H)V\|_{\mathrm{F}}^2 & \qquad & \underset{D}{\text{minimize}} & \|-V(\sqrt{D}-H)V\|_{\mathrm{F}}^2 & \\
\text{(a)} & \text{subject to} & \operatorname{rank} VDV \leq \rho & & \text{subject to} & \operatorname{rank} VDV \leq \rho & \text{(b)} \\
 & & D \in \mathbb{EDM}^N & & & D \in \mathbb{EDM}^N & \\
 & & & & & & \\
 & \underset{D}{\text{minimize}} & \|D-H\|_{\mathrm{F}}^2 & & \underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm{F}}^2 & \\
\text{(c)} & \text{subject to} & \operatorname{rank} VDV \leq \rho & & \text{subject to} & \operatorname{rank} VDV \leq \rho & \text{(d)} \\
 & & D \in \mathbb{EDM}^N & & & D \in \mathbb{EDM}^N &
\end{array}
\tag{340}
$$

Of the auxiliary matrices (§C.9) the centering matrix $V$ (§4.5.1) appears in the literature most often. Substitution of $V_{\mathcal{N}}$ in (a) and (b) produces different results... But $V_{\mathcal{N}}^{\dagger}$ and $V_w$ should yield the same as $V$...

We have not seen (340)(b) posed in the literature... Generally speaking, each formulation produces different results... The analytical solution to problem (340)(a) has been known since 1978. We will see that problems (340)(b), (c), and (d) can be formulated as convex optimization problems in the case $\rho = N-1$... Actually, all four problems can be formulated as convex problems...

In deference to absolute distance, we believe *Problem 2* ((340)(d), §6.3) to be the only one properly posed; considered the most difficult for low desired affine dimension.

Unless sufficient information is provided pertaining to absolute location and orientation of $X$, there can be no unique list corresponding to an EDM. (§4.4) Although provision of such information is antithetical, we will consider the inclusion of such constraints...

**background**

We assume the reader to be familiar with [9, §4, §5]; equivalently, the statement of optimization problems and their characterization. [22] [39] [7] [61] [62] [63] [6] [64] It may seem puzzling, at first, why the search for a problem solution ends abruptly with the presentation of the problem itself. The explanation is: typically, we do not seek analytical solution; rather, if the problem can be expressed in *convex form*, then there exist computer programs that provide unique numerical solution. [3] [65] [66] The goal, then, becomes conversion of a given problem to convex form;[66] a *convex optimization problem* is, conventionally, a convex *objective function* with convex inequality constraint functions and with affine equality constraints. [67, §1] As such problem conversions are not always possible, there is much ongoing research to determine what problem classes have convex expressions. [4] [1] [2] [8] [68]

## 6.1 Given measurement matrix $H$

At the very least, we expect measurements of distance to be nonnegative (axiom 1). Ideally, we want the given measurement matrix $H$ to conform with the first three Euclidean axioms (§4.1), to belong to the intersection of the orthant of nonnegative matrices with the symmetric hollow subspace (§2.1.2.1); *id est*, we want $H$ to belong to the convex cone (§3.4.2)

$$\mathcal{K} \triangleq \mathbb{R}_+^{N\times N} \cap \mathbb{S}_\delta^N \tag{341}$$

[66]This means, for example, that the original problem expression might be a minimization of a constrained objective having many local minima. The equivalent convex problem possesses the same global minimum but no local minima.

Membership to $\mathcal{K}$ can greatly simplify a distance problem but, in practice, $H$ can possess significant measurement uncertainty.

Particularly troubling would be the occurrence of negative measurements, the most egregious of errors. Zeroing negative entries effects *unique* (minimum distance) projection on the orthant of nonnegative matrices $\mathbb{R}_+^{N\times N}$ in isomorphic $\mathbb{R}^{N^2}$ (§A.5.1). When $H$ is not symmetric or hollow, taking its symmetric hollow part is equivalent to orthogonal projection on subspace $\mathbb{S}_\delta^N$ (§2.1.2). Since cone $\mathcal{K}$ (341) is the intersection of an orthant with a subspace, we want to project on that subset of the nonnegative orthant contained in the symmetric hollow subspace; on the nonnegative orthant in $\mathbb{S}_\delta^N$ that is, in fact, the intersection. For that reason alone, the unique projection of $H$ on $\mathcal{K}$ (that $\tilde{H}\in\mathcal{K}$ closest to $H$ in $\mathbb{R}^{N^2}$ in the Euclidean sense) can be obtained by first taking the symmetric hollow part, and only then clipping negative entries of the result to zero. (§A.5.2)

## 6.2 First prevalent problem: Projection on PSD cone

We assume only that the given measurement matrix $H$ is symmetric. The first prevalent problem statement poses a projection [5, §3.12] of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ in subspace $\mathbb{S}^{N-1}$ on a $\rho$-subset of the positive semidefinite cone $\mathbb{S}_+^{N-1}$;

$$\left.\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \le \rho\\ & D\in\mathbb{EDM}^N\end{array}\right\}\quad\text{Problem 1}\tag{342}$$

This optimization problem is convex only when desired affine dimension (§4.5.2) is largest $\rho=N-1$ although its analytical solution is known [69] for all $\rho\le N-1$, being first pronounced in the context of multidimensional scaling by Mardia [70] in 1978: Arranging the eigenvalues $\lambda_i$ of $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ in nonincreasing order for all $i$, $\lambda_i\ge\lambda_{i+1}$ with $v_i$ the corresponding $i^{\text{th}}$ eigenvector,

$$-V_{\mathcal{N}}^T H V_{\mathcal{N}} \triangleq \sum_{i=1}^{N-1}\lambda_i\, v_i v_i^T\tag{343}$$

then the optimal solution to Problem 1 is [42, §2]

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} = \sum_{i=1}^{\rho}\max\{0,\,\lambda_i\} v_i v_i^T\tag{344}$$

### 6.2.1 $\rho$-subset

Once optimal $-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}}$ is found, the technique of §4.8 can be used to determine the optimal distance matrix

$$D^\star \in \mathbb{EDM}^N \tag{345}$$

Prior to determination of $D^\star$, this analytical solution (344) is equivalent to the solution of the generic problem,

$$\begin{array}{cl}\underset{B\in\mathbb{S}^{N-1}}{\text{minimize}} & \|B - -V_{\mathcal{N}}^T H V_{\mathcal{N}}\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} B \leq \rho \\ & B \succeq 0\end{array} \tag{346}$$

Hence Problem 1, where $B \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{S}^{N-1}$ and $D \in \mathbb{S}_\delta^N$, is truly a unique 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 $\rho$ ; called *$\rho$-subset* of the positive semidefinite cone.

**6.2.1.1 Proof.** *Closest EDM Problem 1, convex case.* When desired affine dimension is largest, $\rho = N-1$, the rank function disappears from (342); *videlicet*

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T (D-H) V_{\mathcal{N}}\|_{\mathrm{F}}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{347}$$

In those terms, assuming $D \in \mathbb{S}_\delta^N$, the necessary and sufficient conditions (§A.5.1) for unique projection in isomorphic $\mathbb{R}^{(N-1)^2}$ on the self-dual (128) positive semidefinite cone are:[67] (§2.1.1, (574), §3.6.1.1) (*confer* (544))

$$\begin{array}{l}-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} \succeq 0 \\ -V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} \left(-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} + V_{\mathcal{N}}^T H V_{\mathcal{N}}\right) = \mathbf{0} \\ -V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} \;+\; V_{\mathcal{N}}^T H V_{\mathcal{N}} \succeq 0\end{array} \tag{348}$$

Symmetric $-V_{\mathcal{N}}^T H V_{\mathcal{N}}$ is diagonalizable hence decomposable in terms of its eigenvectors $v$ and eigenvalues $\lambda$ as in (343). Therefore,

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} = \sum_{i=1}^{N-1} \max\{0,\, \lambda_i\} v_i v_i^T \tag{349}$$

[67]These conditions for projection on a convex cone are identical to the Karush-Kuhn-Tucker (KKT) optimality conditions for problem (347).

satisfies (348), optimally solving (347). To see that, recall that these eigenvectors constitute an orthogonal set and

$$-V_{\mathcal{N}}^T D^\star V_{\mathcal{N}} + V_{\mathcal{N}}^T H V_{\mathcal{N}} \;=\; -\sum_{i=1}^{N-1} \min\{0,\,\lambda_i\} v_i v_i^T \tag{350}$$

♦

### 6.2.2 Closest EDM Problem 1, non-convex case

It is curious how seemingly non-convex Problem 1 has such a unique analytical solution. In light of §6.2.1 we need only investigate the more general problem, given $A\in\mathbb{S}^{N-1}$ and desired affine dimension $\rho$ ,

$$\begin{array}{cl}\underset{B\in\mathbb{S}^{N-1}}{\text{minimize}} & \|B-A\|_{\mathrm{F}}^2\\ \text{subject to} & \operatorname{rank} B \leq \rho\\ & B\succeq 0\end{array} \tag{351}$$

whose solution was presented in [69, thm.14.4.2] in 1979. In 1997 Trosset [42] first observed equivalence of this problem to projection on the monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$. He generalized the problem and its solution by admitting spectral projection on any convex subset of $\mathcal{K}_{\mathcal{M}+}$; the nature of Trosset's proof was algebraic. Here we derive the known solution for a $\rho$-subset using instead a geometric argument (subsuming the proof in §6.2.1.1):

**6.2.2.1 Proof.** With diagonalization of the unknown $B=U\Upsilon U^T\in\mathbb{S}^{N-1}$ given $1\leq\rho\leq N-1$ and diagonalizable $A=Q\Lambda Q^T\in\mathbb{S}^{N-1}$, an equivalent statement of problem (351) is

$$\begin{array}{cl}\underset{U,\Upsilon}{\text{minimize}} & \|U\Upsilon U^T - Q\Lambda Q^T\|_{\mathrm{F}}^2\\ \text{subject to} & \delta(\Upsilon)\in\mathcal{K}_{\mathcal{M}+}^{\rho}\\ & U^{-1}=U^T\end{array} \tag{352}$$

where $\delta$ is the linear main-diagonal operator (§C.5), and where

$$\mathcal{K}_{\mathcal{M}+}^{\rho} \triangleq \{\upsilon\in\mathbb{R}^{N-1} \mid \upsilon_1\geq\upsilon_2\geq\cdots\geq\upsilon_\rho\geq\upsilon_{\rho+1}=0=\cdots=\upsilon_{N-1}\geq 0\}\subseteq\mathbb{R}_+^{\rho} \tag{353}$$

is a pointed polyhedral cone, a $\rho$-dimensional subset of the monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$ in $\mathbb{R}^{N-1}$ (§3.6.3.1). Because $U$ is assumed orthogonal, problem (352) is equivalent to:

$$\begin{array}{ll} \underset{U,\Upsilon}{\text{minimize}} & \|\Upsilon - U^TQ\Lambda Q^TU\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}+}^{\rho} \\ & U^{-1} = U^T \end{array} \quad \Leftrightarrow \quad \begin{array}{ll} \underset{R,\Upsilon}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}+}^{\rho} \\ & R^{-1} = R^T \end{array} \tag{354}$$

where $R \triangleq Q^TU$ ; meaning, problem (351) is a unique projection of $R^T\Lambda R$ on a $\rho$-subset of the monotone nonnegative cone $\delta(\mathcal{K}_{\mathcal{M}+}^{\rho})$ in isometrically isomorphic $\mathbb{R}^{(N-1)^2}$.[68] Projection can be accomplished by first projecting $R^T\Lambda R$ orthogonally on the $\rho$-dimensional subspace containing $\mathcal{K}_{\mathcal{M}+}^{\rho}$, and then projecting the result on $\mathcal{K}_{\mathcal{M}+}^{\rho}$ itself: (§A.5.2) 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:

$$\begin{array}{ll} \underset{\tilde{R},\tilde{\Upsilon}}{\text{minimize}} & \|\delta(\tilde{\Upsilon}) - \delta(\tilde{R}^T\Lambda\tilde{R})\|^2 \\ \text{subject to} & \delta(\tilde{\Upsilon}) \in \mathcal{K}_{\mathcal{M}+} \\ & R^{-1} = R^T \end{array} \tag{355}$$

where $\delta(\tilde{\Upsilon}) \in \mathbb{R}^{\rho}$,

$$\mathcal{K}_{\mathcal{M}+} = \{\upsilon \mid \upsilon_1 \geq \upsilon_2 \geq \cdots \geq \upsilon_\rho \geq 0\} \subseteq \mathbb{R}_+^{\rho} \tag{146}$$

is dimensionally redefined, and

$$\tilde{R} \triangleq [r_1\ r_2 \cdots r_\rho] \in \mathbb{R}^{N-1\times\rho} \tag{356}$$

constitutes the first $\rho$ columns of orthogonal variable $R$. Because any permutation matrix is an orthogonal matrix, we may always assume $\delta(\tilde{R}^T\Lambda\tilde{R}) \in \mathbb{R}^{\rho}$ is arranged in nonincreasing order; *id est*,

$$\delta(\tilde{R}^T\Lambda\tilde{R})_i \geq \delta(\tilde{R}^T\Lambda\tilde{R})_{i+1}\ , \quad i = 1 \ldots \rho-1 \tag{357}$$

[68] Isometry is a consequence of the fact, [17, §3.2]

$$<\delta(\Upsilon_1)\,,\,\delta(\Upsilon_2)> \;=\; <\Upsilon_1\,,\,\Upsilon_2>$$

meaning, distances are preserved in the map from $\mathbb{R}^{\rho}$ to the vectorization in $\mathbb{R}^{(N-1)^2}$.

Projection of vector $\delta(\tilde{R}^T\Lambda\tilde{R})$ on convex cone $\mathcal{K}_{\mathcal{M}+}$ requires: (§A.5.1, §3.6.3.1)

$$\begin{aligned} X^\dagger\delta(\tilde{\Upsilon}^\star) &\succeq 0 \\ \delta(\tilde{\Upsilon}^\star)^T\Big(\delta(\tilde{\Upsilon}^\star) - \delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)\Big) &= 0 \\ X^T\Big(\delta(\tilde{\Upsilon}^\star) - \delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)\Big) &\succeq 0 \\ R^{\star^{-1}} &= R^{\star T} \end{aligned} \tag{358}$$

where

$$X^{\dagger T} \triangleq [e_1 - e_2 \quad e_2 - e_3 \quad \cdots \quad e_\rho] \in \mathbb{R}^{\rho\times\rho} \tag{147}$$
$$X = [e_1 \quad e_1 + e_2 \quad e_1 + e_2 + e_3 \quad \cdots \quad \mathbf{1}] \in \mathbb{R}^{\rho\times\rho} \tag{151}$$

Any values $\tilde{R}^\star$ and $\tilde{\Upsilon}^\star$ that satisfy conditions (358) are optimal for problem (354). Then the relationship

$$\delta(\tilde{\Upsilon}^\star)_i = \max\{0\,,\ \delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)_i\}\,, \quad i = 1 \ldots \rho \tag{359}$$

specifies an optimal solution. We may choose

$$R^\star = I\ , \qquad \Upsilon^\star_{ii} = \begin{cases} \max\{0\,,\ \Lambda_{ii}\}\,, & i = 1 \ldots \rho \\ 0\,, & i = \rho + 1 \ \ldots\ N-1 \end{cases} \tag{360}$$

♦

### 6.2.3 Problem 1 in spectral norm

When instead we pose the matrix 2-norm (*spectral norm*) in problem (342) for the convex case $\rho = N-1$, then the new problem

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}}\|_2 \\ \text{subject to} & D \in \mathbb{EDM}^N \end{array} \tag{361}$$

is convex although its solution is not necessarily unique because the spectral norm is not a strictly convex function (§2.2.1);[69] giving rise to *oblique* projection (§A) on the positive semidefinite cone. Indeed, its solution set includes

[69]For each and every $|t| \leq 2$, for example, $\begin{bmatrix} 2 & 0 \\ 0 & t \end{bmatrix}$ has the same spectral norm.

the Frobenius solution (344) for the convex case. [9, new§8.1.1, old p.261] *Singular value problem* (361) is equivalent to

$$\begin{array}{ll}\underset{\mu, D}{\text{minimize}} & \mu \\ \text{subject to} & -\mu I \preceq -V_{\mathcal{N}}^T(D-H)V_{\mathcal{N}} \preceq \mu I \\ & D \in \mathbb{EDM}^N \end{array} \tag{362}$$

where

$$\mu^\star = \max_i \left\{ \left|\lambda\left(-V_{\mathcal{N}}^T(D^\star - H)V_{\mathcal{N}}\right)_i\right| \,,\ i=1\ldots N-1 \right\} \tag{363}$$

the maximum absolute *eigen*value (due to matrix symmetry).

For lack of a unique solution here, we prefer the Frobenius rather than spectral norm.

## 6.3 Second prevalent problem: Projection on EDM cone in $\sqrt{d_{ij}}$

Assume we are given a nonnegative measurement matrix

$$H = [h_{ij}] \in \mathbb{R}_+^{N\times N} \tag{364}$$

Let $\Delta = [\Delta_{ij}]$ be an unknown matrix of absolute distance such that $d_{ij} = \Delta_{ij}^2$ ; *id est*,

$$D = [d_{ij}] \overset{\Delta}{=} \Delta \circ \Delta \in \mathbb{EDM}^N \tag{365}$$

where $\circ$ denotes the Hadamard product. The original statement of the second closest-EDM problem has been considered difficult to solve, in the past, in any desired affine dimension $\rho$ (232) because the problem's objective function

$$\sum_{i,j}(\Delta_{ij} - h_{ij})^2 \;=\; \|\Delta - H\|_{\mathrm{F}}^2 \tag{366}$$

is expressed distinctly in the natural coordinates (absolute distance) with respect to the constraints:

$$\left.\begin{array}{ll}\underset{\Delta}{\text{minimize}} & \|\Delta - H\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T(\Delta\circ\Delta)V_{\mathcal{N}} \leq \rho \\ & \Delta\circ\Delta \in \mathbb{EDM}^N \end{array}\right\} \quad \text{Problem 2} \tag{367}$$

Although not obvious, this second prevalent (non-convex) problem is a projection of $H$ in the natural coordinates on a $\rho$-subset of the convex cone of Euclidean distance matrices $\mathbb{EDM}^N$ in subspace $\mathbb{S}^N_\delta$. (Figure 26(b), §6.3.1)

When $\rho = N-1$, the rank constraint disappears but a non-convex problem remains:

$$\begin{array}{ll}\underset{\Delta}{\text{minimize}} & \sum_{i,j} \Delta_{ij}^2 - 2h_{ij}\,\Delta_{ij} \;+\; h_{ij}^2 \\ \text{subject to} & \Delta\circ\Delta \in \mathbb{EDM}^N\end{array} \tag{368}$$

Problem (368) is transformed to an equivalent convex problem via the substitution $\sqrt{d_{ij}} \leftarrow \Delta_{ij}$ : [71] [49, §13.6]

$$\sum_{i,j} d_{ij} - 2h_{ij}\sqrt{d_{ij}} \;+\; h_{ij}^2 \;\leftarrow\; \sum_{i,j} \Delta_{ij}^2 - 2h_{ij}\,\Delta_{ij} \;+\; h_{ij}^2 \tag{369}$$

For any given $i$ 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 because $d_{ij} + h_{ij}^2$ is affine (convex). Because the sum of any number of convex functions in $D$ remains convex [9, §3] and because the *feasible set*[70] is convex in $D$, we get a convex problem for $\rho = N-1$

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \sum_{i,j} d_{ij} - 2h_{ij}\sqrt{d_{ij}} \;+\; h_{ij}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{370}$$

equivalent to non-convex problem (368).

The existence of a unique (global) solution $D^\star$ for this second prevalent problem depends upon $H$ being nonnegative.

#### 6.3.1 EDM cone in $\sqrt{d_{ij}}$ remains convex

Defining the entry-wise square root matrix,

$$\sqrt{D} \triangleq \Delta = [\sqrt{d_{ij}}\,] \tag{371}$$

we have the convex optimization problem equivalent to (370) whose objective is expressed in the natural (absolute distance $\sqrt{d_{ij}}$ ) coordinates: for

[70]The feasible set of an optimization problem is the set of all variable values, belonging to the intersection of the objective and constraint function domains, that satisfy all the constraints.

nonnegative $H$,

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm F}^2\\ \text{subject to} & D\in\mathbb{EDM}^N\end{array}\tag{372}$$

The *Bunt-Motzkin theorem* asserts: (§A.5) If $\mathcal{C}\subseteq\mathbb{R}^n$ is a nonempty and closed set and if for every $x$ in $\mathbb{R}^n$ there is a unique Euclidean projection of $x$ on $\mathcal{C}$, then $\mathcal{C}$ is convex. We hypothesize that theorem to be applicable without loss of generality (for all $N>0$) to the projection posed in (372) for every $H\in\mathbb{R}_+^{N\times N}$ because $\mathbb{EDM}^N\subset\mathbb{R}_+^{N\times N}$. Problem (372) is an orthogonal projection of $H$ (in the natural coordinates) in isomorphic $\mathbb{R}^{N^2}$ on the cone of Euclidean distance matrices. Uniqueness of projection is guaranteed by the Frobenius norm that is a strictly convex function. [9, old§6.1] By the theorem, that uniqueness implies the EDM cone remains convex when represented in the natural coordinates; call it

$$\sqrt{\mathbb{EDM}}^N \triangleq \{\,[\sqrt{d_{ij}}\,]\mid D=[d_{ij}]\in\mathbb{EDM}^N\}\tag{373}$$

Schoenberg's discoveries in 1938 about isomorphic metric spaces [54, §6] (*confer* §4.13) imply that $\sqrt{\mathbb{EDM}}^N$ is identical to $\mathbb{EDM}^N$ to within an isometric isomorphism (§2.1.1.1)...[71] We infer, $\sqrt{\mathbb{EDM}}^N$ is a proper cone; *id est*, the EDM cone remains a nonempty pointed closed convex cone when represented in the natural coordinates. (We had a hint of this for $N=2$ in Figure 27 and for $N=3$ in Figure 26.)

### 6.3.2 Equivalent semidefinite program, Problem 2

Convex problem (370) (hence (372)) is easily solved for its global minimum by any *interior point method* [22] [8] [72] [73] and requires no further modification. Nevertheless, we translate (370) to an equivalent *semidefinite program* (SDP) for a pedagogical reason that will become clear in §6.3.3. Substituting a new matrix variable $Y=[y_{ij}]$,

$$y_{ij}\leftarrow h_{ij}\sqrt{d_{ij}}\tag{374}$$

[71]Using Schoenberg's terminology, the $n$-dimensional Euclidean space having the Euclidean metric raised to the 1/2 power on it is a metric space "imbeddable" [17, §2.8-8] in a real Hilbert space.

we propose that (370) and (372) are each equivalent to the SDP

$$\begin{array}{ll}\underset{D,Y}{\text{minimize}} & \sum\limits_{i,j} d_{ij} - 2y_{ij} + h_{ij}^2 \\ \text{subject to} & \begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0, \quad i,j=1\ldots N \\ & D \in \mathbb{EDM}^N \end{array} \tag{375}$$

To see that, recall $d_{ij} \geq 0$ is implicit (§4.6.1) to $D \in \mathbb{EDM}^N$ (250). So when $h_{ij}$ is nonnegative,

$$\begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0 \;\Leftrightarrow\; h_{ij}\sqrt{d_{ij}} \geq \sqrt{y_{ij}^2} \tag{376}$$

Because negative $y_{ij}$ will not minimize the objective function, nonnegativity of $y_{ij}$ is implicit in (375). Further, minimization of the objective function implies maximization of $y_{ij}$ that is bounded above. Hence, as desired, $y_{ij} \to h_{ij}\sqrt{d_{ij}}$ as optimization proceeds.

If the given matrix $H$ is nonnegative and symmetric,

$$H = [h_{ij}] \in \mathbb{R}_+^{N\times N} \cap \mathbb{S}^N \tag{377}$$

then $Y = H \circ \sqrt{D}$ must belong to $\mathbb{R}_+^{N\times N} \cap \mathbb{S}_\delta^N$. Then because, for $Y \in \mathbb{S}_\delta^N$, (§C.9.3)

$$\|\sqrt{D} - H\|_{\mathrm{F}}^2 \;=\; \sum_{i,j} d_{ij} - 2y_{ij} + h_{ij}^2 \;=\; -N \operatorname{tr}\Big(V_{\mathcal{N}}^\dagger (D - 2\,Y) V_{\mathcal{N}}\Big) + \sum_{i,j} h_{ij}^2 \tag{378}$$

convex problem (375) is equivalent to the SDP

$$\begin{array}{ll}\underset{D,Y}{\text{minimize}} & -\operatorname{tr}\Big(V_{\mathcal{N}}^\dagger (D - 2\,Y) V_{\mathcal{N}}\Big) \\ \text{subject to} & \begin{bmatrix} d_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0, \quad j > i = 1\ldots N-1 \\ & Y \in \mathbb{S}_\delta^N \\ & D \in \mathbb{EDM}^N \end{array} \tag{379}$$

where the constants $h_{ij}^2$ have been arbitrarily dropped from the objective.

### 6.3.3 Minimization of affine dimension in Problem 2

When the desired affine dimension $\rho$ is diminished, the rank function becomes reintroduced into problem (375) that is then rendered difficult to solve because the feasible set loses convexity in $\mathbb{S}_\delta^N$. Indeed, the rank function is quasiconcave (§2.2.2); meaning, its superlevel sets [9, old§2.1.6] (*confer* (38)) are convex. A remedy developed in [74] [75] [76] introduces the *convex envelope* (cenv) of the rank function. 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 $\mathcal{C}$. The convex envelope of the rank function is proportional to the trace function when its argument is constrained to be symmetric and positive semidefinite. The trace thus represents the best convex lower bound on rank.

Substituting the rank envelope for the rank function in Problem 2, for $D\in\mathbb{EDM}^N$,

$$\operatorname{cenv}\operatorname{rank}(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \operatorname{cenv}\operatorname{rank}(-V_{\mathcal{N}}^\dagger D V_{\mathcal{N}}) \;\propto\; -\operatorname{tr}(V_{\mathcal{N}}^\dagger D V_{\mathcal{N}}) \tag{380}$$

and for $\rho\leq N-1$, $\sqrt{D}=[\sqrt{d_{ij}}\,]$ as in (371), and nonnegative $H$, we have the convex optimization problem

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \|\sqrt{D}-H\|_{\mathrm{F}}^2\\ \text{subject to} & -\operatorname{tr}(V_{\mathcal{N}}^\dagger D V_{\mathcal{N}})\leq\kappa\,\rho\\ & D\in\mathbb{EDM}^N\end{array} \tag{381}$$

where $\kappa\in\mathbb{R}_+$ is a constant determined by cut and try. The equivalent SDP makes $\kappa$ variable: for nonnegative symmetric $H$,

$$\begin{array}{cl}\underset{D,Y,\kappa}{\text{minimize}} & \kappa\,\rho+2\operatorname{tr}(V_{\mathcal{N}}^\dagger Y V_{\mathcal{N}})\\ \text{subject to} & \begin{bmatrix} d_{ij} & y_{ij}\\ y_{ij} & h_{ij}^2\end{bmatrix}\succeq 0, \quad j>i=1\ldots N-1\\ & -\operatorname{tr}(V_{\mathcal{N}}^\dagger D V_{\mathcal{N}})\leq\kappa\,\rho\\ & Y\in\mathbb{S}_\delta^N\\ & D\in\mathbb{EDM}^N\end{array} \tag{382}$$

which is the same as (379). As the problem is stated, the desired affine dimension $\rho$ yields to the variable scale factor $\kappa$; $\rho$ is effectively ignored. Yet the result is an illuminant for (379) and it equivalents; when the given measurement matrix $H$ is nonnegative and symmetric, finding the closest EDM $D$ as in problem (370), (372), (375), or (379) implicitly entails minimization of affine dimension (*confer* §4.6.3, §4.9.4). In other words, those problems are each inherently equivalent to problem (382).

### 6.3.4 Quasiconcavity of $-V_{\mathcal{N}}^T\sqrt{D}\,V_{\mathcal{N}}$

Now consider the function $g : \mathbb{S}^N \to \mathbb{S}^{N-1}$, for $\sqrt{D} = [\sqrt{d_{ij}}\,]$ (371), (*confer* §4.12)

$$g(D) \;=\; -V_{\mathcal{N}}^T\sqrt{D}\,V_{\mathcal{N}} \tag{383}$$

having $\operatorname{dom} g = \mathbb{EDM}^N$ and superlevel sets

$$\mathcal{L}_\nu \;=\; \{D \in \mathbb{EDM}^N \mid -V_{\mathcal{N}}^T\sqrt{D}\,V_{\mathcal{N}} \succeq \nu I\,\} \tag{384}$$

Assuming validity of (311),

$$-\,V_{\mathcal{N}}^T\sqrt{D}\,V_{\mathcal{N}} \succeq 0 \;\Leftarrow\; D \in \mathbb{EDM}^N \tag{385}$$

and given

$$\sqrt{D} \in \sqrt{\mathbb{EDM}}^N \;\Leftrightarrow\; D \in \mathbb{EDM}^N \tag{386}$$

that is self evident, nonlinear function $g$ therefore has superlevel sets $\mathcal{L}_\nu$ equal to the intersection of the nonnegative orthant $\mathbb{R}_+^{N\times N}$ with translations of $\mathbb{EDM}^N$ in $\mathbb{S}^N$; *videlicet*, for each and every $\nu \in \mathbb{R}$,

$$-\,V_{\mathcal{N}}^T\sqrt{D}\,V_{\mathcal{N}} \succeq \nu I \;\;\Leftrightarrow\;\; -V_{\mathcal{N}}^T\Big(\sqrt{D} - \nu\, V_{\mathcal{N}}^{\dagger T} V_{\mathcal{N}}^{\dagger}\Big)V_{\mathcal{N}} \succeq 0 \tag{387}$$

Because all the superlevel sets are convex, then $g$ must be quasiconcave (§2.2.2) in $D$ on its domain.

### 6.3.5 Constraint on affine dimension, alternating projection

When one desires affine dimension $\rho$ diminished further below what can be achieved via rank minimization as in (382) or equivalently (379), one resorts to the numerical technique known as *alternating projection.* [56, §2.2] [42, §3.1] [2] [77] Specifically, we solve the following two-phase problem sequence in

$$(k, j) = \{0 \ldots \infty\} \times \{0, 1\} \tag{388}$$

until convergence: given measurement matrix $H \in \mathbb{R}_+^{N\times N} \cap \mathbb{S}^N$, $\rho < N-1$, and $\sqrt{D}^{(0,1)} = H$,

$$\left.\begin{array}{ll}\underset{\Delta}{\text{minimize}} & \|\Delta - \sqrt{D}^{(k,1)}\|_\mathrm{F}^2\\ \text{subject to} & \Delta\circ\Delta \in \mathbb{EDM}^N\end{array}\right\}\quad j=0$$

$$\left.\begin{array}{ll}\underset{D}{\text{minimize}} & \|-V_\mathcal{N}^T\left(\sqrt{D} - \Delta^{(k,0)}\right)V_\mathcal{N}\|_\mathrm{F}^2\\ \text{subject to} & \operatorname{rank} V_\mathcal{N}^T D V_\mathcal{N} \le \rho\\ & D \in \mathbb{EDM}^N\end{array}\right\}\quad j=1 \tag{389}$$

Assuming (385) is correct,

$$\Delta \in \mathbb{EDM}^N \Leftarrow \Delta\circ\Delta \in \mathbb{EDM}^N \tag{390}$$

so the phase-1 objective is formulated in terms of $\sqrt{D}$ instead of $D$ as in Problem 1 (342); problem (389,1) is a projection of $-V_\mathcal{N}^T\Delta^{(k,0)}V_\mathcal{N}$ (in the natural coordinates $\sqrt{d_{ij}}$ ) on a $\rho$-subset (§6.2.1) of the positive semidefinite cone.

Phase 0. Problem (389,0) is the unique projection of absolute distance $\sqrt{D}^{(k,1)}$ on the EDM cone in the natural coordinates; the same as (372) and equivalent to (379) hence easily solved.

Phase 1. Because of the close correspondence between the boundaries of the PSD and EDM cones (§5.1), projection of $-V_\mathcal{N}^T\Delta^{(k,0)}V_\mathcal{N}$ on the PSD cone in (389,1) corresponds to projection of $\Delta^{(k,0)}$ on the EDM cone... Yet projection that is minimum-distance to the PSD cone does not necessarily mean that the corresponding projection on the EDM cone must also be... So, problem (389,1) can be interpreted as an oblique projection of $\Delta^{(k,0)}$ in the natural coordinates on that non-convex subset of the EDM cone comprising all EDMs whose corresponding lists $X$ have affine dimension no greater than $\rho$. (§4.5.2) When $\rho < N-1$, that subset belongs to the boundary of the EDM cone.

and so on...

Non-convex set. No guarantee of global optimal solution. [57] adds constraints to $X$ to limit the number of generating lists...

## 6.4 Third prevalent problem: Projection on EDM cone in $d_{ij}$

Assume the given measurement matrix $H$ to be nonnegative (§6.1) as in (364). Reformulating Problem 2 in terms of EDM $D$ changes the problem considerably:

$$\left.\begin{array}{ll}\underset{D}{\text{minimize}} & \|D-H\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq \rho \\ & D \in \mathbb{EDM}^N\end{array}\right\} \quad \text{Problem 3} \tag{391}$$

This third prevalent non-convex problem is a projection of $H$ on a $\rho$-subset of the convex cone of Euclidean distance matrices $\mathbb{EDM}^N$ in subspace $\mathbb{S}_\delta^N$ (Figure 26(a)). Because the coordinates of projection are distance-squared and $H$ now holds distance-squared measurements, the solution to Problem 3 is generally different than that of Problem 2. We speculate this third problem to be prevalent only because it was thought easier to solve than Problem 2.

When the subset is the entire EDM cone, $\rho = N-1$, this third problem becomes obviously convex because the objective function

$$\|D-H\|_{\mathrm{F}}^2 = \sum_{i,j}(d_{ij}-h_{ij})^2 \tag{392}$$

is a strictly convex quadratic in $D$ ((11)(34)§F.2) [9, old§6.1];

$$\begin{array}{ll}\underset{D}{\text{minimize}} & \sum\limits_{i,j} d_{ij}^2 - 2h_{ij}\,d_{ij} + h_{ij}^2 \\ \text{subject to} & D \in \mathbb{EDM}^N\end{array} \tag{393}$$

In the past, this convex problem was solved numerically by means of alternating projection. [78] [79] [35, §1] Despite more efficient contemporary methods of solution, we choose to translate (393) to an equivalent SDP because we have a good SDP solver. We will use the same substitution technique as for the second prevalent problem:

### 6.4.1 Equivalent semidefinite programs

Now assume the given measurement matrix $H$ to be nonnegative and symmetric as in (377). For $Y = [y_{ij}]$, and $\partial \triangleq [d_{ij}^2] = D \circ D$ distance-square squared, we substitute

$$\begin{aligned} y_{ij} &\leftarrow h_{ij}\, d_{ij} \\ \partial_{ij} &\leftarrow d_{ij}^2 \end{aligned} \tag{394}$$

Similarly to the development in §6.3.2, we then propose: problem (393) is equivalent to the SDP, (*confer* (378))

$$\begin{array}{cl} \underset{\partial\,,\,Y}{\text{minimize}} & -\operatorname{tr}\Big(V_{\mathcal{N}}^{\dagger}(\partial - 2\,Y)V_{\mathcal{N}}\Big) \\ \text{subject to} & \begin{bmatrix} \partial_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0, \quad j > i = 1 \ldots N-1 \\ & \dfrac{Y}{H} \in \mathbb{EDM}^N \\ & \partial \in \mathbb{S}_\delta^N \cap \mathbb{R}_+^{N\times N} \end{array} \tag{395}$$

where $Y/H \overset{\Delta}{=} [y_{ij}/h_{ij}]$, $h_{ij} \neq 0$. For the same reasons as before, (*confer* (376))

$$\begin{bmatrix} \partial_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0 \;\Leftrightarrow\; h_{ij}\, d_{ij} \geq \sqrt{y_{ij}^2}\;, \quad \partial_{ij} \geq 0 \tag{396}$$

and $y_{ij} \rightarrow h_{ij}\, d_{ij}$ as optimization proceeds. The striking similarity of problem (395) to (379) cannot go unnoticed, but the possibility of division by zero here is problematic.

#### 6.4.1.1 Schur-form semidefinite program.

The division in problem (395) motivates another formulation: Moving the objective function to the constraints in (393) makes an equivalent *second-order cone program.*

$$\begin{array}{cl} \underset{D,\,t}{\text{minimize}} & t \\ \text{subject to} & \|D - H\|_{\mathrm{F}} \leq t \\ & D \in \mathbb{EDM}^N \end{array} \tag{397}$$

We can transform this problem to an equivalent semidefinite program via matrix vectorization (§2.1.1); [80]

$$\begin{array}{cl} \underset{D,\,t}{\text{minimize}} & t \\ \text{subject to} & \begin{bmatrix} tI & \operatorname{vec}(D-H) \\ \operatorname{vec}^T(D-H) & t \end{bmatrix} \succeq 0 \\ & D \in \mathbb{EDM}^N \end{array} \tag{398}$$

a program that follows from the Schur complement (§C.3), and characterized by great sparsity which strongly suggests that an even simpler representation of this problem exists. Yet the projection on distance-squared data has lost its intuitive appeal.

### 6.4.2 Minimization of affine dimension in Problem 3

When the desired affine dimension $\rho$ is diminished, problem (391) is difficult to solve [35, §3] because the feasible set loses convexity in $\mathbb{R}^{N(N-1)/2}$. Substituting the rank envelope into Problem 3 (as for Problem 2 in §6.3.3), for nonnegative $H$ we have

$$\begin{array}{cl} \underset{D}{\text{minimize}} & \|D-H\|_{\mathrm{F}}^2 \\ \text{subject to} & -\operatorname{tr}(V_{\mathcal{N}}^\dagger D V_{\mathcal{N}}) \leq \kappa\,\rho \\ & D \in \mathbb{EDM}^N \end{array} \tag{399}$$

where here $\kappa \in \mathbb{R}_+$ is a constant that can be determined by cut and try. Problem (399) is a convex optimization problem in any affine dimension $\rho$; an approximation to the projection on that subset of the EDM cone containing EDMs with corresponding affine dimension no greater than $\rho$.
... for nonnegative symmetric $H$,

$$\begin{array}{cl} \underset{\partial\,,\,Y}{\text{minimize}} & -\operatorname{tr}\Big(V_{\mathcal{N}}^\dagger(\partial - 2\,Y)V_{\mathcal{N}}\Big) \\ \text{subject to} & \begin{bmatrix} \partial_{ij} & y_{ij} \\ y_{ij} & h_{ij}^2 \end{bmatrix} \succeq 0\,, \quad j>i=1\ldots N-1 \\ & -\operatorname{tr}(V_{\mathcal{N}}^\dagger \dfrac{Y}{H} V_{\mathcal{N}}) \leq \kappa\,\rho \\ & \dfrac{Y}{H} \in \mathbb{EDM}^N \\ & \partial \in \mathbb{S}_\delta^N \cap \mathbb{R}_+^{N\times N} \end{array} \tag{400}$$

We do not see the equivalence of this rank-constrained problem to problems (393) and (395) like we saw for its counterpart (382) in Problem 2.

### 6.4.3 alternating projections for a lower-rank solution

...

### 6.4.4 Projection interpretation of Problem 3

Assume only that measurement matrix $H$ is symmetric. Proof closely follows §6.2.2.1.

$$\left.\begin{array}{ll}\underset{D}{\text{minimize}} & \|-D - -H\|_{\mathrm{F}}^2 \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^T D V_{\mathcal{N}} \leq \rho \\ & D \in \mathbb{EDM}^N \end{array}\right\} \quad \text{Problem 3} \tag{391}$$

**6.4.4.1 Proof.** With diagonalization of the unknown EDM $D$,

$$-D \stackrel{\Delta}{=} U \Upsilon U^T \in \mathbb{S}_\delta^N \tag{401}$$

given diagonalizable $H \in \mathbb{S}^N$ with $-H \stackrel{\Delta}{=} Q\Lambda Q^T$ and given desired affine dimension $1 \leq \rho \leq N-1$, Problem 3 is equivalently stated:

$$\begin{array}{ll}\underset{U,\Upsilon}{\text{minimize}} & \|U\Upsilon U^T - Q\Lambda Q^T\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_\lambda^\varphi \\ & U^{-1} = U^T \\ & \delta(U\Upsilon U^T) = \mathbf{0} \end{array} \tag{402}$$

where $\varphi \stackrel{\Delta}{=} \operatorname{rank} D \leq \rho + 1 \leq N$ (p.77) conservatively relates $\rho$ to $\varphi$, and where

$$\mathcal{K}_\lambda^\varphi \stackrel{\Delta}{=} \{\lambda \in \mathbb{R}^N \mid \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{\varphi-1} \geq \lambda_\varphi = 0 = \cdots = \lambda_{N-1} \geq 0 \geq \lambda_N \,,\ \mathbf{1}^T\lambda = 0\} \subset \mathbb{R}^\varphi \tag{403}$$

is a pointed polyhedral cone, a $\varphi$-dimensional subset of the spectral cone $\mathcal{K}_\lambda$ for $-\mathbb{EDM}^N$ (323). Because $U$ is assumed orthogonal, problem (402) is equivalent to:

$$\begin{array}{ll}\underset{R,\Upsilon}{\text{minimize}} & \|\Upsilon - R^T\Lambda R\|_{\mathrm{F}}^2 \\ \text{subject to} & \delta(\Upsilon) \in \mathcal{K}_\lambda^\varphi \\ & R^{-1} = R^T \\ & \delta(QR\Upsilon R^T Q^T) = \mathbf{0} \end{array} \tag{404}$$

where $R \stackrel{\Delta}{=} Q^T U \in \mathbb{R}^{N\times N}$; meaning, Problem 3 is a unique projection of $R^T\Lambda R$ on a $\varphi$-subset of the spectral cone $\delta(\mathcal{K}_\lambda^\varphi)$ in isometrically isomorphic $\mathbb{R}^{N^2}$. Projection can be accomplished by first projecting $R^T\Lambda R$ orthogonally on the $\varphi$-dimensional subspace containing $\mathcal{K}_\lambda^\varphi$ , and then projecting the result on $\mathcal{K}_\lambda^\varphi$ itself: (§A.5.2) Projection on that subspace amounts to zeroing all entries of $R^T\Lambda R$ off its main diagonal and the $\varphi^{\text{th}}$ through $N-1^{\text{th}}$ entries along its main diagonal. Then we have the equivalent problem:

$$\begin{array}{cl}\underset{\tilde{R},\tilde{\Upsilon}}{\text{minimize}} & \|\delta(\tilde{\Upsilon})-\delta(\tilde{R}^T\Lambda\tilde{R})\|^2\\ \text{subject to} & \delta(\tilde{\Upsilon})\in\mathcal{K}_\lambda\\ & R^{-1}=R^T\\ & \delta(QR\Upsilon R^TQ^T)=\mathbf{0}\end{array}\tag{405}$$

where

$$\delta(\tilde{\Upsilon})\triangleq\begin{bmatrix}\Upsilon_{11}\\ \Upsilon_{22}\\ \vdots\\ \Upsilon_{\varphi-1,\varphi-1}\\ \Upsilon_{NN}\end{bmatrix}\in\mathbb{R}^\varphi\tag{406}$$

where

$$\mathcal{K}_\lambda=\{\lambda\in\mathbb{R}^\varphi\mid\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_{\varphi-1}\geq 0\geq\lambda_\varphi\,,\ \mathbf{1}^T\lambda=0\}\subset\mathbb{R}^\varphi\tag{319}$$

is dimensionally redefined, and where

$$\tilde{R}\triangleq[r_1\ r_2\cdots r_{\varphi-1}\ r_N]\in\mathbb{R}^{N\times\varphi}\tag{407}$$

constitutes the first $\varphi-1$ columns and last column of orthogonal variable $R$. When $\varphi=N$, then $\tilde{R}=R$. Because any permutation matrix is an orthogonal matrix, we may always assume $\delta(\tilde{R}^T\Lambda\tilde{R})\in\mathbb{R}^\varphi$ to be arranged in nonincreasing order; *id est*,

$$\delta(\tilde{R}^T\Lambda\tilde{R})_i\geq\delta(\tilde{R}^T\Lambda\tilde{R})_{i+1}\ ,\quad i=1\ldots\varphi-1\tag{408}$$

Projection of vector $\delta(\tilde{R}^T\Lambda\tilde{R})$ on convex cone $\mathcal{K}_\lambda$ requires: (§A.5.1, §4.14.2)

$$\begin{aligned}
\begin{bmatrix} A \\ \mathbf{1}^T \\ -\mathbf{1}^T \end{bmatrix}\delta(\tilde{\Upsilon}^\star) &\succeq 0 && \text{(a)}\\
\delta(\tilde{\Upsilon}^\star)^T\Big(\delta(\tilde{\Upsilon}^\star)-\delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)\Big) &= 0 && \text{(b)}\\
(\tilde{V}_{\mathcal{N}}^T A^T)^\dagger\,\tilde{V}_{\mathcal{N}}^T\Big(\delta(\tilde{\Upsilon}^\star)-\delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)\Big) &\succeq 0 && \text{(c)}\\
\delta\big(QR^\star\Upsilon^\star R^{\star T}Q^T\big) &= \mathbf{0} && \text{(d)}\\
{R^\star}^{-1} &= R^{\star T} && \text{(e)}
\end{aligned} \tag{409}$$

where, for $\tilde{V}_{\mathcal{N}}\in\mathbb{R}^{\varphi\times\varphi-1}$,

$$A = \begin{bmatrix} I & \mathbf{0} \end{bmatrix} \in \mathbb{R}^{\varphi-1\times\varphi} \qquad (321) \tag{410}$$

$$(\tilde{V}_{\mathcal{N}}^T A^T)^\dagger\,\tilde{V}_{\mathcal{N}}^T = \begin{bmatrix} I & -\mathbf{1} \end{bmatrix} \in \mathbb{R}^{\varphi-1\times\varphi} \tag{411}$$

Any values $\tilde{R}^\star$ and $\Upsilon^\star$ that satisfy conditions (409) are optimal for problem (404). Then the relationship...

$$\delta(\tilde{\Upsilon}^\star)_i = \left\{\begin{array}{ll} \max\{0\,,\ \delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)_i\}\,, & i=1\ldots\varphi-1 \\ -\sum\limits_{j=1}^{\varphi-1}\max\{0\,,\ \delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)_j\}\,, & i=\varphi \end{array}\right. \tag{412}$$

specifies an optimal solution provided (409)(d) and (e) are satisfied and $r_\varphi^\star$ is chosen so

$$\delta(\tilde{R}^{\star T}\Lambda\tilde{R}^\star)_\varphi = \delta(\tilde{\Upsilon}^\star)_\varphi \tag{413}$$

satisfies complementarity condition (409)(b)... ♦

# 7 EDM completion

inequality constraints only; no fixed data...

applications in [44, in cit.]...

barrier problem...

Intriguing is the question of whether the list in $X$ may be reconstructed given an incomplete EDM. We have already examined this problem for a small example given on page 65 and then revisited in §4.7.3 and §4.9.4.1. When the number of points $N$ exceeds 4, it is no longer convenient to use the fifth Euclidean requirement as we did in §4.9.4.1; we need a more general method.

Other researchers [27] [81] have formulated this completion problem in a non-convex way. We will utilize the convexity of $-V_{\mathcal{N}}^T\mathcal{D}(X)V_{\mathcal{N}}$ (§4.10) to reconstruct the list.

Objective is real (not matrix-valued) when you use the equivalent formulation (175). $z$ becomes another variable, though.

Minimize rank...

$$\begin{array}{cl}\underset{D}{\text{minimize}} & \operatorname{tr}(-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}})\\ \text{subject to} & <A_k\,, D> \;=\; h_{ij}\,, \quad k=1\ldots M\\ & \text{or } D\circ\Phi = H\\ & D\in\mathbb{EDM}^N\end{array} \tag{414}$$

Of interest here is Trosset's comment:

> *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 [27]

# 8 Linear 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. [82, pg.9]

**Theorem.** *Geršgorin discs.* [24, §6.1] For $p\in\mathbb{R}^m_+$ given $A\in\mathbb{S}^m$, all the eigenvalues of $A$ belong to the union of $m$ closed intervals on the real line;

$$\lambda(A)\in\bigcup_{i=1}^m\left\{\xi\in\mathbb{R}\ \mid\ |\xi-A_{ii}|\leq\varrho_i\ \triangleq\ \frac{1}{p_i}\sum_{\substack{j=1\\ j\neq i}}^m p_j|A_{ij}|\right\}=\bigcup_{i=1}^m[A_{ii}-\varrho_i\ ,\ A_{ii}+\varrho_i] \tag{415}$$

*Furthermore, if a union of $k$ of these $m$ [intervals] forms a connected region that is disjoint from all the remaining $n-k$ [intervals], then there are precisely $k$ eigenvalues of $A$ in this region.* ◇

## 8.1 $m=2$

To apply the theorem to determine positive semidefiniteness of $A$, we observe that for each $i$ we must have

$$A_{ii}\geq\varrho_i \tag{416}$$

Suppose, for example, $A\in\mathbb{S}^2$. Vectorizing $A$ for $m=2$ we set

$$a\triangleq[A_{11}\ A_{12}\ A_{22}]^T\in\mathbb{R}^{m(m+1)/2} \tag{417}$$

in isomorphic $\mathbb{R}^{m(m+1)/2}$. Then we have $m2^{m-1}=4$ inequalities, in the matrix entries $A_{ij}$ and the Geršgorin parameters $p\in\mathbb{R}^2_+$,

$$\begin{aligned}p_1A_{11}&\geq\pm p_2A_{12}\\ p_2A_{22}&\geq\pm p_1A_{12}\end{aligned} \tag{418}$$

(a)

(b)

(c)

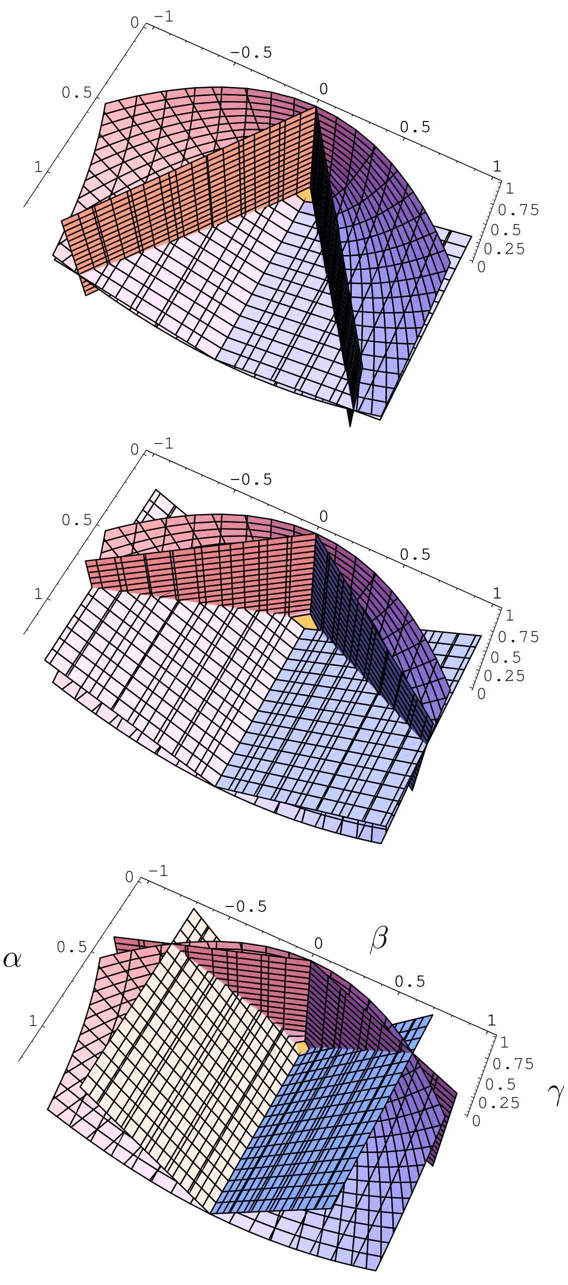



Figure 28: Polyhedral proper cone $\mathcal{K}$ belonging to PSD cone in isomorphic $\mathbb{R}^{\mathbf{3}}$ as predicted by *Geršgorin discs theorem* for $A \in \mathbb{S}^{\mathbf{2}}$ and (a) $p = [1/2 \quad 1]^T$, (b) $p = [1 \quad 1]^T$, (c) $p = [2 \quad 1]^T$. Hyperplanes supporting $\mathcal{K}$ intersect along boundary of PSD cone. Four extreme directions of polyhedral cone are coincident with four extreme directions of PSD cone.

that describe an intersection of four halfspaces in $a\in\mathbb{R}^{\mathbf{3}}$ creating the polyhedral proper cone $\mathcal{K}$ illustrated in Figure 28. Drawn truncated in isomorphic $\mathbb{R}^{\mathbf{3}}$ are the hyperplanes supporting $\mathcal{K}$, and the boundary of the positive semidefinite (PSD) cone $\mathbb{S}_+^{\mathbf{2}}$ (§2.1.3) in the subspace of symmetric $2\times 2$ matrices.

Created by means of Geršgorin discs, $\mathcal{K}$ always belongs to the PSD cone for any nonnegative value of $p\in\mathbb{R}_+^m$. Hence, any point in $\mathcal{K}$ corresponds to some positive semidefinite matrix $A$. As we shall soon posit for the general case, only the extreme directions of $\mathcal{K}$ intersect the PSD cone boundary...

When $m=2$ in particular, we observe that the four extreme directions of $\mathcal{K}$ are extreme directions of the PSD cone. As $p_1/p_2$ increases in value from 0, two extreme directions of $\mathcal{K}$ sweep the entire boundary of the PSD cone, and the interior of $\mathcal{K}$ sweeps the interior of the PSD cone. Because the entire PSD cone can be swept by $\mathcal{K}$, the dynamic system of linear inequalities

$$X^\dagger a \triangleq \begin{bmatrix} p_1 & \pm p_2 & 0 \\ 0 & \pm p_1 & p_2 \end{bmatrix} a \succeq 0 \tag{419}$$

where $X\in\mathbb{R}^{m(m+1)/2\times m2^{m-1}}$, can replace a constraint $A\succeq 0$; *id est*, for $\mathcal{K}=\{z \mid X^\dagger z\succeq 0\}\subseteq\mathbb{S}_+^m$,

$$X^\dagger a\succeq 0 \;\Rightarrow\; A\succeq 0 \tag{420}$$

$$a\in\mathcal{K} \;\Rightarrow\; A\in\mathbb{S}_+^m \tag{421}$$

where $X\in\mathbb{R}^{\mathbf{3}\times\mathbf{4}}$.

## 8.2 $m=3$

Moving to the next level, suppose $A\in\mathbb{S}^{\mathbf{3}}$. Vectorizing $A$ for $m=3$,

$$a \triangleq [A_{11}\ A_{12}\ A_{22}\ A_{13}\ A_{23}\ A_{33}]^T\in\mathbb{R}^{m(m+1)/2} \tag{422}$$

so we get

$$\begin{aligned} p_1A_{11} &\geq \pm p_2A_{12}\pm p_3A_{13} \\ p_2A_{22} &\geq \pm p_1A_{12}\pm p_3A_{23} \\ p_3A_{33} &\geq \pm p_1A_{13}\pm p_2A_{23} \end{aligned} \tag{423}$$

If we vary $p\in\mathbb{R}_+^{\mathbf{3}}$ to sweep the PSD cone as before, then the dynamic system of linear inequalities

$$X^\dagger a \triangleq \begin{bmatrix} p_1 & \pm p_2 & 0 & \pm p_3 & 0 & 0 \\ 0 & \pm p_1 & p_2 & 0 & \pm p_3 & 0 \\ 0 & 0 & 0 & \pm p_1 & \pm p_2 & p_3 \end{bmatrix} a \succeq 0 \tag{424}$$

where $X \in \mathbb{R}^{\mathbf{6\times 12}}$, can replace a constraint $A \succeq 0$ as in (420).

When $m=3$, the sign inversions account for a total of $m2^{m-1}=12$ inequalities. The number of inequalities increases geometrically with dimension because they have a geometrical interpretation; indeed, the linear inequalities describe halfspaces whose intersection forms a polyhedral proper cone $\mathcal{K}$ that belongs to the PSD cone $\mathbb{S}_+^m$ in isomorphic $\mathbb{R}^{m(m+1)/2}$.

## 8.3 Boundary intersection, polyhedral and PSD cones

In the six-dimensional case ($m=3$), the boundary of the PSD cone is no longer constituted completely by its extreme directions (symmetric rank-one matrices); now the boundary comprises all symmetric positive semidefinite rank-one and rank-two matrices. The extreme directions of $\mathcal{K}$ belong to the boundary of the PSD cone, as before, but no longer necessarily correspond to its extreme directions.

To see that, we must find the extreme directions of $\mathcal{K}$. Because $\mathcal{K}$ is a proper cone, its extreme directions are respectively inward-normal to each facet of the dual cone $\mathcal{K}^*$. (§3.6.2.1) Likewise, the inward normals to facets of $\mathcal{K}$ are the extreme directions of $\mathcal{K}^*$; we have those twelve normals in the columns of $X^{\dagger T}$. Decomposing $\mathcal{K}^*$ into its simplicial parts as in §3.6.4...

## 8.4 Semidefinite optimization via linear programming

A natural question arises as to whether it is possible to solve a semidefinite optimization problem by substituting linear inequality (420) for the semidefinite constraint. The basic idea is to fix the Geršgorin parameters $p$ and then solve a linear program in the vectorized-matrix variable $a$ (417) (422). Having found the optimal linear solution, so begins a sequence of linear programs (each with incrementally new $p$) that hopefully converges to the solution of the original semidefinite problem. If we think of the parameters $p$ as variables, it is obvious that they have a nonlinear relationship with the matrix variable entries. How or whether the sequence converges depends upon the properties of the problem's constrained objective [9, §4] as a function of $p$.

Yet implicit to the *Geršgorin discs theorem* is the presumption that matrix $A$ is known in advance...

### 8.4.1 Example: Boolean least squares

Consider, in particular, a semidefinite relaxation of an NP-hard problem; *Boolean least squares*: for fixed $C \in \mathbb{R}^{k\times n}$, $s\in\mathbb{R}^k$, and variable $\alpha\in\mathbb{R}^n$,

$$\begin{array}{ll}\underset{\alpha}{\text{minimize}} & \|C\alpha - s\|^2\\ \text{subject to} & \alpha_i^2 = 1\,, \quad i=1\ldots n\end{array} \tag{425}$$

The problem is difficult because the variable is quantized having only two allowable states. Defining $A \triangleq \alpha\alpha^T$,

$$\|C\alpha - s\|_2^2 \;=\; \operatorname{tr}(C^TCA) - 2s^TC\alpha + s^Ts \tag{426}$$

The relaxation $A \succeq \alpha\alpha^T$ facilitates transformation to a *semidefinite program* [9, §4] [62] [22] via Schur complement (§C.3), [...] (§C.5)

$$\begin{array}{ll}\underset{A,\alpha}{\text{minimize}} & \operatorname{tr}(C^TCA) - 2s^TC\alpha + s^Ts\\ \text{subject to} & \delta(A) = \mathbf{1}\,, \quad \begin{bmatrix} A & \alpha\\ \alpha^T & 1\end{bmatrix} \succeq 0\end{array} \tag{427}$$

Constraining $A$ to be dyadic (§C.7) would be intractable. Yet if solution $A$ has rank 1, then solution $\alpha$ is optimal for the Boolean least squares problem (425). Otherwise, the optimal objective of (427) is a lower bound for the Boolean problem, and $\alpha$ is an approximate solution to that combinatorial problem.

To illustrate the conversion of that semidefinite program (427) to a sequence of linear programs, consider $n=2$ (the case $m=n+1=3$ in §8.2) which yields comparison with respect to the positive semidefinite cone in the six-dimensional isomorphic subspace of symmetric matrices; we get a $3\times 3$ semidefinite constraint in (427) having vectorized variable

$$a \triangleq [A_{11}\;\; A_{12}\;\; A_{22}\;\; \alpha_1\;\; \alpha_2\;\; \beta]^T \in \mathbb{R}^{m(m+1)/2} \tag{428}$$

and vectorized constant $g \triangleq [G_{11}\;\; 2G_{12}\;\; G_{22}]^T \in \mathbb{R}^{n(n+1)/2}$ where $G \triangleq C^TC \in \mathbb{S}^n$ and $\beta$ is constrained to be 1. By discretizing the Geršgorin parameters $p$, (427) is converted:

$$\begin{array}{ll}\underset{p}{\text{minimize}} & \tau \triangleq \left\{\begin{array}{ll}\underset{a}{\text{minimize}} & \begin{bmatrix}g^T & -2s^TC & 0\end{bmatrix} a \;+\; s^Ts\\ \text{subject to} & \Delta\, a = \mathbf{1}\,, \quad X^\dagger a \succeq 0\end{array}\right.\\ \text{subject to} & p \succeq 0\end{array} \tag{429}$$

where $X^\dagger \in \mathbb{R}^{m2^{m-1}\times m(m+1)/2}$ is the matrix of Geršgorin parameters $p \in \mathbb{R}_+^m$ defined in (424), and

$$\Delta = \begin{bmatrix} 1\,0\,0\,0\,0\,0 \\ 0\,0\,1\,0\,0\,0 \\ 0\,0\,0\,0\,0\,1 \end{bmatrix} \in \mathbb{R}^{m\times m(m+1)/2} \tag{430}$$

Of interest is how the objective varies with $p$. Illustrated in Figure 29 is typical swan-like objective data for a random selection of $C$ and $s$. Obviously the objective is not quasiconvex in $p$. Yet the objective seems to be characterized by a global minimum but no local minima. The objective exhibits long troughs of near-zero directional derivative in the direction of the channel. A physical description might be: water poured in any one spot could find the global minimum.

The remaining question is whether that global minimum in the swan corresponds to the optimal value of the objective from the original semidefinite problem (427)...

(a)

(b)

(c)

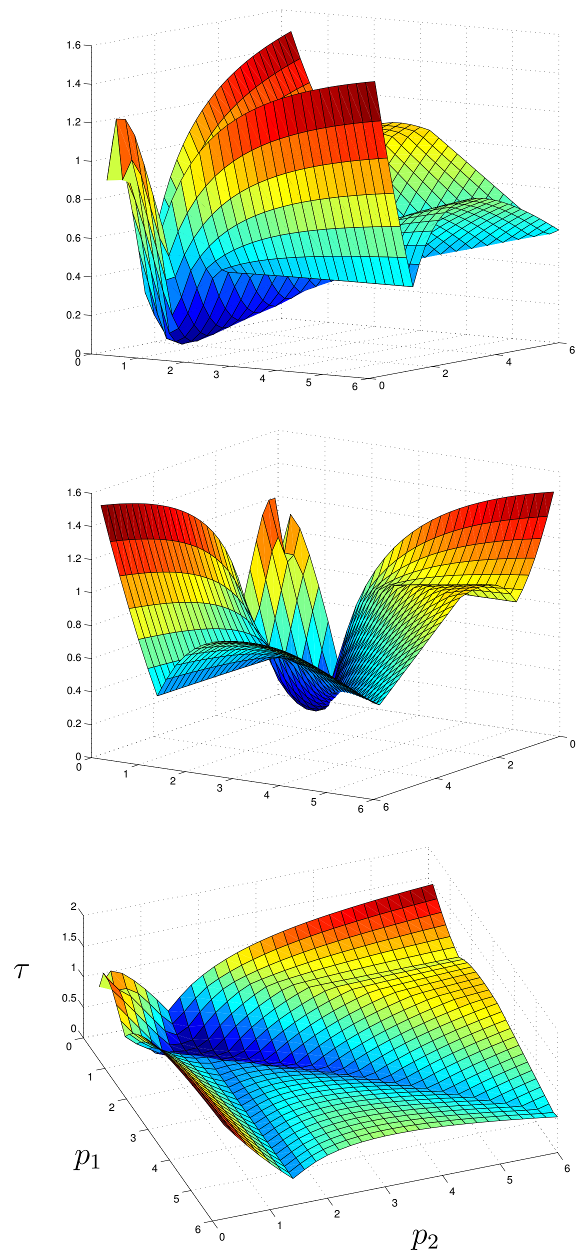



Figure 29: Minimized objective $\tau$ of linear program sequence (429) as function of $p_1$ and $p_2$, from $p \in \mathbb{R}^{\mathbf{3}}$, for $p_3 = 1$ and $C \in \mathbb{R}^{\mathbf{3}\times\mathbf{2}}$ while $s$ is set to a column from $C$ plus a random vector of low amplitude. Three plots show the same data from three different view points. Color indicates absolute level. The swan-like appearance is somewhat independent of selection of two variables from $p$.

# 9 Least squares problem solving via EDM

# 10 Piano Tuning

# 11 Optical character recognition

Account for variation in character representation as higher dimensional rotation.

# 12 Spectral analysis

## 12.1 Discrete Fourier series

The set of all symmetric matrices $\mathbb{S}^M$ forms a subspace in $\mathbb{R}^{M\times M}$ (§2.1.2), so for it there exists a standard orthonormal basis;

$$E_{ij} = \begin{cases} e_i e_i^T\,, & i=j=1\ldots M \\ \frac{1}{\sqrt{2}}\big(e_i e_j^T + e_j e_i^T\big)\,, & 1\leq i<j\leq M \end{cases} \tag{431}$$

where there are $M(M+1)/2$ standard basis matrices $E_{ij}\in\mathbb{S}^M$ formed from the standard basis vectors $e_i\in\mathbb{R}^M$. Let $\mathcal{C}_1$ be any element of $\mathbb{S}^M$. The vector inner product $<E_{ij}\,,\,\mathcal{C}_1>$ (§2.1.1) is a coefficient of projection (§A.3), and so any element of $\mathcal{C}$ can be written as a discrete Fourier series. [23, §2.2.3]

$$\mathcal{C}_1 = \sum_{\substack{i,j=1\\ j\geq i}}^{M} <E_{ij}\,,\,\mathcal{C}_1>\; E_{ij} \tag{432}$$

That Fourier series is a sum of orthogonal projections on the vectorized range of the standard basis matrices; an orthogonal projection on the subspace $\mathbb{S}^M$.

Fourier's name is attached to a series whenever its basis for the signal space is a complete orthonormal set. [23, §2.2.3] [17, §3.5, §3.6] The discrete case of the Fourier series is distinguished from its continuous counterpart by the finite number of terms required to represent a finite-dimensional signal. [83, §8.1] [84] [85] Thus if $\mathcal{C}_1$ were some nonsymmetric matrix, the right-hand side of (432) would remain an orthogonal projection on $\mathbb{S}^M$ but no longer an equality, hence no longer a Fourier series.

In the present case, $\mathcal{C}$ is assumed to be in $\mathbb{S}^M$ which is a convex set. From the *image theorem* in §2.1, it follows that $<E_{ij}\,,\,\mathcal{C}>$ is a convex set whenever $\mathcal{C}$ is. More generally, when $\mathcal{C}_1$ belongs to any convex set $\mathcal{C}$ of dimension $M$, *Caratheodory's theorem* [11] [10] [39] guarantees that no more than $M+1$ terms, in some linear combination of distinct elements from $\mathcal{C}$, are required to faithfully represent it. The orthonormal basis $E_{ij}$ of the Fourier series (432) is replaced, in that circumstance, with a set of extreme directions (§3.4.4) from $\mathcal{C}$, that is not necessarily unique.

Because any symmetric matrix can be diagonalized [86, §6.4], $\mathcal{C}_1 \in \mathbb{S}^M$ has a decomposition in terms of its *eigenmatrices* $q_i q_i^T$ (§A.3.3.1) and eigenvalues $\lambda_i$ ,

$$\mathcal{C}_1 \;=\; Q\Lambda Q^T = \sum_{i=1}^{M} \lambda_i \, q_i q_i^T \tag{433}$$

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. If we simultaneously rotate (§C.6) all the standard basis matrices into alignment with the eigenmatrices of $\mathcal{C}_1$ by applying a traditional *similarity transformation*, [19, §5.6]

$$QE_{ij}Q^T = \begin{cases} q_i q_i^T \,, & i = j = 1 \ldots M \\ \frac{1}{\sqrt{2}}\big(q_i q_j^T \,+\, q_j q_i^T\big)\,, & 1 \leq i < j \leq M \end{cases} \tag{434}$$

a remarkable thing happens to the Fourier series:

$$\begin{aligned}
\mathcal{C}_1 \;&=\; \sum_{\substack{i,j=1\\ j\geq i}}^{M} <QE_{ij}Q^T, \mathcal{C}_1> \; QE_{ij}Q^T \\
&=\; \sum_{i=1}^{M} <q_i q_i^T, \mathcal{C}_1> \; q_i q_i^T \;+\; \sum_{\substack{i,j=1\\ j> i}}^{M} <QE_{ij}Q^T, Q\Lambda Q^T> \; QE_{ij}Q^T \\
&=\; \sum_{i=1}^{M} <q_i q_i^T, \mathcal{C}_1> \; q_i q_i^T \\
&=\; \sum_{i=1}^{M} \lambda_i \, q_i q_i^T
\end{aligned} \tag{435}$$

The eigenvalues are clearly coefficients of orthogonal projection of $\mathcal{C}_1$ on the vectorized range of its eigenmatrices; (§A.3.3.1) $\mathcal{C}_1$ is a sum of one-dimensional projections. [19, §3.4] The remaining $M(M-1)/2$ Fourier series coefficients for $i \neq j$ are zeroed by the projection. Because the projection is on a rotated standard basis for the subspace $\mathbb{S}^M$, it remains an orthogonal projection on $\mathbb{S}^M$.

Each element of $\mathcal{C}$ generally brings a different eigenmatrix, so the *image theorem* does not apply to $<q_i q_i^T, \mathcal{C}>$, as it did to $<E_{ij}\,, \mathcal{C}>$, because $q_i$ is generally a nonlinear function of $\mathcal{C}_1 \in \mathcal{C}$. So, unfortunately, we may *not* conclude that the $i^{\text{th}}$ eigenvalue of all matrices in the subspace of symmetric matrices $\mathbb{S}^M$ forms a convex set; neither may we conclude that the $i^{\text{th}}$

eigenvalue of all matrices in the positive semidefinite cone $\mathbb{S}_+^M$ forms a convex set. Yet the set of all *circulant* matrices (§12.3) forms a subspace in $\mathbb{R}^{M\times M}$ whose members all have the same eigenvectors; the orthogonal basis from the DFT. So each eigenvalue of a circulant matrix comes from a convex set of eigenvalues.

From Laurent's paper on semidefinite and integer programming pg.6 ... Horn pg.432...

$$\max_{UU^T=I_k} \operatorname{tr} UU^T\mathcal{C}_1 \;=\; \sum_{i=1}^{k}\lambda_i \tag{436}$$

$$\operatorname{tr} QQ^T\mathcal{C}_1 \;=\; <QQ^T,\, \mathcal{C}_1> \;=\; \sum_{i=1}^{M}\lambda_i \tag{437}$$

$\mathcal{C}_1$ is projected orthogonally on the vectorized range of $Q$.

## 12.2 DFT

The discrete Fourier transform (DFT) is a staple of the digital signal processing community. [83] In essence, the DFT is a correlation of a rectangularly windowed sequence (or *discrete signal*) with exponentials whose frequencies are equally spaced on the unit circle.[72] The DFT of the sequence $f \triangleq [f(i),\ i\!=\!0 \ldots n\!-\!1] \in \mathbb{R}^n$ is, in traditional form,[73]

$$F(k) = \sum_{i=0}^{n-1} f(i)\, e^{-j\,i2\pi k/n} \tag{438}$$

for $k \in \{0 \ldots n-1\}$ and $j = \sqrt{-1}$. The implicit window on $f$ in (438) is rectangular. The sequence $F \triangleq [F(k),\ k\!=\!0 \ldots n\!-\!1] \in \mathbb{C}^n$ is considered a spectral analysis of the sequence $f$; *id est*, the $F(k)$ are amplitudes of exponentials which when combined, give back the original sequence,

$$f(i) = \frac{1}{n} \sum_{k=0}^{n-1} F(k)\, e^{j\,i2\pi k/n} \tag{439}$$

The argument $k$ of $F$ indexes the discrete frequencies $2\pi k/n$ of the exponentials $e^{j\,i2\pi k/n}$ in the synthesis equation (439).

The matrix form of the DFT is written

$$F = W^H f \tag{440}$$

where the *DFT matrix* is []

$$W \triangleq \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & e^{j2\pi/n} & e^{j4\pi/n} & \cdots & e^{j(n-1)2\pi/n} \\ 1 & e^{j4\pi/n} & e^{j8\pi/n} & \cdots & e^{j(n-1)4\pi/n} \\ 1 & e^{j6\pi/n} & e^{j12\pi/n} & \cdots & e^{j(n-1)6\pi/n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & e^{j(n-1)2\pi/n} & e^{j(n-1)4\pi/n} & \cdots & e^{j(n-1)^2 2\pi/n} \end{bmatrix} \in \mathbb{C}^{n\times n} \tag{441}$$

which is characterized by

$$W^T = W \tag{442}$$

$$W^{-1} = \frac{1}{n} W^H \tag{443}$$

[72] That is the unit circle in the $z$ plane; $z = e^{sT}$ where $s = \sigma + j\omega$ is the traditional Laplace frequency, $\omega$ is the Fourier frequency in radians $2\pi f$, while $T$ is the sample period.

[73] The convention is lowercase for the sequence and uppercase for its transform.

where the superscript $H$ denotes the conjugate (Hermitian) transpose. Similarly, the IDFT is

$$f = \frac{1}{n} W F \tag{444}$$

Direct computation of (440) or (444) would require on the order of $n^2$ operations for large $n$. The solution to the computational problem of evaluating the DFT for large $n$ culminated in the development of the fast Fourier transform (FFT) algorithm whose intensity is proportional to $n \log(n)$.

## 12.3 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.

Circulant.ps... set of circulant EDMs is a polyhedral cone.

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 [87], any circulant matrix $C$ may be represented,

$$C = \frac{1}{n} W \Lambda W^H \tag{445}$$

where $\Lambda = \delta(W^H f)$.
which is in the final form of (435),...show this.

The set of all circulant matrices forms a subspace. Hence it must follow that any linear combination of circulant matrices remains circulant; for all $\mu, \zeta \in \mathbb{R}$,

$$\mu C_1 + \zeta C_2 = \frac{1}{n} W (\mu \Lambda_1 + \zeta \Lambda_2) W^H \tag{446}$$

is circulant. From §12.1 we know that each eigenvalue comes from a convex set of eigenvalues. The relation (446) 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 convex cone in the subspace of circulant matrices. -Reader 35C

For $C$ circulant, where the first row is some time sequence $c_0, c_1, c_2, \ldots$, let $X = C^T$. Then (178)

$$\mathcal{D}(C^T) \;=\; k_i \, \mathbf{1}\mathbf{1}^T \,-\, 2\, C C^T \tag{447}$$

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.

## 12.4 DFT via EDM

Do this again in inner-product form (191)...

The DFT (438) is separable in the real and the imaginary part; meaning, the analysis exhibits no dependency between the two parts when the sequence is real; *videlicet*,

$$F(k)=\sum_{i=0}^{n-1} f(i)\,\cos(i2\pi k/n)-j\sum_{i=0}^{n-1} f(i)\,\sin(i2\pi k/n) \tag{448}$$

It follows then, to relate the DFT to our work with EDMs, we should separately consider the Euclidean distance-squared between the sequence and each part of the complex exponentials. Augmenting the real list $\{x_\ell\in\mathbb{R}^n,\ \ell=1\ldots N\}$ will be the new imaginary list $\{y_\ell\in\mathbb{R}^n,\ \ell=1\ldots N\}$ where

$$\begin{aligned}
x_1 \;=\; y_1 \;&\stackrel{\Delta}{=}\; [f(i),\, i=0\ldots n-1]\in\mathbb{R}^n\\
x_\ell &\stackrel{\Delta}{=} [\ \cos(i2\pi(\ell-2)/n),\, i=0\ldots n-1]\in\mathbb{R}^n, \quad \ell\in\{2\ldots N\}\\
y_\ell &\stackrel{\Delta}{=} [-\sin(i2\pi(\ell-2)/n),\, i=0\ldots n-1]\in\mathbb{R}^n, \quad \ell\in\{2\ldots N\}
\end{aligned} \tag{449}$$

where $N=n+1$, and where the [ ] bracket notation means a vector made from a sequence. The row-1 entries (columns $\ell\in\{2\ldots N\}$) of EDM

$$D(X)\stackrel{\Delta}{=}[d(x_m\,,x_\ell)] \tag{450}$$

are

$$\begin{aligned}
d(x_1,x_\ell) &= \|x_\ell-x_1\|^2\\
&= \sum_{i=0}^{n-1}(\cos(i2\pi(\ell-2)/n)\;-\;f(i))^2\\
&= \sum_{i=0}^{n-1}\cos^2(i2\pi(\ell-2)/n)\;+\;f^2(i)\;-\;2f(i)\cos(i2\pi(\ell-2)/n)\\
&= \tfrac{1}{4}\Big(2n+1+\tfrac{\sin(2\pi(\ell(2n-1)+2)/n)}{\sin(2\pi(\ell-2)/n)}\Big)\;+\;\tfrac{1}{n}\sum_{k=0}^{n-1}|F(k)|^2\;-\;2\,\mathrm{Re}F(\ell-2)
\end{aligned} \tag{451}$$

where the Fourier summation is from the Parseval relation [23] [83] [88] [85] for the DFT.[74] For the imaginary list we have a separate EDM

$$D(Y)\stackrel{\Delta}{=}[d(y_m\,,y_\ell)] \tag{452}$$

[74]The Fourier summation $\sum|F(k)|^2/n$ replaces $\sum f^2(i)$; we arbitrarily chose not to mix domains. Some physical systems, such as Magnetic Resonance Imaging devices, naturally produce signals originating in the Fourier domain. [89]

whose row-1 entries (columns $\ell \in \{2 \ldots N\}$) are

$$\begin{aligned} d(y_1, y_\ell) &= \|y_\ell - y_1\|^2 \\ &= \sum_{i=0}^{n-1} (\sin(i2\pi(\ell-2)/n) \ + \ f(i))^2 \\ &= \sum_{i=0}^{n-1} \sin^2(i2\pi(\ell-2)/n) \ + \ f^2(i) \ + \ 2f(i)\sin(i2\pi(\ell-2)/n) \\ &= \tfrac{1}{4}(2n - 1 - \tfrac{\sin(2\pi(\ell(2n-1)+2)/n)}{\sin(2\pi(\ell-2)/n)}) \ + \ \tfrac{1}{n}\sum_{k=0}^{n-1} |F(k)|^2 \ - \ 2\,\mathrm{Im}F(\ell-2) \end{aligned} \tag{453}$$

where Im takes the imaginary part of its argument. In the remaining rows ($m \in \{2 \ldots N\},\ m < \ell$) of these two EDMs, $D(X)$ and $D(Y)$, we have[75]

$$\begin{aligned} d(x_m, x_\ell) &= \|x_\ell - x_m\|^2 \\ &= \sum_{i=0}^{n-1} (\cos(i2\pi(\ell-2)/n) \ - \ \cos(i2\pi(m-2)/n))^2 \\ &= \tfrac{1}{4}(4n + 2 + \tfrac{\sin(2\pi(\ell(2n-1)+2)/n)}{\sin(2\pi(\ell-2)/n)} + \tfrac{\sin(2\pi(m(2n-1)+2)/n)}{\sin(2\pi(m-2)/n)}) \\ d(y_m, y_\ell) &= \|y_\ell - y_m\|^2 \\ &= \sum_{i=0}^{n-1} (\sin(i2\pi(\ell-2)/n) \ - \ \sin(i2\pi(m-2)/n))^2 \\ &= \tfrac{1}{4}(4n - 2 - \tfrac{\sin(2\pi(\ell(2n-1)+2)/n)}{\sin(2\pi(\ell-2)/n)} - \tfrac{\sin(2\pi(m(2n-1)+2)/n)}{\sin(2\pi(m-2)/n)}) \end{aligned} \tag{454}$$

We observe from these distance-squared equations that only the first row and column of each EDM depends upon the sequence $f(i)$ itself. The remaining entries depend only upon the sequence length $n$.

To relate the EDMs $D(X)$ and $D(Y)$ to the DFT in a useful way, consider the possibility of finding the inverse DFT (IDFT) via either EDM. For reasonable values of $N$, the number of EDM entries $N^2$ can become prohibitively large. Yet the DFT is subject to the same kind of computational intensity. It is neither our purpose nor goal to invent a fast algorithm for doing this, we simply present an example of finding an IDFT by way of the EDM. The technique we use was developed in §4.8:...

[75] $\lim\limits_{i\to 2} \sin(2\pi(i(2n-1)+2)/n)\,/\sin(2\pi(i-2)/n) \ = \ 2n-1$

# 13 Self similarity

Given the length-$M$ real sequence $[f(i),\ i\!=\!0\ldots M\!-\!1] \in \mathbb{R}^M$, we define the *self-similarity function*;[76]

$$A(\ell) \triangleq \frac{1}{2}\sum_{i=0}^{n-1}(f(i) - f(i-\ell))^2 \tag{455}$$

where $n \leq M$ is the window length.

$$x_{i+1} \triangleq f(i) \in \mathbb{R} \tag{456}$$

$$d_{ij} = \begin{cases} (x_i - x_j)^2, & 1 \leq i,j \leq M \\ 0 & \text{otherwise} \end{cases} \tag{457}$$

$$A(\ell) = \frac{1}{2}\sum_{i=1}^{n} d_{i,i-\ell} \tag{458}$$

which is a sum of some diagonal of the EDM $D$. To select the $ij^{\text{th}}$ entry of matrix $\Delta$,

$$\sqrt{d_{ij}} \triangleq e_i^T\Delta e_j \;=\; e_j^T\Delta e_i \;=\; \operatorname{tr}(e_j e_i^T\Delta) = <e_i e_j^T,\, \Delta> \tag{459}$$

where here,

$$D \triangleq \Delta \circ \Delta \tag{460}$$

and where $\circ$ denotes the Hadamard (entry-wise) product. Each scaled entry

$$\sqrt{2d_{ij}} = \sqrt{2}\operatorname{tr}(e_j e_i^T\Delta) = \frac{1}{\sqrt{2}}\operatorname{tr}\big((e_i e_j^T + e_j e_i^T)\Delta\big) \tag{461}$$

is a coefficient of orthogonal projection of $\Delta$ (§A.3.3) on the vectorized range (§2.1.1) of a member of the orthonormal basis for the vector space $\mathbb{S}_\delta^M$ :

$$E_{ij} = \frac{1}{\sqrt{2}}\big(e_i e_j^T + e_j e_i^T\big)\,, \qquad 1 \leq i < j \leq M \tag{462}$$

The self-similarity function is therefore equivalent to the Parseval relation, [23] [83] [88] [85] giving a total energy of projection:

$$A(\ell) = \sum_{\substack{i=1\\ i>\ell}}^{n} \operatorname{tr}(e_i e_{i-\ell}^T D) \;=\; \operatorname{tr}\sum_{\substack{i=1\\ i>\ell}}^{n} e_i e_{i-\ell}^T\, D \tag{463}$$

[76] which is the progenitor of autocorrelation. When $n \to \infty$, $A(\ell) = K - 2R(\ell)$ where, for some constant $K$, $R(\ell)$ is the autocorrelation function.

# A Pseudoinverse, Projection

For all $A\in\mathbb{R}^{m\times n}$, the pseudoinverse [5, §6.12, prob.19] [24, §7.3, prob.9] [25, §5.5.4] [19, App.A]

$$A^\dagger = \lim_{t\to 0^+}(A^TA + t\,I)^{-1}A^T = \lim_{t\to 0^+}A^T(AA^T + t\,I)^{-1} \in \mathbb{R}^{n\times m} \tag{464}$$

is a unique matrix, having[77]

$$\mathcal{R}(A^\dagger) = \mathcal{R}(A^T), \qquad \mathcal{R}(A^{\dagger T}) = \mathcal{R}(A) \tag{465}$$

$$\mathcal{N}(A^\dagger) = \mathcal{N}(A^T), \qquad \mathcal{N}(A^{\dagger T}) = \mathcal{N}(A) \tag{466}$$

that satisfies the *Penrose conditions*: [34] [90, §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 pseudo-inverse whose principal action is to injectively map $\mathcal{R}(A)$ onto $\mathcal{R}(A^T)$. The following relations are reliably true without qualification:

a. $A^{T\dagger} = A^{\dagger T}$
b. $A^{\dagger\dagger} = A$
c. $(AA^T)^\dagger = A^{T\dagger}A^\dagger$
d. $(A^TA)^\dagger = A^\dagger A^{T\dagger}$
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.* [91] [92, exer.7.23]
For $A\in\mathbb{R}^{m\times n}$ and $B\in\mathbb{R}^{n\times k}$,

$$(AB)^\dagger = B^\dagger A^\dagger \tag{467}$$

if and only if

$$\mathcal{R}(A^TAB) \subseteq \mathcal{R}(B) \quad \text{and} \quad \mathcal{R}(BB^TA^T) \subseteq \mathcal{R}(A^T) \tag{468}$$

⋄

[77] Proof of (465) and (466) is by singular value decomposition (§A.2.1).

### A.0.1

When $A$ is invertible, $A^{\dagger}=A^{-1}$, of course; so $A^{\dagger}A=AA^{\dagger}=I$. Otherwise, [93, §5.3.3.1] [92, §7] [94]

| | | |
|---|---|---|
| g. | $A^{\dagger}A=I\,,$ | $\operatorname{rank}A=\min\{m,n\}\,,\quad m\geq n$ |
| h. | $AA^{\dagger}=I\,,$ | $\operatorname{rank}A=\min\{m,n\}\,,\quad m\leq n$ |
| i. | $A^{\dagger}A\omega=\omega\,,$ | $\omega\in\mathcal{R}(A^T)$ |
| j. | $AA^{\dagger}\upsilon=\upsilon\,,$ | $\upsilon\in\mathcal{R}(A)$ |
| k. | $A^{\dagger}A\;=AA^{\dagger}\,,$ | $A$ normal |
| l. | $A^{k\dagger}=A^{\dagger k}\,,$ | $A$ normal, $k$ an integer |

When $A$ is symmetric, $A^{\dagger}$ is symmetric and (§A.2.1)

$$A\succeq 0\;\Leftrightarrow\;A^{\dagger}\succeq 0 \tag{469}$$

## A.1 Idempotent matrices

Projection matrices are square and characterized by *idempotence*, $P^2\!=\!P$; [19, §2.6] [90, §1.3] equivalent to the condition that $P$ be diagonalizable [24, §3.3, prob.3] with eigenvalues $\phi_i\in\{0,1\}$. [50, §4.1, thm.4.1] Solely excepting $P=I$, all projection matrices are neither orthogonal (§C.6) nor invertible. [19, §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 some matrix $A\!\in\!\mathbb{R}^{m\times n}$. All idempotent matrices projecting nonorthogonally on $\mathcal{R}(A)$ may be expressed:

$$P=A(A^{\dagger}+BZ^T) \tag{470}$$

where $\mathcal{R}(P)=\mathcal{R}(A)$,[78] $B\in\mathbb{R}^{n\times k}$ 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*,

$$A^TZ\;=\;A^{\dagger}Z\;=\;\mathbf{0} \tag{471}$$

[78] $\mathcal{R}(P)\!\subseteq\!\mathcal{R}(A)$ is obvious [19, §3.6]. By (493),

$$\begin{aligned}
\mathcal{R}(A^{\dagger}+BZ^T)\;&=\;\{(A^{\dagger}+BZ^T)y\mid y\in\mathbb{R}^m\}\\
&\supseteq\;\{(A^{\dagger}+BZ^T)y\mid y\in\mathcal{R}(A)\}=\mathcal{R}(A^T)\\
\mathcal{R}(P)\;&=\;\{A(A^{\dagger}+BZ^T)y\mid y\!\in\!\mathbb{R}^m\}\\
&\supseteq\;\{A(A^{\dagger}+BZ^T)y\mid (A^{\dagger}+BZ^T)y\in\mathcal{R}(A^T)\}=\mathcal{R}(A)
\end{aligned}$$

Evidently, the collection of nonorthogonal projection matrices on $\mathcal{R}(A)$ is an affine set $\mathcal{P}_k = \left\{A(A^\dagger + BZ^T) \mid B \in \mathbb{R}^{n\times k}\right\}$.

### A.1.1 Eigendecomposition

When a matrix $X \in \mathbb{R}^{m\times m}$ is *diagonalizable*, [19, §5.6]

$$X \;=\; S\Lambda S^{-1} \;=\; [s_1 \cdots s_m]\; \Lambda \begin{bmatrix} w_1^T \\ \vdots \\ w_m^T \end{bmatrix} \;=\; \sum_{i=1}^{m} \lambda_i\, s_i w_i^T \tag{472}$$

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

$$XS = S\Lambda \tag{473}$$

$w_i^T \in \mathbb{C}^m$ are linearly independent *left*-eigenvectors of $X$ constituting the rows of $S^{-1}$ defined by [24]

$$S^{-1}X = \Lambda S^{-1} \tag{474}$$

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.

**A.1.1.1** 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 [23, §2.2.4] [24] because neither set of left or right eigenvectors is necessarily an orthogonal set. Consequently, each dyad from a diagonalization is an independent (§C.7.1) *non*orthogonal projection matrix because

$$s_i w_i^T s_i w_i^T = s_i w_i^T \tag{475}$$

(whereas the dyads of singular value decomposition are not inherently projectors (*confer* (499))).

### A.1.2 Biorthogonal decomposition

In fact, any nonorthogonal projector $P^2 = P \in \mathbb{R}^{m\times m}$ on $\mathcal{R}(U)$ may be characterized by a biorthogonality condition $Q^T U = I$ (§C.7.1.1); (*confer* (470))

$$P = UQ^T, \qquad Q^T U = I \tag{476}$$

where $\mathcal{R}(P)=\mathcal{R}(U)$,[79] $\mathcal{N}(P)=\mathcal{N}(Q^T)$ (604), and where, in general, (*confer* (496))[80]

$$P^T \neq P\,, \qquad P^\dagger \neq P\,, \qquad \|P\| \neq 1\,, \qquad P \nsucceq 0 \tag{477}$$

and $P$ is not non-expansive (497). To verify assertion (476) we observe that because idempotent matrices are diagonalizable [24, §3.3, prob.3], they must have the form (472)

$$P \;=\; S\Phi S^{-1} \;=\; \sum_{i=1}^{m} \phi_i\, s_i w_i^T \;=\; \sum_{i=1}^{k\,\leq\, m} s_i w_i^T \tag{478}$$

that is a sum of $k=\operatorname{rank} P$ independent dyadic projectors (§C.7.1) where $\phi_i \in \{0,1\}$ are the eigenvalues of $P$ [50, §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, that are independent and all real.[81] Therefore

$$U = [s_1 \cdots s_k] \in \mathbb{R}^{m\times k} \tag{479}$$

is the full-rank matrix $S\in\mathbb{R}^{m\times m}$ having $m-k$ columns truncated (corresponding to 0 eigenvalues), while

$$Q^T = \begin{bmatrix} w_1^T \\ \vdots \\ w_k^T \end{bmatrix} \in \mathbb{R}^{k\times m} \tag{480}$$

is matrix $S^{-1}$ having the corresponding $m-k$ rows truncated. By the *0 eigenvalues theorem* (§C.4), $\mathcal{R}(U)=\mathcal{R}(P)$, $\mathcal{R}(Q)=\mathcal{R}(P^T)$, and

$$\begin{aligned}
\mathcal{R}(P) \;&=\; \operatorname{span}\{s_i \;\mid\; \phi_i = 1,\ \forall i\}\\
\mathcal{N}(P) \;&=\; \operatorname{span}\{s_i \;\mid\; \phi_i = 0,\ \forall i\}\\
\mathcal{R}(P^T) \;&=\; \operatorname{span}\{w_i \mid \phi_i = 1,\ \forall i\}\\
\mathcal{N}(P^T) \;&=\; \operatorname{span}\{w_i \mid \phi_i = 0,\ \forall i\}
\end{aligned} \tag{481}$$

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[79] Obviously, $\mathcal{R}(P)\subseteq\mathcal{R}(U)$. Because $Q^TU=I$,

$$\begin{aligned}
\mathcal{R}(P) \;&=\; \{UQ^Tx \mid x\in\mathbb{R}^m\}\\
&\supseteq\; \{UQ^TUy \mid y\in\mathbb{R}^k\} \;=\; \mathcal{R}(U)
\end{aligned}$$

[80] Orthonormal decomposition (§A.2.1.1) is a special case of biorthogonal decomposition, so these characteristics (477) are not necessary conditions for biorthogonality.

[81] Eigenvectors of a real matrix corresponding to real eigenvalues must be real. $Ax=\lambda x$. 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.

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 $\mathcal{Q}_k = \{Q \mid Q^TU = I,\ Q \in \mathbb{R}^{m\times k}\}$. Finally, biorthogonality is a sufficient condition for idempotence;

$$P^2 \;=\; \sum_{i=1}^{k} s_i w_i^T \;\sum_{j=1}^{k} s_j w_j^T \;=\; P \tag{482}$$

*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,

$$Px \;=\; UQ^Tx \;=\; \sum_{i=1}^{k} w_i^T x\, s_i \tag{483}$$

When $x$ is in the range of $P$, say $x = U\xi$, then $x = Px = UQ^TU\xi = U\xi$ and the expansion is unique because the eigenvectors are linearly independent.

The direction of nonorthogonal projection is always orthogonal to $\mathcal{R}(Q)$; *id est*, for $Px \in \mathcal{R}(U)$,

$$Px - x \;\perp\; \mathcal{R}(Q) \text{ in } \mathbb{R}^m \tag{484}$$

### A.1.3 $I - P$

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

$$I - P \;=\; S(I - \Phi)S^{-1} \;=\; \sum_{i=1}^{m} (1-\phi_i)\, s_i w_i^T \tag{485}$$

where $(1-\phi_i) \in \{1, 0\}$ are the eigenvalues of $I-P$ whose eigenvectors $s_i\,, w_i$ are identical to those of $P$ in (478).[82] A consequence of that complementary

[82] For $\mu \in \mathbb{R}$, all square $A$, and for $\lambda(A)$ a vector holding the eigenvalues of $A$, $\lambda(I+\mu A) = \mathbf{1} + \mu\lambda(A)$ because $A = MJM^{-1}$ and $I + \mu A = M(I+\mu J)M^{-1}$ where $J$ is the Jordan form for $A$; [19, §5.6] *id est*, $\delta(J) = \lambda(A)$ (§C.5), so $\lambda(I+\mu A) = \delta(I+\mu J)$ because $I + \mu J$ is also a Jordan form.

relationship is the fact, [95, §2] [96, §2] for $P^2 = P \in \mathbb{R}^{m\times m}$,

$$\begin{aligned}
\mathcal{R}(P) &= \operatorname{span}\{s_i \mid \phi_i = 1,\ \forall i\} = \operatorname{span}\{s_i \mid (1-\phi_i) = 0,\ \forall i\} = \mathcal{N}(I-P)\\
\mathcal{N}(P) &= \operatorname{span}\{s_i \mid \phi_i = 0,\ \forall i\} = \operatorname{span}\{s_i \mid (1-\phi_i) = 1,\ \forall i\} = \mathcal{R}(I-P)\\
\mathcal{R}(P^T) &= \operatorname{span}\{w_i \mid \phi_i = 1,\ \forall i\} = \operatorname{span}\{w_i \mid (1-\phi_i) = 0,\ \forall i\} = \mathcal{N}(I-P^T)\\
\mathcal{N}(P^T) &= \operatorname{span}\{w_i \mid \phi_i = 0,\ \forall i\} = \operatorname{span}\{w_i \mid (1-\phi_i) = 1,\ \forall i\} = \mathcal{R}(I-P^T)
\end{aligned} \tag{486}$$

that is easy to see from (478) and (485). 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* [17, §3.3] of $\mathcal{R}(P)$ is equivalent to $\mathcal{N}(P)$;[83] *id est*,

$$\mathcal{R}(P)\oplus\mathcal{N}(P) = \mathcal{R}(P^T)\oplus\mathcal{N}(P^T) = \mathcal{R}(P^T)\oplus\mathcal{N}(P) = \mathcal{R}(P)\oplus\mathcal{N}(P^T) = \mathbb{R}^m \tag{487}$$

because $\mathcal{R}(P)\oplus\mathcal{R}(I-P) = \mathbb{R}^m$. For idempotent $P\in\mathbb{R}^{m\times m}$, consequently,

$$\operatorname{rank} P + \operatorname{rank}(I-P) = m \tag{488}$$

**Theorem.** *Rank/Trace.* [50, §4.1, prob.9] (*confer* (498))

$$P^2 = P \iff \operatorname{rank} P = \operatorname{tr} P \quad\text{and}\quad \operatorname{rank}(I-P) = \operatorname{tr}(I-P) \tag{489}$$

$\diamond$

Summarizing, nonorthogonal projector $P$ is a linear operator characterized by idempotence but not symmetry nor positive semidefiniteness nor non-expansiveness (497).

## A.2 Symmetric idempotent matrices

When idempotent matrix $P$ is symmetric, $P$ is an orthogonal projector. In other words, the projection $Px$ of vector $x$ on subspace $\mathcal{R}(P)$ is orthogonal; [34] *id est*, for $P^2 = P \in \mathbb{S}^m$,

$$Px - x \perp \mathcal{R}(P) \text{ in } \mathbb{R}^m \tag{490}$$

[83] The same phenomenon occurs with symmetric (non-idempotent) matrices, for example.

Any norm is a convex function [5, §7.8], whereas the Euclidean norm is a strictly convex function. [9, old§6.1] Thus an equivalent condition is: The norm of vector $x-Px$ is the infimum of all *non*orthogonal projections of $x$ on $\mathcal{R}(P)$; [5, §3.3] for $P^2\!=\!P\in\mathbb{S}^m$, $\mathcal{R}(P)\!=\!\mathcal{R}(A)$, and matrices $A\,,B\,,Z$ as defined for (470),

$$\|x-Px\|_2 \;=\; \inf_{B\in\mathbb{R}^{n\times k}} \|x-A(A^\dagger+BZ^T)x\|_2 \tag{491}$$

The infimum is attained for $\mathcal{R}(B)\subseteq\mathcal{N}(A)$ over each and every affine set of nonorthogonal projection matrices indexed by $k$. The proof is straightforward, applying gradients from §F.2, setting the gradient of the squared norm to $\mathbf{0}$,

$$\begin{array}{c}\big(A^TABZ^T-A^T(I-AA^\dagger)\big)\,xx^TA \;=\; \mathbf{0}\\ \Leftrightarrow\\ A^TABZ^Txx^TA=\mathbf{0}\end{array} \tag{492}$$

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 (490) or (491), the projection $Px$ is unique (minimum distance).

We summarize the orthogonal projectors on the four fundamental subspaces:

$$\begin{array}{lllll}
1. & A^\dagger A & :\ \mathbb{R}^n \text{ on } \mathcal{R}(A^\dagger A) & =\mathcal{R}(A^T) \\
2. & AA^\dagger & :\ \mathbb{R}^m \text{ on } \mathcal{R}(AA^\dagger) & =\mathcal{R}(A) \\
3. & I-A^\dagger A & :\ \mathbb{R}^n \text{ on } \mathcal{R}(I-A^\dagger A) & =\mathcal{N}(A) \\
4. & I-AA^\dagger & :\ \mathbb{R}^m \text{ on } \mathcal{R}(I-AA^\dagger\,) & =\mathcal{N}(A^T)
\end{array} \tag{493}$$

Symmetric projector $P$ is positive semidefinite; $P\succeq 0$ (§C.2.5). When skinny matrix $Q\in\mathbb{R}^{m\times k}$ has orthonormal columns, $Q^TQ=I$ and so, by the Penrose conditions, $Q^\dagger=Q^T$. Hence, any $P$ such that

$$P=QQ^T\,, \qquad Q^TQ=I \tag{494}$$

is an orthogonal projector on $\mathcal{R}(P)=\mathcal{R}(Q)$ (604) having, for $Px\in\mathcal{R}(Q)$, (*confer* (484))

$$Px-x \;\perp\; \mathcal{R}(Q) \text{ in } \mathbb{R}^m \tag{495}$$

and $\mathcal{N}(P)\!=\!\mathcal{N}(Q^T)$ [19, §3.3], and is obviously positive semidefinite; necessarily,

$$P^T=P\,, \qquad P^\dagger=P\,, \qquad \|P\|=1\,, \qquad P\succeq 0 \tag{496}$$

Given (494), then $\|Px\| = \|QQ^T x\| = \|Q^T x\|$. Hence all orthogonal projectors are *non-expansive* because

$$\|Px\| \leq \|x\| \quad \forall\, x \tag{497}$$

that follows from Bessel's inequality [17], with equality when $x \in \mathcal{R}(Q)$.

**Theorem.** *Symmetric rank/trace.* (*confer* (489))

$$P^T = P\,, \quad P^2 = P$$
$$\Leftrightarrow$$
$$\operatorname{rank} P \;=\; \operatorname{tr} P \;=\; \|P\|_{\mathrm F}^2 \quad \text{and} \quad \operatorname{rank}(I-P) \;=\; \operatorname{tr}(I-P) \;=\; \|I-P\|_{\mathrm F}^2 \tag{498}$$

$\diamond$

In fact, any real orthogonal projector may be represented as such an *orthonormal decomposition* (494) (§A.2.1.1) [90, §1, prob.42]:

### A.2.1 Singular value decomposition

To verify that assertion (494) for the four fundamental subspaces, we need only to express $A$ using the *skinny singular value decomposition*; [25, §2.5.4] for any $A \in \mathbb{R}^{m\times n}$ and $\eta \overset{\Delta}{=} \min\{m,n\}$,

$$A \;=\; U\Sigma Q^T \;=\; [u_1 \;\cdots\; u_\eta]\;\Sigma \begin{bmatrix} q_1^T \\ \vdots \\ q_\eta^T \end{bmatrix} \;=\; \sum_{i=1}^{\eta} \sigma_i\, u_i q_i^T$$
$$U \in \mathbb{R}^{m\times \min\{m,n\}}, \quad \Sigma \in \mathbb{R}^{\min\{m,n\}\times\min\{m,n\}}, \quad Q \in \mathbb{R}^{n\times\min\{m,n\}} \tag{499}$$

where $U$ and $Q$ are always skinny or square having the property (§C.7.1.1),

$$U^T U = I, \qquad Q^T Q = I \tag{500}$$

Square matrix $\Sigma$ is diagonal; (180) (§C.5)

$$\delta(\delta(\Sigma)) = \Sigma \tag{501}$$

holding the singular values $\sigma_i$ of which the last $\eta-\operatorname{rank} A$ are zero.[84] A point sometimes lost is that any real matrix may be decomposed in terms of its real singular values $\sigma_i$ and *real* matrices $U$ and $Q$ as in (499), where [19, App.A] [25, §2.5.3]

$$\begin{array}{l} \mathcal{R}\{u_i \mid \sigma_i \neq 0\} = \mathcal{R}(A) \\ \mathcal{R}\{u_i \mid \sigma_i = 0\} \subseteq \mathcal{N}(A^T) \\ \mathcal{R}\{q_i \mid \sigma_i \neq 0\} = \mathcal{R}(A^T) \\ \mathcal{R}\{q_i \mid \sigma_i = 0\} \subseteq \mathcal{N}(A) \end{array} \tag{502}$$

The pseudoinverse is nearly synonymous with singular value decomposition because of the elegant expression,

$$A^\dagger = Q\Sigma^\dagger U^T \tag{503}$$

where $\Sigma^\dagger$ simply inverts the nonzero entries of $\Sigma$.

**A.2.1.1 Orthonormal decomposition.** From (503) we have

$$\begin{array}{rclcrcl} AA^\dagger &=& U\Sigma\Sigma^\dagger U^T = \hat{U}\hat{U}^T, & \quad & A^\dagger A &=& Q\Sigma^\dagger\Sigma Q^T = \hat{Q}\hat{Q}^T \\ I - AA^\dagger &=& I - \hat{U}\hat{U}^T = \hat{U}^\perp\hat{U}^{\perp T}, & & I - A^\dagger A &=& I - \hat{Q}\hat{Q}^T = \hat{Q}^\perp\hat{Q}^{\perp T} \end{array} \tag{504}$$

where $\hat{U} \in \mathbb{R}^{m\times \operatorname{rank} A}$ is the matrix $U$ having $\eta-\operatorname{rank} A$ columns (corresponding to singular values zero) truncated, likewise for $\hat{Q} \in \mathbb{R}^{n\times \operatorname{rank} A}$, $\hat{U}^\perp \in \mathbb{R}^{m\times m-\operatorname{rank} A}$ 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 $P$ (494). The relation (504) shows that orthogonal projectors simultaneously possess a biorthogonal decomposition (§A.1.2; *e.g.*, $AA^\dagger$ for skinny-or-square $A$ full rank) and an orthonormal decomposition (*e.g.*, $\hat{U}\hat{U}^T$).

**A.2.1.2 Action of the pseudo-inverse.** nascence nb. pg.39...

[84]For $\eta = n$, $\sigma(A) = \sqrt{\lambda(A^TA)}$ where $\lambda$ denotes eigenvalues. For $\eta = m$, $\sigma(A) = \sqrt{\lambda(AA^T)}$. When $A$ is normal, $\sigma(A) = |\lambda(A)|$.

**A.2.1.3**
**Example.** *Projecting the origin on a hyperplane.* (*confer* §3.2.2.1)
Given the hyperplane description

$$\partial\mathcal{H} = \{x \mid a^T x = b\} \subset \mathbb{R}^n \qquad (62)$$

the orthogonal projection of the origin on that hyperplane is the solution to a minimization problem: (491)

$$\begin{aligned}\|P\mathbf{0} - \mathbf{0}\|_2 &= \inf_{x\in\partial\mathcal{H}} \|x - \mathbf{0}\|_2 \\ &= \inf_{\xi\in\mathbb{R}^{n-1}} \|Z\xi + x_o\|_2\end{aligned} \tag{505}$$

where $P\mathbf{0}$ represents the projection, $x_o$ is any solution to $a^T x = b$, and where the columns of $Z \in \mathbb{R}^{n\times n-1}$ constitute a basis for $\mathcal{N}(a^T)$ so that $x = Z\xi + x_o \in \partial\mathcal{H}$ for all $\xi$.

The infimum is found by setting the gradient (with respect to $\xi$) of the strictly convex norm-squared to zero. We find the argument,

$$\xi = -(Z^T Z)^{-1} Z^T x_o \tag{506}$$

so

$$x = \big(I - Z(Z^T Z)^{-1} Z^T\big) x_o \tag{507}$$

and from (493),

$$x = a(a^T a)^{-1} a^T x_o \tag{508}$$

In words, any point $x_o$ in the hyperplane $\partial\mathcal{H}$ projected on its normal $a$ (*confer* (511)) yields that point in the hyperplane closest to the origin. □

In summary, orthogonal projector $P$ is a linear operator characterized by idempotence, symmetry, positive semidefiniteness, and non-expansiveness. [10, §A.3.1]

## A.3 Projection on a matrix, vectorization interpretation

### A.3.1 Nonorthogonal projection on a vector

Nonorthogonal projection of vector $x$ on the range of vector $y$ is accomplished using a normalized dyad $P_0$ (§C.7); *videlicet*,

$$\frac{<z,x>}{<z,y>}\,y \;=\; \frac{z^Tx}{z^Ty}\,y \;=\; \frac{yz^T}{z^Ty}\,x \;\triangleq\; P_0\,x \tag{509}$$

where $<z,x>/<z,y>$ 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 *non*orthogonal projection is orthogonal to $z$; *id est*,

$$P_0\,x - x \;\perp\; z \tag{510}$$

### A.3.2 Orthogonal projection on a vector

The formula for *orthogonal* projection of vector $x$ on the range of vector $y$ (*one-dimensional* (orthogonal) *projection*) is basic analytic geometry; [46, §1-8] [23, §2.2] [19, §3.2]

$$\frac{<y,x>}{<y,y>}\,y \;=\; \frac{y^Tx}{y^Ty}\,y \;=\; \frac{yy^T}{y^Ty}\,x \;\triangleq\; P_1\,x \tag{511}$$

where $<y,x>/<y,y>$ 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

$$P_1\,x - x \;\perp\; y \tag{512}$$

because $P_1^T = P_1$.

### A.3.3 Projection on a vectorized matrix

We extend formula (511) to vectorized matrices:[85] Given $X, Y \in \mathbb{R}^{m\times n}$, we have the one-dimensional orthogonal projection of $X$ in isomorphic $\mathbb{R}^{mn}$ on

[85] Formula (509) is also extensible. We consider an example in §A.3.3.1.

the vectorized range of $Y$ : (§2.1.1)

$$\frac{<Y\,,\,X>}{<Y\,,\,Y>}\,Y \tag{513}$$

where $<Y\,,\,X>/<Y\,,\,Y>$ is the coefficient of projection. There is opportunity for insight when $Y$ is a dyad $yz^T$ : Instead given $X\in\mathbb{R}^{m\times n}$, $y\in\mathbb{R}^m$, and $z\in\mathbb{R}^n$,

$$\frac{<yz^T,\,X>}{<yz^T,\,yz^T>}\,yz^T \;=\; \frac{y^TXz}{y^Ty\;z^Tz}\,yz^T \tag{514}$$

that is the one-dimensional orthogonal projection of $X$ in isomorphic $\mathbb{R}^{mn}$ on the vectorized range of $yz^T$. To reveal the obscured symmetric projection matrices $P_1$ and $P_2$ we rewrite (514):

$$\frac{y^TXz}{y^Ty\;z^Tz}\,yz^T \;=\; \frac{yy^T}{y^Ty}\,X\,\frac{zz^T}{z^Tz} \;\triangleq\; P_1XP_2 \tag{515}$$

So for dyadic (§C.7) projection matrices, the projection (515) in $\mathbb{R}^{mn}$ is orthogonal if and only if $P_1$ *and* $P_2$ are symmetric.[86] When $P_1$ and $P_2$ as in (515) are rank-one symmetric, (5)

$$\mathcal{R}(\operatorname{vec} P_1XP_2) = \mathcal{R}(\operatorname{vec} yz^T) \text{ in } \mathbb{R}^{mn} \tag{516}$$

and

$$P_1XP_2 - X \;\perp\; yz^T \tag{517}$$

[86]For *orthogonal* projection, the argument outside the inner products $<\cdot>$ in (514) must equal the arguments inside in three places.

For diagonalizable $X\in\mathbb{R}^{m\times m}$ (§A.1.1), 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 $j^{\text{th}}$ dyad 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 [50, §3.2]. Yet when $\mathcal{R}(P_2)=\mathcal{R}(s_k)$, $k\neq j\in\{1\ldots m\}$, then $P_1XP_2 = \mathbf{0}$.

**A.3.3.1 Example.** *Nonorthogonal projection on vectorized matrix.* Any square matrix in $\mathbb{R}^{m\times m}$ may be expressed as a sum of orthogonal projections in isomorphic $\mathbb{R}^{m^2}$ on the vectorized range of the standard basis;

$$X = \sum_{i,j=1}^{m} <e_i e_j^T, X> \ e_i e_j^T \tag{518}$$

where the set of unit matrices forms the standard orthonormal basis;

$$\left\{e_i e_j^T \mid i,j=1\ldots m\right\} \in \mathbb{R}^{m\times m} \tag{519}$$

The transpose matrix is a good example of *non*orthogonal projection on the standard basis:

$$X^T = \sum_{i,j=1}^{m} <\left(e_i e_j^T\right)^T, X> \ e_i e_j^T \tag{520}$$

Any diagonalization $X = S\Lambda S^{-1} = \sum_{i=1}^m \lambda_i\, s_i w_i^T$ (472) may be expressed as a sum of nonorthogonal projections on the vectorized range of its eigenmatrices $P_j \triangleq s_j w_j^T$ ;

$$\begin{aligned}
X &= \sum_{i,j=1}^{m} <\left(S e_i e_j^T S^{-1}\right)^T, X> \ S e_i e_j^T S^{-1} \\
&= \sum_{j=1}^{m} <\left(s_j w_j^T\right)^T, X> \ s_j w_j^T \ + \sum_{\substack{i,j=1 \\ j\neq i}}^{m} <\left(S e_i e_j^T S^{-1}\right)^T, S\Lambda S^{-1}> \ S e_i e_j^T S^{-1} \\
&= \sum_{j=1}^{m} <\left(s_j w_j^T\right)^T, X> \ s_j w_j^T \\
&\triangleq \sum_{j=1}^{m} < P_j^T, X> P_j \ = \sum_{j=1}^{m} s_j w_j^T X s_j w_j^T \ = \sum_{j=1}^{m} P_j X P_j \\
&= \sum_{j=1}^{m} \lambda_j\, s_j w_j^T
\end{aligned} \tag{521}$$

Matrix $X$ is a sum of one-dimensional nonorthogonal projections because the argument inside the projection coefficient $<\cdot>$ differs from the argument outside. The eigenvalues 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 $P_j$ as in (521) is rank one,

$$\mathcal{R}(\operatorname{vec} P_j X P_j) \ = \ \mathcal{R}(\operatorname{vec} s_j w_j^T) \ = \ \mathcal{R}(\operatorname{vec} P_j) \text{ in } \mathbb{R}^{m^2} \tag{522}$$

and

$$P_j X P_j - X \perp w_j s_j^T \tag{523}$$

When $X$ is a symmetric matrix, the eigenmatrices must also be symmetric. Hence the one-dimensional projections become orthogonal. □

### A.3.4 Positive semidefiniteness test as projection

For any given $X \in \mathbb{R}^{m\times m}$, the familiar quadratic construct $y^T X y \geq 0$, over broad domain, is a fundamental test of positive semidefiniteness. (§C.1) It is a fact that $y^T X y$ is always proportional to a coefficient of projection; letting $z$ in formula (514) become $y \in \mathbb{R}^m$, then $P_2 = P_1 = yy^T/y^T y = yy^T/\|yy^T\|$ and formula (515) becomes

$$\frac{<yy^T,\, X>}{<yy^T,\, yy^T>}\, yy^T = \frac{y^T X y}{y^T y}\frac{yy^T}{y^T y} = \frac{yy^T}{y^T y} X \frac{yy^T}{y^T y} \triangleq P_1 X P_1 \tag{524}$$

The product $P_1 X P_1$ is the one-dimensional orthogonal projection of $X$ in isomorphic $\mathbb{R}^{m^2}$ on the vectorized range of $P_1$ because, for $\operatorname{rank} P_1 = 1$ and $P_1^2 = P_1 \in \mathbb{S}^m$,

$$P_1 X P_1 = \frac{y^T X y}{y^T y}\frac{yy^T}{y^T y} = <\frac{yy^T}{y^T y}\,,\, X> \frac{yy^T}{y^T y} = <P_1\,,\, X> P_1 = \frac{<P_1\,,\, X>}{<P_1\,,\, P_1>}\, P_1 \tag{525}$$

The coefficient of orthogonal projection $<P_1\,,\, X> = y^T X y/(y^T y)$ is also known as Rayleigh's quotient. When $P_1$ as in (524) is rank-one symmetric,

$$\mathcal{R}(\operatorname{vec} P_1 X P_1) = \mathcal{R}(\operatorname{vec} yy^T) = \mathcal{R}(\operatorname{vec} P_1) \text{ in } \mathbb{R}^{m^2} \tag{526}$$

and

$$P_1 X P_1 - X \perp yy^T \tag{527}$$

The test for positive semidefiniteness, then, is a test for nonnegativity of the coefficient of projection of $X$ on the vectorized range of each and every extreme direction $yy^T$ (§3.4.4) from the positive semidefinite cone in the subspace of symmetric matrices.

#### A.3.4.1 PXP $\succeq$ 0

In some circumstances, it may be desirable to limit the domain of test; *e.g.*, $\|y\|=1$.[87] 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 $-V^TDV\succeq 0$ determines whether $D\in\mathbb{S}^N_\delta$ is a Euclidean distance matrix. The same test may be stated: For $D\in\mathbb{S}^N_\delta$ (and optionally $\|y\|=1$),

$$D\in\mathbb{EDM}^N \Leftrightarrow -y^TDy \;=\; <yy^T,\, -D> \;\geq\; 0\,,\quad y\in\mathcal{R}(V) \tag{528}$$

The test $-V^TDV\succeq 0$ is therefore equivalent to a test for nonnegativity of the coefficient of orthogonal projection of $-D$ on the vectorized range of each and every 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.)

### A.3.5 PXP misinterpretation for higher rank P

For a projection matrix $P$ of rank greater than 1, $PXP$ is generally not commensurate with $\frac{<P,X>}{<P,P>}P$ as in the dyadic case (525). Yet for a symmetric idempotent matrix $P$ of any rank we are tempted to say $PXP$ is an ortho-

[87] When $y$ becomes the $j^{\text{th}}$ eigenvector $s_j$ of diagonalizable $X$, for example, $<P_1\,,X>$ becomes the $j^{\text{th}}$ eigenvalue: [28, §III]

$$<P_1\,,X>|_{y=s_j} \;=\; \frac{s_j^T\left(\sum\limits_{i=1}^m \lambda_i\, s_i w_i^T\right)s_j}{s_j^Ts_j} \;=\; \lambda_j$$

Similarly for $y=w_j$, the $j^{\text{th}}$ left-eigenvector,

$$<P_1\,,X>|_{y=w_j} \;=\; \frac{w_j^T\left(\sum\limits_{i=1}^m \lambda_i\, s_i w_i^T\right)w_j}{w_j^Tw_j} \;=\; \lambda_j$$

A quandary may arise regarding the potential annihilation of the antisymmetric part of $X$ when $s_j^TXs_j$ 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 $\mathrm{Re}(s_j^HXs_j) = s_j^H(X+X^T)s_j/2$ [24, §7.1] where $(X+X^T)/2$ is the symmetric part of $X$, and $s_j^H$ denotes the conjugate (Hermitian) transpose.

gonal projection of $X$, supported by the following erroneous argument:

> Because of idempotence ($P(PXP)P = PXP$) and symmetry of $P$, we have orthogonality; $PXP - X \perp P$ since $\langle PXP - X\,,\, P\rangle = \operatorname{tr}(P(PXP - X)P) = 0$. When $X \in \mathbb{S}^m$, we may ascribe geometric meaning; $PXP$ is the unique orthogonal projection of $X$ on the vectorized range of $P$ in the isomorphic subspace of symmetric matrices in $\mathbb{R}^{m^2}$.

The fallacy is: $\operatorname{vec} PXP$ does not necessarily belong to the vectorized range of $P$; the most basic requirement for projection on $\operatorname{vec} P$.

## A.4 Projection on a matrix, range/rowspace interpretation

For symmetric projection matrices $P_1$ and $P_2$ of any rank, $P_1XP_2$ is simultaneously the orthogonal projection of $\mathcal{R}(X)$ on $\mathcal{R}(P_1)$ and the orthogonal 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 (499) where here $\eta = \min\{m, p\}$,

$$P_1XP_2 \;=\; \sum_{i=1}^{\eta} \sigma_i\, P_1\, u_i q_i^T P_2 \;=\; \sum_{i=1}^{\eta} \sigma_i\, P_1 u_i\, (P_2\, q_i)^T \tag{529}$$

Recall that $u_i \in \mathcal{R}(X)$ and $q_i \in \mathcal{R}(X^T)$ when the corresponding singular values are nonzero. (§A.2.1) So $P_1$ orthogonally projects $u_i$ on $\mathcal{R}(P_1)$ while $P_2$ orthogonally projects $q_i$ on $\mathcal{R}(P_2)$; *id est*, the range and row-space of any $X$ are respectively projected orthogonally on the ranges of $P_1$ and $P_2$.[88]

With $A_1, B_1, Z_1, A_2, B_2, Z_2$ as defined for (470), for $P_1 = A_1A_1^\dagger \in \mathbb{R}^{m\times m}$ where $A_1 \in \mathbb{R}^{m\times n}$, $Z_1 \in \mathbb{R}^{m\times k}$, and for $P_2 = A_2A_2^\dagger \in \mathbb{R}^{p\times p}$ where $A_2 \in \mathbb{R}^{p\times n}$, $Z_2 \in \mathbb{R}^{p\times k}$,

$$\|X - P_1XP_2\|_{\mathrm F} \;=\; \inf_{B_1,\,B_2 \in \mathbb{R}^{n\times k}} \|X - A_1(A_1^\dagger + B_1Z_1^T)X(A_2^{\dagger T} + Z_2B_2^T)A_2^T\|_{\mathrm F} \tag{530}$$

That means projectors $P_1$ and $P_2$ must be symmetric (*confer* (515)) to achieve the infimum, but may be of any rank:

[88] 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 $j^{\text{th}}$ dyad 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 $P_1XP_2 = \mathbf{0}$.

**A.4.0.1 Proof.** *Minimum Frobenius norm* (530). inf inf [10, §0.1.2]

$$\inf_{B_1,\,B_2}\|X - A_1(A_1^\dagger + B_1Z_1^T)X(A_2^{\dagger T} + Z_2B_2^T)A_2^T\|_F \;=\; \inf_{B_1}\;\inf_{B_2}\|\cdot\|_F \tag{531}$$

Defining $P \triangleq A_1(A_1^\dagger + B_1Z_1^T)$ and losing the remaining subscripts,

$$\inf_B\|X - PX(A^{\dagger T} + ZB^T)A^T\|_F^2 \tag{532}$$

$$= \inf_B \operatorname{tr}\big((X^T - A(A^\dagger + BZ^T)X^TP^T)(X - PX(A^{\dagger T} + ZB^T)A^T)\big) \tag{533}$$

$$= \inf_B \operatorname{tr}\big(X^TX - X^TPX(A^{\dagger T} + ZB^T)A^T - A(A^\dagger + BZ^T)X^TP^TX + A(A^\dagger + BZ^T)X^TP^TPX(A^{\dagger T} + ZB^T)A^T\big) \tag{534}$$

The Frobenius norm is a strictly convex function. [9, old§6.1] Terms not containing $B$ will vanish from the gradient; (§F.2.2)

$$\nabla_B \operatorname{tr}\big(-X^TPXZB^TA^T - ABZ^TX^TP^TX + AA^\dagger X^TP^TPXZB^TA^T + ABZ^TX^TP^TPXA^{\dagger T}A^T + ABZ^TX^TP^TPXZB^TA^T\big) \tag{535}$$

$$= \; -2A^TX^TPXZ + 2A^TAA^\dagger X^TP^TPXZ + 2A^TABZ^TX^TP^TPXZ \tag{536}$$

$$= A^T\big(-X^T + AA^\dagger X^TP^T + ABZ^TX^TP^T\big)PXZ \;=\; \mathbf{0} \tag{537}$$

$$\Leftrightarrow\; \mathcal{R}(B_1) \subseteq \mathcal{N}(A_1) \;\text{ and }\; \mathcal{R}(B_2) \subseteq \mathcal{N}(A_2) \tag{538}$$

The same conclusion is obtained were instead $P^T \triangleq (A_2^{\dagger T} + Z_2B_2^T)A_2^T$ . ♦

## A.5 Projection on convex set

Thus far we have discussed only projection on subspaces. Now we generalize, considering projection on convex sets (objects) in Euclidean space; *convex* sets because then projection is unique. [10, §A.3.1]

Like before (491), the *unique projection* $Px$ of a point $x \in \mathbb{R}^n$ on convex set $\mathcal{C} \subseteq \mathbb{R}^n$ is that point in $\mathcal{C}$ closest to $x$;

$$\|x - Px\|_2 \;=\; \inf_{y\in\mathcal{C}}\|x - y\|_2 \tag{539}$$

In other words, of all points in $\mathcal{C}$, the point $Px$ therein is closest to $x$ in the Euclidean sense.

Also like before, there is an equivalent characterization of projection on a convex set analogous to the orthogonality condition (490) for projection on a subspace:

**Theorem.** *Unique projection on closed convex set.* [10, §A.3.1] A point $Px$ in the closed convex set $\mathcal{C} \subseteq \mathbb{R}^n$ is the unique projection of $x \in \mathbb{R}^n$ on $\mathcal{C}$ if and only if, for all $y \in \mathcal{C}$,

$$<x - Px\,,\, y - Px> \;\leq\; 0 \tag{540}$$

$\diamond$

Unlike before, the operator $P$ is not linear; projector $P$ is a linear operator if and only if the convex set on which projection is made is a subspace. [10, §A.3.1]

**Bunt-Motzkin Theorem.** *Convex set if unique projection.* [14, §7.5] [97] If $\mathcal{C} \subseteq \mathbb{R}^n$ is a nonempty closed set and if for every $x$ in $\mathbb{R}^n$ there is a unique Euclidean projection of $x$ on $\mathcal{C}$, then $\mathcal{C}$ is convex. $\diamond$

### A.5.1 Projection on cone

When the convex set $\mathcal{C}$ is a cone, there is a finer statement of optimality conditions:

**Theorem.** *Unique projection on cone.* [10, §A.3.2] [9, §8] Let $\mathcal{K} \subseteq \mathbb{R}^n$ be a closed convex cone, and $\mathcal{K}^*$ its dual (§3.6). Then $Px$ is the unique projection of $x \in \mathbb{R}^n$ on $\mathcal{K}$ if and only if

$$Px \in \mathcal{K}\,, \quad <Px - x\,,\, Px> \;=\; 0\,, \quad Px - x \in \mathcal{K}^* \tag{541}$$

$\diamond$

As stated, the theorem admits $\mathcal{K}$ having empty interior; *id est*, convex cones in a proper subspace of $\mathbb{R}^n$. In words, $Px$ is the unique projection of $x$ on $\mathcal{K}$ if and only if

1) projection $Px$ lies in $\mathcal{K}$,
2) difference vector $Px - x$ is orthogonal to the projection $Px$,
3) difference vector $Px - x$ lies in the dual cone $\mathcal{K}^*$.

The first and second conditions 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 orthogonality condition (490), we recall the second requirement for projection on a subspace,

$$Px - x \perp \mathcal{R}(P) \;\Leftrightarrow\; Px - x \in \mathcal{R}(P)^{\perp} \tag{542}$$

Yet condition 3 is a generalization of subspace projection; *id est*, for unique projection on a closed convex cone, $\mathcal{K}^*$ plays the role that $\mathcal{R}(P)^{\perp}$ plays for subspace projection; indeed, $\mathcal{K} \oplus -\mathcal{K}^* = \mathbb{R}^n \Rightarrow$ cone $\mathcal{K}$ is closed and convex [12, §2.7]. Recalling that any subspace is a closed convex cone (but not a proper cone (§3.4.2)),

$$\mathcal{K} = \mathcal{R}(P) \;\Leftrightarrow\; \mathcal{K}^* = \mathcal{R}(P)^{\perp} \tag{543}$$

meaning, when a cone is a subspace $\mathcal{R}(P)$, the dual cone becomes its orthogonal complement $\mathcal{R}(P)^{\perp}$. [9, old§1.6.1] Then condition 3 becomes coincident with condition 2.

**Salient properties of projection $Px$ on closed convex cone $\mathcal{K}$**

[10, §A.3.2]

1. $Px = \mathbf{0} \;\Leftrightarrow\; x \in -\mathcal{K}^*$
2. $P\alpha x = \alpha\, Px \;\; \forall\, \alpha \geq 0$
3. $P(-x)\;(\text{on } \mathcal{K}) = -(Px \text{ on } -\mathcal{K})$
4. [Jean – Jacques Moreau]

$$\begin{gathered} x = x_1 + x_2\,, \quad x_1 \in \mathcal{K}\,, \quad x_2 \in -\mathcal{K}^*, \quad x_1 \perp x_2 \\ \Leftrightarrow \\ x_1 = Px \;\; (\text{on } \mathcal{K}) \quad \text{and} \quad x_2 = Px \;\text{ on } -\mathcal{K}^* \end{gathered}$$

**Example.** *Unique projection on nonnegative orthant.* (*confer* (348)) From the *unique projection on cone theorem*, to uniquely project matrix $H \in \mathbb{R}^{m\times n}$ on the self-dual orthant (§3.6.2) of nonnegative matrices $\mathbb{R}_+^{m\times n}$ in isomorphic $\mathbb{R}^{mn}$, the necessary and sufficient conditions are:

$$\begin{aligned} &H^\star \geq \mathbf{0} \\ &\operatorname{tr}\big((H^\star - H)^T H^\star\big) = 0 \\ &H^\star - H \geq \mathbf{0} \end{aligned} \tag{544}$$

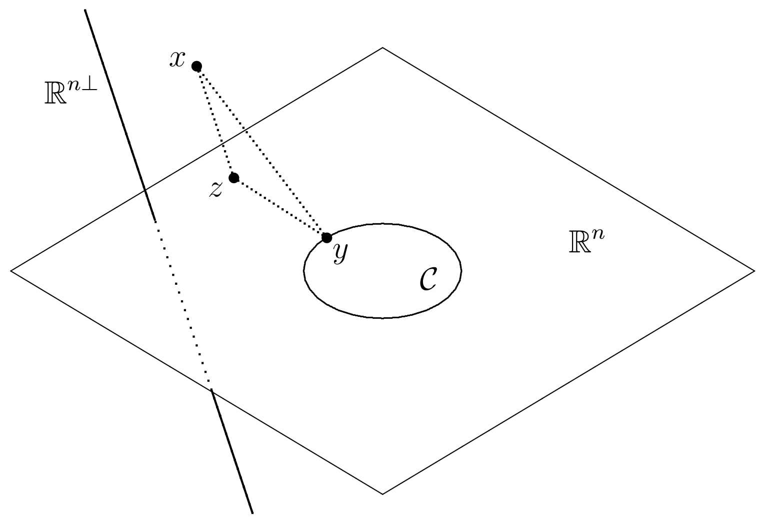


Figure 30: Closed convex set $\mathcal{C}$, whose boundary is drawn, belongs to subspace $\mathbb{R}^n$ represented in the sketch by the diamond drawn without proper perspective. Point $y$ is unique projection of $x$ on $\mathcal{C}$; equivalent to product of orthogonal projection of $x$ on $\mathbb{R}^n$ and unique projection of result $z$ on $\mathcal{C}$.

where the inequalities denote entry-wise comparison. The optimal solution $H^\star$ is simply $H$ having all its negative entries zeroed. $\square$

Similarly, it is easy to show that projecting $H \in \mathbb{R}^{n\times n}$ orthogonally on $\mathbb{S}^n$ 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. Yet projecting $H$ uniquely on the 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* §6.1)

### A.5.2 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 $\mathcal{C}$; *id est*, the ordered product of two individual projections.

To show that, suppose $Px$ on $\mathcal{C}$ is $y$ as illustrated in Figure 30;

$$\|x-y\| \leq \|x-q\| \quad \forall\, q\in\mathcal{C} \tag{545}$$

Further suppose $Px$ on $\mathbb{R}^n$ equals $z$. Then by the *Pythagorean theorem*

$$\|x-y\|^2 = \|x-z\|^2 + \|z-y\|^2 \tag{546}$$

because $x-z \perp z-y$. (490) [5, §3.3] Then point $y$ is also the projection of $z$ on $\mathcal{C}$ because

$$\|z-y\|^2 \;=\; \|x-y\|^2 - \|x-z\|^2 \;\leq\; \|z-q\|^2 \;=\; \|x-q\|^2 - \|x-z\|^2 \quad \forall\, q \in \mathcal{C} \tag{547}$$

The converse is also true. ♦

## A.6 Calculus of variations

When $x$, $Px$, and $y$ are instead continuous real functions of $t$, we have

$$\|x(t)-Px(t)\|^2 \;=\; \int (x(t) - Px(t))^2\, dt \;=\; \inf_{y\in\mathcal{C}} \|x(t)-y(t)\|^2 \;=\; \inf_{y\in\mathcal{C}} \int (x(t) - y(t))^2\, dt \tag{548}$$

Solution is via *calculus of variations.* [5, §7.4]...

# B Volume of a convex polyhedron

Look at Gower82 section 4 [43, §4]
Strang [19] pg.212, Horn [24] pg.477.

No method is known for computing the volume of a general convex polyhedron [98, pg.173]. Amazing that this fundamental question has confounded mathematicians.

Algorithm: many out there on internet.

Volume is a concept in $\mathbb{R}^{\mathbf{3}}$; in higher dimensions called "content". The volume of a pyramid is 1/3 the product of the base area with the height. [37] The volume is independent of the highest vertex location in a pyramid as long as its height remains constant. Volume of any simplex is proportional to the Cayley-Menger determinant.

How to know that a particular distance refers to an interior point? Find the list. If any list member can be expressed as a convex combination of the others, then it is an interior point. [11]

Semidefinite program to minimize volume as in §4.9.3.

Volume of a polyhedron is log concave function of halfspace description parameter. [Reader, pg.78] Volume is log of piecewise linear concave function. -Boyd

Applying the results from §4.7,

$$\int_{\mathcal{S}} dp(y)dy \tag{549}$$

where $p(y) = X\sqrt{2}V_{\mathcal{N}}\, y$ from (260), and $\mathcal{S}$ is the unit simplex in $\mathbb{R}_+^{N-1}$ (§3.5.3). Because $y$ is a vector, the integral equation is an abbreviation for a multiple integration. Suppose for example that $N=3$, then $y\in\mathbb{R}_+^{\mathbf{2}}$ so (549) becomes

$$\int\!\!\int_{\mathcal{S}} dp(y)\, dy_1\, dy_2 \tag{550}$$

P. Gritzman and V. Klee, "On the complexity of some basic problems in computational convexity: II. volume and mixed volumes. Technical report TR:94-31, DIMACS, Rutgers University, NJ, 1994

Lasserre J.B. and E.S. Zeron(2001) "A Laplace transform algorithm for the volume of a convex polytope". Journal of the ACM 48, pp. 1126--1140.

# C Linear Algebra

## C.1 Semidefiniteness: domain of test

The most fundamental necessary and sufficient test for positive semidefiniteness of $A\in\mathbb{R}^{n\times n}$ is:

$$x^TA\,x \geq 0\,, \quad \text{for each and every } x\in\mathbb{R}^n \text{ such that } \|x\|=1 \tag{551}$$

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 $x^TAx$ is nonnegative for particular $x=x_o$ , then it is nonnegative for any $\alpha x_o$ 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) are admitted to the set of positive semidefinite matrices (555); an unnecessary prohibitive constraint.

### C.1.1 Symmetry *versus* semidefiniteness

We call (551) *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 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*,

$$A = \frac{(A+A^T)}{2} + \frac{(A-A^T)}{2} \tag{552}$$

Because, for all real $A$, the antisymmetric part vanishes under real test,

$$x^T\frac{(A-A^T)}{2}\,x = 0 \tag{553}$$

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 (551). Because eigenvalue-signs of a symmetric matrix translate unequivocally to its semidefiniteness, the eigenvalues that determine semidefiniteness are always those of the *symmetrized* matrix. (§C.2) 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 (551), that presumption is typically bolstered with compelling examples from the physical sciences where symmetric matrices occur within the exposition of natural phenomena.[89] [99, §52]

Perhaps a better explanation of this pervasive presumption of symmetry comes from Horn and Johnson [24, §7.1] whose perspective[90] is the *complex* matrix, thus necessitating the complex domain of test throughout their treatise. They explain, if $A\in\mathbb{C}^{n\times n}$

> *... and if $x^HAx$ 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 $x^HAx$ comes from the Hermitian part $(A+A^H)/2$ of $A$;

$$\operatorname{Re}(x^HAx) = x^H\frac{A+A^H}{2}\,x \tag{554}$$

rather,

$$x^HAx \in \mathbb{R} \;\Leftrightarrow\; A^H = A \tag{555}$$

because the imaginary part of $x^HAx$ comes from the anti-Hermitian part $(A-A^H)/2$;

$$\operatorname{Im}(x^HAx) = x^H\frac{A-A^H}{2}\,x \tag{556}$$

that vanishes for nonzero $x$ if and only if $A=A^H$. So the Hermitian symmetry assumption is unnecessary, according to Horn and Johnson, *not* because non-Hermitian matrices could be regarded positive semidefinite, rather

---

[89] Symmetric matrices certainly arise frequently in the our chosen subject matter as well.

[90] A totally complex perspective is not necessarily more advantageous. The positive semidefinite cone, for example, is *not* self-dual (§3.6.1.2) in the subspace of Hermitian matrices. [28, §II]

because non-Hermitian (includes nonsymmetric real) matrices are not comparable on the real line under $x^HAx$. Yet that complex edifice is dismantled in the test of real matrices (551) because the domain of test is no longer necessarily complex; meaning, $x^TAx$ 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 (551), then nonsymmetric real matrices are admitted to the realm of semidefinite matrices because they become comparable on the real line. One noteworthy exception occurs for rank-one matrices $\Psi = uv^T$ where $u$ and $v$ are real vectors: $\Psi$ is positive semidefinite if and only if $\Psi$ is symmetric. (§C.2.6) 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.

### C.1.2 Example: nonsymmetric positive definite product

Horn and 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.* [24, §7.6, prob.10] [50, §6.2, §3.2]

Implicitly in their statement, $A$ and $B$ are assumed individually Hermitian, and the domain of test is assumed complex.

We show that assertion to be false for real matrices under (551) that adopts a real domain of test.

$$A^T = A = \begin{bmatrix} 3 & 0 & -1 & 0 \\ 0 & 5 & 1 & 0 \\ -1 & 1 & 4 & 1 \\ 0 & 0 & 1 & 4 \end{bmatrix}, \qquad \lambda(A) = \begin{bmatrix} 5.9 \\ 4.5 \\ 3.4 \\ 2.0 \end{bmatrix} \tag{557}$$

$$B^T = B = \begin{bmatrix} 4 & 4 & -1 & -1 \\ 4 & 5 & 0 & 0 \\ -1 & 0 & 5 & 1 \\ -1 & 0 & 1 & 4 \end{bmatrix}, \qquad \lambda(B) = \begin{bmatrix} 8.8 \\ 5.5 \\ 3.3 \\ 0.24 \end{bmatrix} \tag{558}$$

$$(AB)^T \neq AB = \begin{bmatrix} 13 & 12 & -8 & -4 \\ 19 & 25 & 5 & 1 \\ -5 & 1 & 22 & 9 \\ -5 & 0 & 9 & 17 \end{bmatrix}, \qquad \lambda(AB) = \begin{bmatrix} 36. \\ 29. \\ 10. \\ 0.72 \end{bmatrix} \tag{559}$$

$$\tfrac{1}{2}(AB + (AB)^T) = \begin{bmatrix} 13 & 15.5 & -6.5 & -4.5 \\ 15.5 & 25 & 3 & 0.5 \\ -6.5 & 3 & 22 & 9 \\ -4.5 & 0.5 & 9 & 17 \end{bmatrix}, \quad \lambda\big(\tfrac{1}{2}(AB + (AB)^T)\big) = \begin{bmatrix} 36. \\ 30. \\ 10. \\ 0.014 \end{bmatrix} \tag{560}$$

By (561), positive definiteness of the product $AB$ is affirmed by the eigenvalues in (560), yet $AB$ is not symmetric.[91] The anomaly is resolved by choosing to exclude nonsymmetric matrices, as do Horn, Johnson, and Zhang; they do so by expanding the domain of test to $\mathbb{C}^n$.

## C.2 Proper statements of positive semidefiniteness

We state several fundamental facts regarding the positive semidefiniteness of real matrix $A$ and the product $AB$ of real matrices under the fundamental test (551). Only one of them requires proof, as it departs from the standard texts, while those remaining are well established or obvious. Ironically, the restriction to real $x$ in the test complicates these facts when compared to the corresponding facts for the complex case.

For $A \in \mathbb{R}^{n\times n}$, let $\lambda\big(\frac{1}{2}(A + A^T)\big) \in \mathbb{R}^n$ denote the eigenvalues of symmetrized matrix $A$.[92]

- For $A \in \mathbb{R}^{n\times n}$, (§C.2.1)

$$\lambda(A + A^T) \succeq 0 \;\Leftrightarrow\; A + A^T \succeq 0 \;\Leftrightarrow\; A \succeq 0 \tag{561}$$

- Matrix symmetry is not intrinsic to positive semidefiniteness;

$$A^T = A, \quad \lambda(A) \succeq 0 \;\Rightarrow\; A \succeq 0 \tag{562}$$

$$\lambda(A) \succeq 0 \;\Leftarrow\; A^T = A, \quad A \succeq 0 \tag{563}$$

[91] It is a little more difficult to find a counter-example in $\mathbb{R}^{\mathbf{2\times2}}$ or $\mathbb{R}^{\mathbf{3\times3}}$; which may have served to advance any confusion.

[92] The symmetrization of $A$ is $(A + A^T)/2$. $\lambda\big(\frac{1}{2}(A + A^T)\big) = \lambda(A + A^T)/2$.

- If $A^T = A$ then
$$\lambda(A) \succeq 0 \;\Leftrightarrow\; A \succeq 0 \tag{564}$$

- For $A \in \mathbb{R}^{m\times n}$,
$$A^TA \succeq 0\,, \qquad AA^T \succeq 0 \tag{565}$$
because, for dimensionally compatible vector $x$, $x^TA^TAx = \|Ax\|_2^2$, $x^TAA^Tx = \|A^Tx\|_2^2$.

- For $A, B \in \mathbb{S}^n$, product $AB$ is symmetric if and only if $AB$ is commutative;
$$(AB)^T = AB \;\Leftrightarrow\; AB = BA \tag{566}$$

- For $A, B \in \mathbb{R}^{n\times n}$ and $AB = BA$,
$$A \succeq 0,\; B \succeq 0 \;\Rightarrow\; \lambda(A + A^T)_i\, \lambda(B + B^T)_i \geq 0 \;\; \forall i \;\;\not\Leftrightarrow\;\; AB \succeq 0 \tag{567}$$
For example, $X^2$ is generally *not* positive semidefinite unless $X$ is symmetric; then (565) applies.

- For $A, B \in \mathbb{S}^n$ and $AB = BA$,
$$A \succeq 0,\; B \succeq 0 \;\Rightarrow\; \lambda(A)_i\, \lambda(B)_i \geq 0 \;\; \forall i \;\;\Leftrightarrow\;\; AB \succeq 0 \tag{568}$$
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, [19, §5.6] we have $A = S\Lambda S^T$ and $B = T\Delta T^T$, where $\Lambda$ and $\Delta$ are real diagonal matrices while $S$ and $T$ are orthogonal matrices. Because $(AB)^T = AB$, then $T$ must equal $S$, [24, §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 (561). 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 (561), and so all products $\lambda(A)_i\, \lambda(B)_i$ must be nonnegative; meaning, $\mathrm{sgn}(\lambda(A)) = \mathrm{sgn}(\lambda(B))$. We may, therefore, conclude nothing about the semidefiniteness of $A$ and $B$. ♦

### C.2.1

**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 [19, §6]

$$A\succeq 0 \;\Leftrightarrow\; \lambda\big(\tfrac{1}{2}(A+A^T)\big)\succeq 0 \tag{569}$$

$$A\succ 0 \;\Leftrightarrow\; \lambda\big(\tfrac{1}{2}(A+A^T)\big)\succ 0 \tag{570}$$

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 [24, §7.7, prob.1]

$$A\succeq B \;\Rightarrow\; \lambda\big(\tfrac{1}{2}(A+A^T)\big)\succeq\lambda\big(\tfrac{1}{2}(B+B^T)\big) \tag{571}$$

$\diamond$

### C.2.2

**Theorem.** *Positive (semi)definite matrix.*
$A\in\mathbb{S}^M$ is positive semidefinite if and only if for each and every real vector $w$ of unit norm, $\|w\|=1$,[93] (551)

$$A\succeq 0 \;\;\Leftrightarrow\;\; \operatorname{tr}(ww^TA) \;=\; w^TAw \;\geq\; 0 \tag{572}$$

Matrix $A\in\mathbb{S}^M$ is positive definite if and only if for each and every $\|w\|=1$,

$$A\succ 0 \;\;\Leftrightarrow\;\; \operatorname{tr}(ww^TA) \;=\; w^TAw \;>\; 0 \tag{573}$$

Further, for $W,A\in\mathbb{S}_+^M$ [4, §2.6.1, exer.2.8] [62, §3.1],

$$\operatorname{tr}(WA)=0 \;\Leftrightarrow\; WA \;=AW \;=\; \mathbf{0} \tag{574}$$

Matrices $A$ and $W$ are *simultaneously diagonalizable* [24] in that circumstance. $\diamond$

---

[93] The traditional condition requiring *all* $w\in\mathbb{R}^M$ 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. Further, relations (572) and (573) remain true when $ww^T$ is replaced with "each and every" $W\in\mathbb{S}_+^M$ [9, old§1.6.1] of unit norm, but this condition is also more than what is necessary.

### C.2.3

**Corollary.** *Positive (semi)definite symmetrical products.*

- If matrix $A \in \mathbb{S}^M$ is positive (semi)definite then, for any matrix $Z$ of compatible dimension, $Z^T\!AZ$ is positive *semi*definite.

- 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.

- $A \in \mathbb{S}^M$ is positive (semi)definite if and only if there exists a nonsingular $Z$ such that $Z^T\!AZ$ is positive (semi)definite. [24, 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. [*ibidem*][94]

$\diamond$

### C.2.4

**Theorem.** *Positive (semi)definite principal submatrices.*[95]

- $A \in \mathbb{S}^M$ 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.

$\diamond$

---

[94] Using the interpretation in §A.3.4.1, 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.

[95] A recursive condition for positive (semi)definiteness, this theorem is a synthesis of facts from [24, §7.2] [19, §6.3]. Principal submatrices are formed by discarding any subset of rows and columns having the same indices. There are $M!/(1!(M-1)!)$ principal $1\times 1$ submatrices, $M!/(2!(M-2)!)$ principal $2\times 2$ 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.

### C.2.5

**Theorem.** *Symmetric projector semidefinite.* [30, §6] [100, p.55] [29, §III] For symmetric idempotent matrices $P$ and $R$,

$$\begin{gathered} P, R \succeq 0 \\ P \succeq R \;\Leftrightarrow\; \mathcal{R}(P) \supseteq \mathcal{R}(R) \;\Leftrightarrow\; \mathcal{N}(P) \subseteq \mathcal{N}(R) \end{gathered} \tag{575}$$

Projector $P$ is never positive definite [86, §6.5, prob.20] unless it is the identity matrix. $\diamond$

### C.2.6

**Theorem.** *Symmetric positive semidefinite.* Given real matrix $\Psi$ with $\operatorname{rank}\Psi = 1$,

$$\Psi \succeq 0 \;\Leftrightarrow\; \Psi = \Psi^T \tag{576}$$

$\diamond$

**Proof.** Any rank-one matrix must have the form $\Psi = uv^T$. (§C.7) Suppose $\Psi$ is symmetric; *id est*, $v = u$. For all $y \in \mathbb{R}^M$, $y^T u\, u^T y \geq 0$. Conversely, suppose $uv^T \succeq 0$. We know $uv^T \succeq 0 \;\Leftrightarrow\; uv^T + vu^T \succeq 0 \;\Leftrightarrow$ 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 §C.1.2 shows.

## C.3 Schur complement

Consider the block matrix $G$: Given $A^T = A$ and $C^T = C$, then [1]

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} &\succeq 0 \\ \Leftrightarrow \;\; A \succeq 0, \;\; B^T(I - AA^\dagger) = \mathbf{0}, \;\; C - B^T A^\dagger B &\succeq 0 \\ \Leftrightarrow \;\; C \succeq 0, \;\; B(I - CC^\dagger) = \mathbf{0}, \;\; A - BC^\dagger B^T &\succeq 0 \end{aligned} \tag{577}$$

where $A^\dagger$ denotes the Moore-Penrose (pseudo)inverse (§A). In the first instance, $I - AA^\dagger$ is a symmetric projection matrix orthogonally projecting on $\mathcal{N}(A^T)$. (§493) It is apparently required that $\mathcal{R}(B) \perp \mathcal{N}(A^T)$; 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 $\mathcal{R}(B^T) \perp \mathcal{N}(C^T)$; which precludes $C = \mathbf{0}$ for $B$ nonzero. Again, $C \succ 0 \Rightarrow C^\dagger = C^{-1}$. So we get,

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} &\succeq 0 \\ \Leftrightarrow \;\; A \succ 0, \;\; C - B^T A^{-1} B &\succeq 0 \\ \Leftrightarrow \;\; C \succ 0, \;\; A - BC^{-1} B^T &\succeq 0 \end{aligned} \tag{578}$$

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,

$$\begin{aligned} G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} &\succ 0 \\ \Leftrightarrow \;\; A \succ 0, \;\; C - B^T A^{-1} B &\succ 0 \\ \Leftrightarrow \;\; C \succ 0, \;\; A - BC^{-1} B^T &\succ 0 \end{aligned} \tag{579}$$

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 $A - BC^{-1}B^T$. [93, §4.8]

### C.3.1 Determinant

$$G = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \tag{580}$$

We consider again a matrix $G$ partitioned similarly to (577), but not necessarily positive (semi)definite, where $A\,,C\in\mathbb{S}^m$.

- When $A$ is invertible,

$$\det G \;=\; \det A \;\; \det(C - B^TA^{-1}B) \tag{581}$$

When $C$ is invertible,

$$\det G \;=\; \det C \;\; \det(A - BC^{-1}B^T) \tag{582}$$

- When $B$ is full rank and skinny, $C = \mathbf{0}$, and $A \succeq 0$, then [9, §10]

$$\det G \neq 0 \;\Leftrightarrow\; A + BB^T \succ 0 \tag{583}$$

When $B$ is a (column) vector, then for all $C\in\mathbb{R}$ and all $A$ of dimension compatible with $G$,

$$\det G \;=\; \det(A)C - B^TA_{cof}^TB \tag{584}$$

while for $C\neq 0$,

$$\det G \;=\; C\,\det(A - \frac{1}{C}BB^T) \tag{585}$$

- When $B$ is full rank and fat, $A = \mathbf{0}$, and $C \succeq 0$, then

$$\det G \neq 0 \;\Leftrightarrow\; C + B^TB \succ 0 \tag{586}$$

When $B$ is a row vector, then for $A\neq 0$ and all $C$ of dimension compatible with $G$,

$$\det G \;=\; A\,\det(C - \frac{1}{A}B^TB) \tag{587}$$

while for all $A\in\mathbb{R}$,

$$\det G \;=\; \det(C)A - BC_{cof}^TB^T \tag{588}$$

where $A_{cof}$ and $C_{cof}$ are matrices of cofactors [19, §4] (the *adjugates*) respectively corresponding to $A$ and $C$.

### C.3.2 Rank

Fazel's rank theorem...

## C.4 *0 eigenvalues theorem*

**Theorem.** *Number of* 0 *eigenvalues.* For any $A \in \mathbb{R}^{m\times n}$,

$$\operatorname{rank}(A) + \dim \mathcal{N}(A) = n \tag{589}$$

by *conservation of dimension.* [24, §0.4.4] For any square $A \in \mathbb{R}^{m\times m}$, the number of 0 eigenvalues is at least equal to $\dim \mathcal{N}(A)$,

$$\dim \mathcal{N}(A) \;\le\; \text{number of } 0 \text{ eigenvalues} \;\le\; m \tag{590}$$

while the eigenvectors corresponding to those 0 eigenvalues belong to $\mathcal{N}(A)$. [19, §5.1][96] For diagonalizable $A$ (§A.1.1), 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 $\mathcal{R}(A)$.

Likewise, for any $A \in \mathbb{R}^{m\times n}$,

$$\operatorname{rank}(A^T) + \dim \mathcal{N}(A^T) = m \tag{591}$$

For any square $A \in \mathbb{R}^{m\times m}$, the number of 0 eigenvalues is at least equal to $\dim \mathcal{N}(A^T) = \dim \mathcal{N}(A)$ (590) while the *left-eigenvectors* (eigenvectors of $A^T$) corresponding to those 0 eigenvalues belong to $\mathcal{N}(A^T)$. For $A$ diagonalizable, 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 $\mathcal{R}(A^T)$. $\diamond$

---

[96] We take as given the well-known fact that the number of 0 eigenvalues cannot be less than the dimension of the nullspace. We offer an example of the converse:

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

$\dim \mathcal{N}(A) = 2$, $\lambda(A) = \{0, 0, 0, 1\}$; three eigenvectors in the nullspace but only two are independent. The right-hand side of (590) is tight for nonzero matrices; *e.g.*, (§C.7) dyad $uv^T \in \mathbb{R}^{m\times m}$ has $m$ 0-eigenvalues when $u \in v^\perp$.

**Proof.** First we show that 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: [Alison Kay Hottes]

If $A\in\mathbb{R}^{m\times m}$ is full rank (invertible), then all $m=\operatorname{rank}(A)$ eigenvalues are nonzero. [19, §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. [19, §5.2] Eigenvectors of a real matrix corresponding to zero eigenvalues must be real.[97] Thus $A$ has at least $m-\operatorname{rank}(A)$ eigenvalues equal to 0.

Now suppose $A$ has more than $m-\operatorname{rank}(A)$ eigenvalues equal to 0. Then there are more than $m$–$\operatorname{rank}(A)$ linearly independent eigenvectors associated with 0 eigenvalues, and each of those eigenvectors must be in $\mathcal{N}(A)$. Thus there are more than $m-\operatorname{rank}(A)$ linearly independent vectors in $\mathcal{N}(A)$; a contradiction.

Therefore diagonalizable $A$ has $\operatorname{rank}(A)$ nonzero eigenvalues and exactly $m-\operatorname{rank}(A)$ 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 that when $A$ is diagonalizable, the real and imaginary parts of the eigenvectors, corresponding to nonzero eigenvalues, span $\mathcal{R}(A)$:

Any diagonalizable matrix $A\in\mathbb{R}^{m\times m}$ must possess a complete set of linearly independent eigenvectors. Further, the right-eigenvectors 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 (472) (§A.1.1), assuming 0 eigenvalues are ordered last,

$$A \;=\; \sum_{i=1}^{m}\lambda_i\; s_i w_i^T \;=\; \sum_{\substack{i=1\\ \lambda_i\neq 0}}^{k\,\leq\, m}\lambda_i\; s_i w_i^T \tag{592}$$

From the *linear independence theorem* (§C.7.1), the dyads $\{s_i w_i^T\}$ must be independent because each set of eigenvectors are; hence $\operatorname{rank}A=k$, the

[97] 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, $As_i^*=\mathbf{0}\ \Rightarrow\ As_i=As_i^*\ \Rightarrow\ s_i=s_i^*$.

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 (592), we get the partial summation

$$\begin{aligned}\lambda_i\, s_i w_i^T + \lambda_i^*\, s_i^* w_i^{*T} &= 2\,\mathrm{Re}(\lambda_i\, s_i w_i^T)\\ &= 2\big(\mathrm{Re}\, s_i\ \mathrm{Re}(\lambda_i\, w_i^T) - \mathrm{Im}\, s_i\ \mathrm{Im}(\lambda_i\, w_i^T)\big)\end{aligned} \tag{593}$$

where[98] $\lambda_i^* = \lambda_{i+1}$ , $s_i^* = s_{i+1}$ , and $w_i^* = w_{i+1}$ . Then (592) is equivalently written

$$A = 2\sum_{\substack{i\\ \lambda\in\mathbb{C}\\ \lambda_i\neq 0}} \mathrm{Re}\, s_{2i}\ \mathrm{Re}(\lambda_{2i}\, w_{2i}^T) - \mathrm{Im}\, s_{2i}\ \mathrm{Im}(\lambda_{2i}\, w_{2i}^T) \ + \sum_{\substack{j\\ \lambda\in\mathbb{R}\\ \lambda_j\neq 0}} \lambda_j\ s_j w_j^T \tag{594}$$

The summation (594) shows that $A$ is a linear combination of real and imaginary parts of its right-eigenvectors corresponding to nonzero eigenvalues. Therefore, the $k$ vectors $\{\mathrm{Re}\, s_i\,, \mathrm{Im}\, s_i \mid \lambda_i \neq 0,\ i\in\{1\ldots m\}\}$ must span the range of diagonalizable matrix $A$.

The argument is similar regarding the span of the left-eigenvectors. ♦

## C.5 Main diagonal $\delta$ operator, trace

When linear function $\delta$ 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;

$$\delta(A) \in \mathbb{R}^N \quad (180)$$

Operating on a vector, $\delta$ naturally returns a diagonal matrix. Operating recursively on a diagonal matrix $\Lambda\in\mathbb{R}^{N\times N}$, $\delta(\delta(\Lambda))$ returns $\Lambda$ itself;

$$\delta^2(\Lambda) \triangleq \delta(\delta(\Lambda)) \triangleq \Lambda \in \mathbb{R}^{N\times N} \tag{595}$$

Defined in this manner, linear operator $\delta$ is self-adjoint [17, §3.10]; *videlicet*, for $y\in\mathbb{R}^N$, (§2.1.1)

$$\delta(A)^T y = <\delta(A)\,,\, y> = <A\,, \delta(y)> = \mathrm{tr}\big(A^T \delta(y)\big) \tag{596}$$

[98] The complex conjugate of $w$ is denoted $w^*$, while its Hermitian transpose is denoted by $w^H = w^{*T}$.

This notation is efficient as illustrated in the following examples where $A\circ B$ denotes the Hadamard product [24] [25, §1.1.4] of matrices of like size: for $A\,,B\in\mathbb{R}^{N\times N}$,

1. $\delta(A+B)=\delta(A)+\delta(B)$

2. $\delta(cA)=c\,\delta(A)\,,\quad c\in\mathbb{R}$

3. $\delta(AB)=(A\circ B^T)\mathbf{1}=(B^T\circ A)\mathbf{1}$

4. $\delta(AB)^T=\mathbf{1}^T(A^T\circ B)=\mathbf{1}^T(B\circ A^T)$

5. $$\begin{aligned}\operatorname{tr}(A^TB)&=\operatorname{tr}(AB^T)=\operatorname{tr}(BA^T)=\operatorname{tr}(B^TA)\\&=\mathbf{1}^T(A\circ B)\mathbf{1}=\mathbf{1}^T\delta(AB^T)=\delta(A^TB)^T\mathbf{1}\end{aligned}$$

6. $$\begin{aligned}y^TB\,\delta(A)&=\operatorname{tr}\big(B\,\delta(A)y^T\big)=\operatorname{tr}\big(\delta(B^Ty)A\big)=\operatorname{tr}\big(A\,\delta(B^Ty)\big)\\&=\delta(A)^TB^Ty=\operatorname{tr}\big(y\,\delta(A)^TB^T\big)=\operatorname{tr}\big(A^T\delta(B^Ty)\big)=\operatorname{tr}\big(\delta(B^Ty)A^T\big)\end{aligned}$$

7. For $\lambda=[\lambda_i]\in\mathbb{R}^k$ and $x=[x_i]\in\mathbb{R}^k$, $\sum\limits_i\lambda_i/x_i\;=\;\lambda^T\delta(x)^{-1}\mathbf{1}$.

8. For any permutation matrix $\Xi$ and dimensionally compatible vector $y$ or matrix $A$,

$$\begin{aligned}\delta(\Xi\,y)\;&=\;\Xi\,\delta(y)\,\Xi^T\\\delta(\Xi\,A\,\Xi^T)&=\Xi\,\delta(A)\end{aligned}$$

   So given any permutation matrix $\Xi$ and any compatible matrix $B$, for example,

$$\delta^2(B)=\;\Xi\,\delta^2(\Xi^TB\,\Xi)\Xi^T$$

9. For $A\in\mathbb{S}_+^N$ and $\beta\in\mathbb{R}$, [9, new§B.1.5]

$$\begin{array}{rcll}\beta\operatorname{tr}A&=&\underset{X\in\mathbb{S}^N}{\text{maximize}}&\operatorname{tr}(XA)\\&&\text{subject to}&X\preceq\beta I\end{array}$$

## C.6 Orthogonal matrix

The characteristic [19, §2.6, §3.4] [86, §6.5] [24, §2.1]

$$Q^{-1} = Q^T \tag{597}$$

defines an orthogonal matrix $Q$ employed to effect vector rotation; for $x \in \mathbb{R}^n$,

$$\|Qx\| = \|x\| \tag{598}$$

Applying definition (597) to $Q^T$ we see it is also an orthogonal matrix. Hence the rows and columns of $Q$ respectively form an orthonormal set. All permutation matrices, for example, are orthogonal matrices.

An orthogonal matrix for point-wise reflection is additionally characterized by symmetry;

$$Q^{-1} = Q^T = Q \tag{599}$$

The Householder matrix (§C.8.1) is an example of a symmetric orthogonal (reflection) matrix. Any reflection matrix is related to some projection matrix $P$ of orthogonal projection by [90, §1, prob.44]

$$Q = I - 2P \tag{600}$$

Yet $P$ is, generally, neither orthogonal nor invertible. Reflection is with respect to $\mathcal{R}(P)^{\perp}$. Matrix $2P-I$ represents anti-reflection. Every orthogonal matrix can be expressed as the product of a rotation and a reflection.

Each eigenvalue of an orthogonal matrix has magnitude 1, while only the identity matrix can be simultaneously positive definite and orthogonal. The collection of all orthogonal matrices of particular dimension does not form a convex set.

Orthogonal matrices are also employed to rotate or reflect other matrices: [25, §12.4.1] The product $Q^TA$ will rotate $A \in \mathbb{R}^{n\times n}$ in the vectorization sense in $\mathbb{R}^{n^2}$ because (§2.1.1.1)

$$\|Q^TA\|_{\mathrm{F}} = \sqrt{\operatorname{tr}(A^TQQ^TA)} = \|A\|_{\mathrm{F}} \tag{601}$$

(likewise for $AQ$). Were $A$ symmetric, such a rotation would depart from $\mathbb{S}^n$. One remedy is to instead form the product $Q^TAQ$ because

$$\|Q^TAQ\|_{\mathrm{F}} = \sqrt{\operatorname{tr}(Q^TA^TQQ^TAQ)} = \|A\|_{\mathrm{F}} \tag{602}$$

This rotation of $A$ in the vectorization sense has an added benefit: the simultaneous rotation/reflection of range and rowspace.[99] We see that by recalling, any matrix can be expressed in terms of its singular value decomposition $A = U\Sigma W^T$ (499) where $\delta^2(\Sigma) = \Sigma$, $\mathcal{R}(U) \supseteq \mathcal{R}(A)$, and $\mathcal{R}(W) \supseteq \mathcal{R}(A^T)$.

# Simple matrices

## C.7 Rank-one (dyadic) matrix

Any matrix formed from the outer product of two vectors,

$$\Psi = uv^T \in \mathbb{R}^{M\times N} \tag{603}$$

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 $\Psi$. [24, §0.4, (§1.4, prob.1, $M=N$)] For matrix products $AB^T$, in general, we have

$$\mathcal{R}(AB^T) \subseteq \mathcal{R}(A), \qquad \mathcal{N}(AB^T) \supseteq \mathcal{N}(B^T) \tag{604}$$

with equality when $B = A$ [19, §3.3, §3.6][100] or when $B^TA = I$ (that means $A$ has no nullspace (p.193)). Yet for all nonzero dyads we have

$$\mathcal{R}(uv^T) = \mathcal{R}(u), \qquad \mathcal{N}(uv^T) = \mathcal{N}(v^T) \equiv v^\perp \tag{605}$$

where $\dim v^\perp = N-1$.

When $u$ and $v$ are normalized, the pseudoinverse is the transposed dyad. Otherwise,

$$\Psi^\dagger \;=\; (uv^T)^\dagger \;=\; \frac{vu^T}{\|u\|^2\,\|v\|^2} \tag{606}$$

and

$$\|\Psi\| \;=\; \|uv^T\| \;=\; \|u\|\,\|v\| \tag{607}$$

[99] The product $Q^TAQ$ 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 (493) of matrix $A$.

[100] $\mathcal{R}(AA^T) \subseteq \mathcal{R}(A)$ is obvious.

$$\begin{aligned}\mathcal{R}(AA^T) \;&=\; \{AA^Ty \mid y \in \mathbb{R}^m\}\\ &\supseteq\; \{AA^Ty \mid A^Ty \in \mathcal{R}(A^T)\} = \mathcal{R}(A) \text{ by (493)3.}\end{aligned}$$

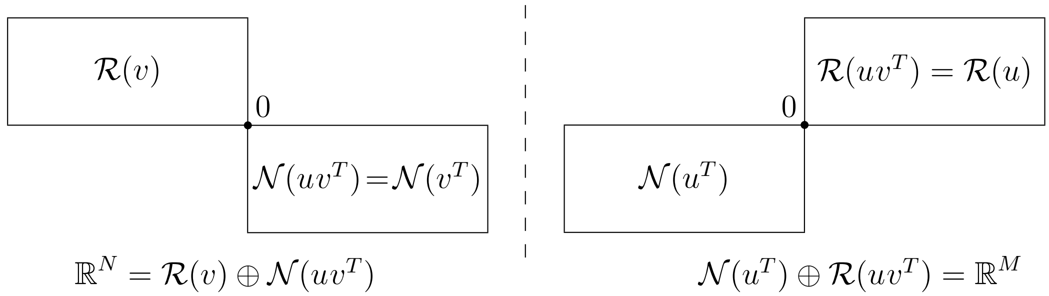


Figure 31: The four fundamental subspaces [86, §3.6] of any dyad $uv^T \in \mathbb{R}^{M\times N}$. $\Psi = uv^T$ is a mapping from $\mathbb{R}^N$ to $\mathbb{R}^M$. The map from $\mathcal{R}(v)$ to $\mathcal{R}(u)$ is one-to-one and onto. [19, §3.1]

When dyad $uv^T \in \mathbb{R}^{N\times N}$ is square, $uv^T$ has at least $N-1$ zero eigenvalues and corresponding eigenvectors spanning $v^\perp$. The remaining eigenvector $u$ spans the range of $uv^T$ with corresponding eigenvalue

$$\lambda = v^T u = \operatorname{tr}(uv^T) \tag{608}$$

The determinant is the product of the eigenvalues; so, it is always true that

$$\det \Psi = \det(uv^T) = 0 \tag{609}$$

When $\lambda = 1$, the square dyad is a nonorthogonal projector on its range ($\Psi^2 = \Psi$, §A.1). It is quite possible that $u \in v^\perp$ making the remaining eigenvalue zero $\lambda = 0$ along with the first $N-1$ zero eigenvalues; *id est*, $uv^T$ is nonzero but its eigenvalues could all be zero. (So the dyad is not always diagonalizable (§A.1.1) because the eigenvectors are not always independent.) In other words, eigenvector $u$ may belong simultaneously to the nullspace and to the range of the dyad. The explanation is, simply, because $u$ and $v$ share the same dimension, $\dim u = M = \dim v = N$. Figure 31 shows the four fundamental subspaces for the dyad. [19, §3.1] Linear operator $\Psi$ is a mapping from one vector space to another; $\Psi : \mathbb{R}^N \rightarrow \mathbb{R}^M$. Vector spaces $\mathbb{R}^N$ and $\mathbb{R}^M$ remain distinct when $M = N$;

$$\begin{gathered} u \in \mathcal{R}(uv^T), \qquad u \in \mathcal{N}(uv^T) \Leftrightarrow v^T u = 0 \\ \mathcal{R}(uv^T) \cap \mathcal{N}(uv^T) = \{\emptyset\} \end{gathered} \tag{610}$$

**rank-one modification**

If $A$ is any nonsingular matrix of compatible dimension and

$$1 + v^T A^{-1} u \neq 0$$

then [101, App.6] [50, §2.3, prob.16]

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1} uv^T A^{-1}}{1 + v^T A^{-1} u} \tag{611}$$

**dyadic symmetry**

In the specific circumstance that $v = u$, then $uu^T$ is symmetric, rank-one, and positive semidefinite. In fact, (§C.2.6)

$$uv^T \succeq 0 \;\Leftrightarrow\; v = u \tag{612}$$

### C.7.1 Dyadic independence

Now we consider a sum of dyads like (603) as encountered in diagonalization and singular value decomposition.

**Definition.** *Dyadic linear independence.* [102, pg.29, thm.11] [103, pg.2] The set of $k$ dyads

$$\left\{ s_i w_i^T \mid i = 1 \ldots k \right\} \tag{613}$$

where $s_i \in \mathbb{C}^M$ and $w_i \in \mathbb{C}^N$, is said to be linearly independent iff

$$\operatorname{rank}\left( \Upsilon \;\triangleq\; \sum_{i=1}^{k} s_i w_i^T \;=\; SW^T \right) = \; k \tag{614}$$

where $S \triangleq [s_1 \cdots s_k] \in \mathbb{C}^{M \times k}$, $W \triangleq [w_1 \cdots w_k] \in \mathbb{C}^{N \times k}$, and $\Upsilon \in \mathbb{C}^{M \times N}$. $\diamond$

As defined, dyadic independence does not preclude the existence of a null-space $\mathcal{N}(\Upsilon)$, nor does it imply $\Upsilon$ is full rank. In the absence of an assumption of independence, generally, $\operatorname{rank} \Upsilon \leq k$. Conversely, any rank-$k$ matrix can be written in the form $\Upsilon$. [24, §0.4.6(e), (§1.4, prob.2, $M = N$)]

**Theorem.** *Linear independence.* The vectors $\{s_i \in \mathbb{C}^M,\ i=1\ldots k\}$ are linearly independent and the vectors $\{w_i \in \mathbb{C}^N,\ i=1\ldots k\}$ are linearly independent if and only if the dyads $\{s_i w_i^T,\ i=1\ldots k\}$ are linearly independent. $\diamond$

**Proof.** Linear independence of $k$ dyads is identical to definition (614).
$\Longrightarrow$ Suppose $\{s_i\}$ and $\{w_i\}$ are each linearly independent sets. Invoking Sylvester's rank inequality, [24, §0.4] [50, §2.4]

$$\operatorname{rank} S + \operatorname{rank} W - k \ \leq\ \operatorname{rank}(SW^T) \ \leq\ \min\{\operatorname{rank} S,\ \operatorname{rank} W\} \ \ (\leq\ k) \tag{615}$$

Then $k \leq \operatorname{rank}(SW^T) \leq k$ that implies the dyads are independent.
$\Longleftarrow$ Conversely, suppose $\operatorname{rank}(SW^T) = k$. Then $k \leq \min\{\operatorname{rank} S,\ \operatorname{rank} W\} \leq k$ that implies the vector sets are each independent. ♦

**C.7.1.1 Biorthogonality condition, nullspace.** Dyads characterized by a biorthogonality condition are independent; *id est*, for $S \in \mathbb{C}^{M\times k}$ and $W \in \mathbb{C}^{N\times k}$, if $W^TS = I$ then $\operatorname{rank}(SW^T) = k$ because then $\operatorname{rank} S = \operatorname{rank} W = k \leq M = N$ (*e.g.*, §A.1.2).

To see that, because of the *linear independence theorem* we need only show: $\mathcal{N}(S) = \mathbf{0} \ \Leftrightarrow\ \exists\ B \ \ni\ BS = I$. (Left inverse is not unique.)
$\Longleftarrow$ Assume $BS = I$. Then $\mathcal{N}(BS) = \mathbf{0} = \{x \mid BSx = \mathbf{0}\} \supseteq \mathcal{N}(S)$. (604)
$\Longrightarrow$ 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: $\mathcal{N}(W) = \mathbf{0} \ \Leftrightarrow\ \exists\ S \ \ni\ S^TW = I$. ♦

Dyads produced by diagonalization, for example, are independent because of their inherent biorthogonality. (§A.1.1.1) The converse is generally false; *id est*, linearly independent dyads are not necessarily biorthogonal.

Under the biorthogonality condition $W^TS = I$, nullspace $\mathcal{N}(SW^T)$ must be equivalent to $\mathcal{N}(W^T)$: $\mathcal{N}(SW^T) \supseteq \mathcal{N}(W^T)$ is obvious.

$$\mathcal{N}(SW^T) \ =\ \{x \mid SW^Tx = \mathbf{0}\} \ \subseteq\ \{x \mid W^TSW^Tx = \mathbf{0}\} \ =\ \mathcal{N}(W^T) \tag{616}$$

## C.8 Elementary matrix

A matrix of the form

$$E = I - \zeta u v^T \in \mathbb{R}^{N\times N} \tag{617}$$

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.* [90] 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

$$\lambda = 1 - \zeta v^T u \tag{618}$$

corresponds to eigenvector $u$. (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.)

$$\det E \;=\; 1 - \operatorname{tr}\!\big(\zeta u v^T\big) \;=\; \lambda \tag{619}$$

[101, App.7] If $\lambda \neq 0$ then $E$ is invertible; [93]

$$E^{-1} = I + \frac{\zeta}{\lambda} u v^T \tag{620}$$

Eigenvectors corresponding to zero eigenvalues belong to $\mathcal{N}(E)$, and the number of zero eigenvalues must be at least $\dim \mathcal{N}(E)$ that, here, can be at most 1. (§C.4) 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 ($E^2 = E$, §A.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 (617) 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,

$$\mathcal{R}(E) = \mathcal{N}(v^T), \qquad \mathcal{N}(E) = \mathcal{R}(u), \qquad v^T u = 1/\zeta \tag{621}$$

illustrated in Figure 32, which is opposite to the assignment of subspaces for a dyad (Figure 31). Otherwise, $\mathcal{R}(E) = \mathbb{R}^N$.

When $E = E^T$,

$$\|E\| = \max\{1\,, |\lambda|\} \tag{622}$$

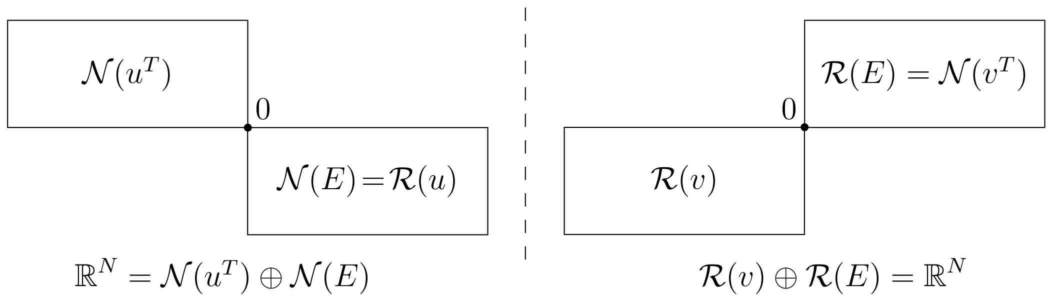


Figure 32: The four fundamental subspaces [86, §3.6] of elementary matrix $E$ when $v^Tu = 1/\zeta$ .

### C.8.1 Householder matrix

An elementary matrix is called a Householder matrix $H$ when, for nonzero vector $u$ , $E$ has the form [25, §5.1.2] [93, §4.10.1] [19, §7.3] [24, §2.2]

$$H = I - 2\frac{uu^T}{u^Tu} \tag{623}$$

which is a symmetric orthogonal (reflection) matrix ($H^{-1}=H^T=H$ (§C.6)). 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;

$$\|H\| = 1 \tag{624}$$

For example, the permutation matrix

$$\Xi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{625}$$

is a Householder matrix. Not all permutation matrices are Householder matrices, although all permutation matrices are orthogonal matrices. [19, §3.4]

## C.9 Auxiliary $V$-matrices

### C.9.1 $V$ matrix

It will become convenient to define a matrix $V$ that arises naturally as a consequence of translating the geometric center $\alpha_g$ (§4.5.1) to the origin. In place of $X - \alpha_g \mathbf{1}^T$ we may write $XV$ as in (221) where

$$V \triangleq I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^N \tag{626}$$

is an elementary matrix called a *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 $N^{\text{th}}$ eigenvalue equals 0. The number of zero eigenvalues must equal $\dim \mathcal{N}(V) = 1$, by the *0 eigenvalues theorem* (§C.4), because $V = V^T$ is diagonalizable. Because

$$V\mathbf{1} = \mathbf{0} \tag{627}$$

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 $V^2 = V$ and $V^T = V$, the elementary matrix $V$ is also a projection matrix (§A.2) projecting orthogonally on its range $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$ that has dimension $N-1$. The $\{0,1\}$ eigenvalues also indicate that diagonalizable $V$ is a projection matrix. [50, §4.1, thm.4.1] The symmetry of $V$ denotes orthogonal projection; [34] hence (496)

$$V^T = V\,, \qquad V^{\dagger} = V\,, \qquad \|V\| = 1\,, \qquad V \succeq 0 \tag{628}$$

Matrix $V$ is also circulant. (§12.3) 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.

### C.9.2 Matrix $V_w$

Here is a skinny matrix having the same range as $V$ but with orthonormal columns: [81]

$$V_w \triangleq \begin{bmatrix} \frac{-1}{\sqrt{N}} & \frac{-1}{\sqrt{N}} & \cdots & \frac{-1}{\sqrt{N}} \\ 1+\frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & \frac{-1}{N+\sqrt{N}} \\ \frac{-1}{N+\sqrt{N}} & \ddots & \cdots & \frac{-1}{N+\sqrt{N}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & 1+\frac{-1}{N+\sqrt{N}} \end{bmatrix} \in \mathbb{R}^{N\times N-1} \tag{629}$$

We defined three auxiliary $V$ matrices, $V$, $V_{\mathcal{N}}$ (199), and $V_w$, that share some common attributes listed in Table C.9.4. For example, $V$ can be expressed

$$V = V_w V_w^T = V_{\mathcal{N}} V_{\mathcal{N}}^\dagger \tag{630}$$

but $V_w^T V_w = I$ that means $V$ is an orthogonal projector (494), and

$$V_w^\dagger = V_w^T\,, \qquad \|V_w\| = 1 \tag{631}$$

### C.9.3 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. $(I - e_1\mathbf{1}^T)V_{\mathcal{N}} = \begin{bmatrix} \mathbf{0} & \sqrt{2}V_{\mathcal{N}} \end{bmatrix} V_{\mathcal{N}} = V_{\mathcal{N}}$
4. $V_{\mathcal{N}}^\dagger = \sqrt{2}\begin{bmatrix} -\frac{1}{N}\mathbf{1} & I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \end{bmatrix} \in \mathbb{R}^{N-1\times N}, \qquad \left(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^{N-1}\right)$
5. $V_{\mathcal{N}}^\dagger\mathbf{1} = \mathbf{0}$
6. $V_{\mathcal{N}}^\dagger V_{\mathcal{N}} = I$
7. $[V_{\mathcal{N}} \quad \frac{1}{\sqrt{2}}\mathbf{1}]^{-1} = \begin{bmatrix} V_{\mathcal{N}}^\dagger \\ \frac{\sqrt{2}}{N}\mathbf{1}^T \end{bmatrix}$
8. $V^T = V = V_{\mathcal{N}}V_{\mathcal{N}}^\dagger = I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}^N$

9. $$\begin{array}{c} D\in\mathbb{EDM}^N \\ DD^\dagger\mathbf{1}=\mathbf{1} \\ \mathbf{1}^TD^\dagger D=\mathbf{1}^T \end{array} \qquad [47,\ \S2]$$

10. $$\begin{array}{l} D=[d_{ij}]\in\mathbb{S}_\delta^N \\ \operatorname{tr}(-V\,D\,V)=\operatorname{tr}(-V_{\mathcal{N}}^\dagger DV_{\mathcal{N}})=\frac{1}{N}\mathbf{1}^TD\,\mathbf{1}=\frac{1}{N}\operatorname{tr}(\mathbf{1}\mathbf{1}^TD)=\frac{1}{N}\sum_{i,j}d_{ij} \end{array}$$

Any elementary matrix $E\in\mathbb{S}^N$ of the particular form,[101] for $k_1\,,k_2\in\mathbb{R}$,

$$E=k_1\,I-k_2\,\mathbf{1}\mathbf{1}^T \tag{632}$$

will make $\operatorname{tr}(ED)$ proportional to $\sum d_{ij}$.

11. $$\begin{array}{l} D=[d_{ij}]\in\mathbb{S}_\delta^N \\ \operatorname{tr}(-V_{\mathcal{N}}^TDV_{\mathcal{N}})=\sum_j d_{\mathbf{1}j} \end{array}$$

### C.9.4 Auxiliary $V$-matrix Table

| | $\dim V$ | $\operatorname{rank} V$ | $\mathcal{R}(V)$ | $\mathcal{N}(V^T)$ | $V^TV$ | $VV^T$ | $VV^\dagger$ |
|---|---|---|---|---|---|---|---|
| $V$ | $N\times N$ | $N-1$ | $\mathcal{N}(\mathbf{1}^T)$ | $\mathcal{R}(\mathbf{1})$ | $V$ | $V$ | $V$ |
| $V_{\mathcal{N}}$ | $N\times(N-1)$ | $N-1$ | $\mathcal{N}(\mathbf{1}^T)$ | $\mathcal{R}(\mathbf{1})$ | $\frac{1}{2}(I+\mathbf{1}\mathbf{1}^T)$ | $\frac{1}{2}\begin{bmatrix} N-1 & -\mathbf{1}^T \\ -\mathbf{1} & I \end{bmatrix}$ | $V$ |
| $V_w$ | $N\times(N-1)$ | $N-1$ | $\mathcal{N}(\mathbf{1}^T)$ | $\mathcal{R}(\mathbf{1})$ | $I$ | $V$ | $V$ |

[101] 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. [104]

# D $-V_{\mathcal N}^T D V_{\mathcal N}$ nesting

From (241) 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 [25] [24] [19] and have the same form as $T$; *videlicet*,

$$\left\{\begin{array}{lcll}
-V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow 1} &=& \emptyset\;, & \text{(o)}\\[6pt]
-V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow 2} &=& [d_{12}] \in \mathbb{S}_+\;, & \text{(a)}\\[6pt]
-V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow 3} &=& \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} \end{bmatrix} = T \in \mathbb{S}_+^{\mathbf 2}\;, & \text{(b)}\\[6pt]
-V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow 4} &=& \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) & \frac{1}{2}(d_{12}+d_{14}-d_{24}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} & \frac{1}{2}(d_{13}+d_{14}-d_{34}) \\ \frac{1}{2}(d_{12}+d_{14}-d_{24}) & \frac{1}{2}(d_{13}+d_{14}-d_{34}) & d_{14} \end{bmatrix}, & \text{(c)}\\[6pt]
&\vdots&&\\
-V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow i} &=& \begin{bmatrix} -V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow i-1} & \nu(i) \\ \nu^T(i) & d_{1i} \end{bmatrix} \in \mathbb{S}_+^{i-1}, & \text{(d)}\\
&\vdots&&\\
-V_{\mathcal N}^T D V_{\mathcal N} &=& \begin{bmatrix} -V_{\mathcal N}^T D V_{\mathcal N}|_{N\leftarrow N-1} & \nu(N) \\ \nu^T(N) & d_{1N} \end{bmatrix} \in \mathbb{S}_+^{N-1} & \text{(e)}
\end{array}\right\} \tag{633}$$

where[102]

$$\nu(i) \triangleq \frac{1}{2}\begin{bmatrix} d_{12}+d_{1i}-d_{2i} \\ d_{13}+d_{1i}-d_{3i} \\ \vdots \\ d_{1,i-1}+d_{1i}-d_{i-1,i} \end{bmatrix} \in \mathbb{R}^{i-2}, \quad i > 2 \tag{634}$$

[102] $-V^T D V|_{N\leftarrow 1} = 0 \in \mathbb{S}_+^{\mathbf 0}$ (§C.9.1)

Bordered symmetric matrices in the form (633d) are known to have *intertwined* [19, §6.4] (or *interlaced* [24, §4.3]) eigenvalues; (*confer* §4.14.1) that means, for the particular submatrices (633a) and (633b),

$$\sigma_2 \le d_{12} \le \sigma_1 \tag{635}$$

where $d_{12}$ is the eigenvalue of the submatrix (633a), and $\sigma_1, \sigma_2$ are the eigenvalues of $T$ (633b)(241). Intertwining in (635) predicts that should $d_{12}$ become zero, then $\sigma_2$ must go to zero.[103] The eigenvalues are similarly intertwined for submatrices (633b) and (633c);

$$\gamma_3 \le \sigma_2 \le \gamma_2 \le \sigma_1 \le \gamma_1 \tag{636}$$

where $\gamma_1, \gamma_2, \gamma_3$ are the eigenvalues of submatrix (633c). Intertwining likewise predicts that should $\sigma_2$ become zero (a possibility revealed in §D.1), then $\gamma_3$ must go to zero. Combining results so far for $N = 2, 3, 4$: (635) (636)

$$\gamma_3 \le \sigma_2 \le d_{12} \le \sigma_1 \le \gamma_1 \tag{637}$$

The preceding logic extends by induction through the remaining members of the sequence (633).

## D.1 Tightening the triangle inequality

Now we apply the Schur complement from §C.3 to tighten the triangle inequality. We find that the gains by doing so are modest. From §D we identify

$$G \triangleq -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 4} \tag{638}$$

$$A \triangleq T = -V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 3} \tag{639}$$

both positive semidefinite by assumption, $B = \nu(4)$ defined in (634), and $C = d_{14}$. Using the latter non-strict form of (577), $C \ge 0$ by assumption (§4.6.1) and $CC^\dagger = I$. So by the *positive semidefinite ordering of eigenvalues theorem* (§C.2.1),

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}}|_{N\leftarrow 4} \succeq 0 \;\Leftrightarrow\; T \succeq d_{14}^{-1}\nu(4)\nu^T(4) \;\Rightarrow\; \left\{\begin{array}{l} \sigma_1 \ge d_{14}^{-1}\|\nu(4)\|^2 \\ \sigma_2 \ge 0 \end{array}\right. \tag{640}$$

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 $T$.

[103] If $d_{12}$ were zero, eigenvalue $\sigma_2$ becomes zero (243) because $d_{13}$ must then be equal to $d_{23}$; *id est*, $d_{12} = 0 \Leftrightarrow x_1 = x_2$. (47)

### D.1.1 Example revisitation

Applying the inequality for $\sigma_1$ in (640) to the *small completion problem* on page 65, Figure 20 (*confer* §4.7.3, §4.9.4.1), the lower bound on $\sqrt{d_{14}}$ , 1.236 in (173), is tightened to 1.289 . The correct value of $\sqrt{d_{14}}$ to three significant figures is 1.414 .

# E MATLAB programs...

## E.1 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 2002
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;
```

## E.2 Map of the USA

### E.2.1 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

%Execution time for factor=4 is less than 2 minutes
%on Pentium III @700MHz laptop, 256MB RAM.
%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
```

#### E.2.1.1 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';
```

### E.2.2 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
```

# F Matrix Calculus

## F.1 Gradient, directional derivative, Taylor series

### F.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

$$\nabla f(x) \triangleq \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^K \tag{641}$$

while the second-order gradient of the twice differentiable real function with respect to its vector domain is traditionally called the *Hessian*;

$$\nabla^2 f(x) \triangleq \begin{bmatrix} \frac{\partial^2 f(x)}{\partial^2 x_1} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_K} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial^2 x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_K \partial x_1} & \frac{\partial^2 f(x)}{\partial x_K \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial^2 x_K} \end{bmatrix} \in \mathbb{S}^K \tag{642}$$

The gradient of vector-valued function $v(x):\mathbb{R}\to\mathbb{R}^M$ on real domain is

$$\nabla v(x) \triangleq \begin{bmatrix} \frac{\partial v_1(x)}{\partial x} & \frac{\partial v_2(x)}{\partial x} & \cdots & \frac{\partial v_M(x)}{\partial x} \end{bmatrix} \in \mathbb{R}^M \tag{643}$$

while the second order gradient is

$$\nabla^2 v(x) \triangleq \begin{bmatrix} \frac{\partial^2 v_1(x)}{\partial x^2} & \frac{\partial^2 v_2(x)}{\partial x^2} & \cdots & \frac{\partial^2 v_M(x)}{\partial x^2} \end{bmatrix} \in \mathbb{R}^M \tag{644}$$

The gradient of vector-valued function $h(x):\mathbb{R}^K\to\mathbb{R}^M$ on vector domain is

$$\nabla h(x) \triangleq \begin{bmatrix} \frac{\partial h_1(x)}{\partial x_1} & \frac{\partial h_2(x)}{\partial x_1} & \cdots & \frac{\partial h_M(x)}{\partial x_1} \\ \frac{\partial h_1(x)}{\partial x_2} & \frac{\partial h_2(x)}{\partial x_2} & \cdots & \frac{\partial h_M(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \frac{\partial h_1(x)}{\partial x_K} & \frac{\partial h_2(x)}{\partial x_K} & \cdots & \frac{\partial h_M(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^{K\times M} \tag{645}$$

while the second-order gradient has a three-dimensional matrix representation called *cubix*;

$$\nabla^2 h(x) \triangleq \begin{bmatrix} \nabla\frac{\partial h_1(x)}{\partial x_1} & \nabla\frac{\partial h_2(x)}{\partial x_1} & \cdots & \nabla\frac{\partial h_M(x)}{\partial x_1} \\ \nabla\frac{\partial h_1(x)}{\partial x_2} & \nabla\frac{\partial h_2(x)}{\partial x_2} & \cdots & \nabla\frac{\partial h_M(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial h_1(x)}{\partial x_K} & \nabla\frac{\partial h_2(x)}{\partial x_K} & \cdots & \nabla\frac{\partial h_M(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^{K\times M\times K} \tag{646}$$

where the gradient of each real entry is with respect to vector $x$ as in (641). The gradient of real function $g(X) : \mathbb{R}^{K\times L} \rightarrow \mathbb{R}$ on matrix domain is

$$\nabla g(X) \triangleq \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L} \tag{647}$$

while the second-order gradient has a four-dimensional matrix representation called *quartix*;

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla\frac{\partial g(X)}{\partial X_{11}} & \nabla\frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g(X)}{\partial X_{21}} & \nabla\frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g(X)}{\partial X_{K1}} & \nabla\frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L} \tag{648}$$

where the gradient of each real entry is with respect to matrix $X$ as in (647). The cubix and quartix representations are not unique as they may be rotated; *e.g.*, for the cubix in (646), we can have $\mathbb{R}^{K\times K\times M}$ or $\mathbb{R}^{M\times K\times K}$.

### F.1.2 Product rule

Given $f : \mathbb{R}^{K\times L} \rightarrow \mathbb{R}^{\ell\times M}$ and $g : \mathbb{R}^{K\times L} \rightarrow \mathbb{R}^{\ell\times N}$,

$$\nabla_X\big(f(X)^T g(X)\big) = \nabla_X(f)\, g \;+\; \nabla_X(g)\, f \tag{649}$$

**Example.** *Cubix.*
Suppose $f(X):\mathbb{R}^{\mathbf{2}\times\mathbf{2}}\!\to\mathbb{R}^{\mathbf{2}} = X^Ta$ and $g(X):\mathbb{R}^{\mathbf{2}\times\mathbf{2}}\!\to\mathbb{R}^{\mathbf{2}} = Xb$. We wish to find (Table F.2.1)

$$\nabla_X\big(f(X)^T g(X)\big) = \nabla_X\, a^TX^2b \tag{650}$$

using the product rule. Formula (649) calls for

$$\nabla_X\, a^TX^2b = \nabla_X(X^Ta)\,Xb \;+\; \nabla_X(Xb)\,X^Ta \tag{651}$$

Consider the first of the two terms:

$$\begin{aligned}\nabla_X(f)\,g \;&= \nabla_X(X^Ta)\,Xb\\ &= \left[\begin{array}{cc} \frac{\partial(X^Ta)}{\partial X_{11}} & \frac{\partial(X^Ta)}{\partial X_{12}}\\[4pt] \frac{\partial(X^Ta)}{\partial X_{21}} & \frac{\partial(X^Ta)}{\partial X_{22}}\end{array}\right] Xb\end{aligned} \tag{652}$$

The gradient of $X^Ta$ forms a cubix in $\mathbb{R}^{\mathbf{2}\times\mathbf{2}\times\mathbf{2}}$.

$$\nabla_X(X^Ta)\,Xb \;=\; \left[\begin{array}{cccc} \frac{\partial(X^Ta)_1}{\partial X_{11}} & & \frac{\partial(X^Ta)_1}{\partial X_{12}} & \\ & \frac{\partial(X^Ta)_2}{\partial X_{11}} & & \frac{\partial(X^Ta)_2}{\partial X_{12}} \\ \frac{\partial(X^Ta)_1}{\partial X_{21}} & & \frac{\partial(X^Ta)_1}{\partial X_{22}} & \\ & \frac{\partial(X^Ta)_2}{\partial X_{21}} & & \frac{\partial(X^Ta)_2}{\partial X_{22}} \end{array}\right] \left[\begin{array}{c} (Xb)_1 \\[12pt] (Xb)_2 \end{array}\right] \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$$

Because the gradient of the product (650) 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 third dimension of the cubix (indicated by dotted line segments);

$$\begin{aligned}\nabla_X(X^Ta)\,Xb \;&= \left[\begin{array}{cc} \left[\begin{array}{cc} a_1 & 0 \end{array}\right] & \left[\begin{array}{cc} 0 & a_1 \end{array}\right] \\[4pt] \left[\begin{array}{cc} a_2 & 0 \end{array}\right] & \left[\begin{array}{cc} 0 & a_2 \end{array}\right] \end{array}\right] \left[\begin{array}{c} b_1X_{11}+b_2X_{12} \\ b_1X_{21}+b_2X_{22} \end{array}\right]\\ &= \left[\begin{array}{cc} a_1(b_1X_{11}+b_2X_{12}) & a_1(b_1X_{21}+b_2X_{22}) \\ a_2(b_1X_{11}+b_2X_{12}) & a_2(b_1X_{21}+b_2X_{22}) \end{array}\right]\\ &= \; ab^TX^T\end{aligned} \tag{653}$$

where the cubix is written as a matrix of row-vectors. In like manner for the second term $\nabla_X(g)\, f$,

$$\begin{aligned}\nabla_X(Xb)\,X^Ta \;&=\; \begin{bmatrix} \begin{bmatrix} b_1 & 0 \end{bmatrix} & \begin{bmatrix} b_2 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & b_1 \end{bmatrix} & \begin{bmatrix} 0 & b_2 \end{bmatrix} \end{bmatrix} \begin{bmatrix} X_{11}a_1 + X_{21}a_2 \\ X_{12}a_1 + X_{22}a_2 \end{bmatrix} \\ &=\; X^Tab^T \end{aligned} \tag{654}$$

□

### F.1.3 Chain rule

Given $f : \mathbb{R}^{K\times L} \to \mathbb{R}^{n\times m}$ and $g : \mathbb{R}^{m\times n} \to \mathbb{R}^{M\times N}$, [*sic*] [32, §15.7]

$$\nabla_X\, g\big(f(X)^T\big) = \nabla_X f^T\, \nabla_f\, g \tag{655}$$

$$\nabla_X^2\, g\big(f(X)^T\big) \;=\; \nabla_X\big(\nabla_X f^T\, \nabla_f\, g\big) \;=\; \nabla_X^2 f\; \nabla_f\, g \;+\; \nabla_X f^T\, \nabla_f^2 g\; \nabla_X f \tag{656}$$

These formulae remain correct when the gradients produce higher-dimensional representations:

### F.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 $\nabla g$ and $\nabla^2 g$ over $\operatorname{dom} g$ which is an open set. We seek simple expressions for the first and second directional derivatives, both in $\mathbb{R}^{M\times N}$, dubbed $\overset{\to Y}{dg}$ and $\overset{\to Y}{dg^2}$ respectively.

Assuming that the limit exists, we may state the partial derivative of the $mn^{\text{th}}$ entry of $g$ with respect to the $kl^{\text{th}}$ entry of $X$;

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} \;=\; \lim_{\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \tag{657}$$

where $e_k$ is the $k^{\text{th}}$ standard basis vector in $\mathbb{R}^K$ while $e_l$ is the $l^{\text{th}}$ standard basis vector in $\mathbb{R}^L$. The total number of partial derivatives equals $KLMN$ while the gradient is defined in their terms; the $mn^{\text{th}}$ entry of the gradient is

$$\nabla g_{mn}(X) \triangleq \begin{bmatrix} \frac{\partial g_{mn}(X)}{\partial X_{11}} & \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial g_{mn}(X)}{\partial X_{21}} & \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L} \tag{658}$$

while the gradient is a quartix

$$\nabla g(X) \triangleq \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L}$$

$$= \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times M\times N} \tag{659}$$

By simply rotating our perspective of the four-dimensional representation of the gradient matrix, we found a second equivalent expression for the quartix in (659). If $M=N=K=3$ and $L=1$, then the entries of $\nabla g$ could be written into the cells of a cube like Rubik's. [34] If $L>1$, then the entries of $\nabla g$ are matrices requiring a fourth dimension for their representation.

When the limit for $\Delta t\in\mathbb{R}$ exists, it is easy to show by substitution of variables in (657)

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \lim_{\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \tag{660}$$

which may be interpreted as the change in $g_{mn}$ at $X$ when the change in $X_{kl}$ is equal to $Y_{kl}$, the $kl^{\text{th}}$ entry of $Y\in\mathbb{R}^{K\times L}$. 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 $mn^{\text{th}}$ entry of the directional derivative is the corresponding total differential [32, §15.8]

$$dg_{mn}(X)|_{dX\to Y} = \sum_{k,l} \frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \operatorname{tr}\big(\nabla g_{mn}(X)^T Y\big) \tag{661}$$

$$= \sum_{k,l} \lim_{\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T) - g_{mn}(X)}{\Delta t} \tag{662}$$

$$= \lim_{\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, Y) - g_{mn}(X)}{\Delta t} \tag{663}$$

$$= \left.\frac{d}{dt}\right|_{t=0} g_{mn}(X+t\,Y) \tag{664}$$

where $t \in \mathbb{R}$. Assuming finite $Y$, equation (663) is called the *Gateaux differential* [39, App.A.5] [10, §D.2.1] [15, §5.28] whose existence is implied by the existence of the *Fréchet differential*, the sum in (661). [5, §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 $Y$.[104] Hence the directional derivative,

$$\overset{\rightarrow Y}{dg}(X) \triangleq \left.\begin{bmatrix} dg_{11}(X) & dg_{12}(X) & \cdots & dg_{1N}(X) \\ dg_{21}(X) & dg_{22}(X) & \cdots & dg_{2N}(X) \\ \vdots & \vdots & & \vdots \\ dg_{M1}(X) & dg_{M2}(X) & \cdots & dg_{MN}(X) \end{bmatrix}\right|_{dX \rightarrow Y} \in \mathbb{R}^{M\times N}$$

$$= \begin{bmatrix} \operatorname{tr}\big(\nabla g_{11}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{12}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{1N}(X)^T Y\big) \\ \operatorname{tr}\big(\nabla g_{21}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{22}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{2N}(X)^T Y\big) \\ \vdots & \vdots & & \vdots \\ \operatorname{tr}\big(\nabla g_{M1}(X)^T Y\big) & \operatorname{tr}\big(\nabla g_{M2}(X)^T Y\big) & \cdots & \operatorname{tr}\big(\nabla g_{MN}(X)^T Y\big) \end{bmatrix}$$

$$= \begin{bmatrix} \sum\limits_{k,l} \frac{\partial g_{11}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{12}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{1N}(X)}{\partial X_{kl}} Y_{kl} \\ \sum\limits_{k,l} \frac{\partial g_{21}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{22}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{2N}(X)}{\partial X_{kl}} Y_{kl} \\ \vdots & \vdots & & \vdots \\ \sum\limits_{k,l} \frac{\partial g_{M1}(X)}{\partial X_{kl}} Y_{kl} & \sum\limits_{k,l} \frac{\partial g_{M2}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum\limits_{k,l} \frac{\partial g_{MN}(X)}{\partial X_{kl}} Y_{kl} \end{bmatrix} \tag{665}$$

from which it follows

$$\overset{\rightarrow Y}{dg}(X) = \sum_{k,l} \frac{\partial g(X)}{\partial X_{kl}} Y_{kl} \tag{666}$$

Yet for all $X \in \operatorname{dom} g$, any $Y \in \mathbb{R}^{K\times L}$, and some open interval of $t \in \mathbb{R}$,

$$g(X + t\,Y) = g(X) \;+\; t\,\overset{\rightarrow Y}{dg}(X) \;+\; o(t^2) \tag{667}$$

which is the first-order Taylor expansion about $X$. [10, §0.4.1] [32, §18.4] [61, §2.3.4] Differentiation with respect to $t$ and subsequent $t$-zeroing isolates the second term of the expansion. Thus differentiating and zeroing $g(X+t\,Y)$

[104] Although $Y$ is a matrix, we may regard it as a vector in $\mathbb{R}^{KL}$.

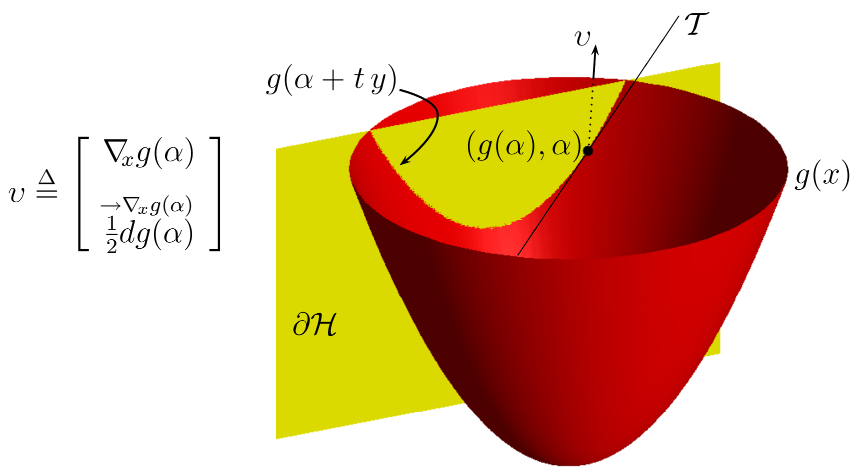


Figure 33: Drawn is a convex quadratic bowl in $\mathbb{R}^{\mathbf{3}}$; $g(x) = x^T x : \mathbb{R}^{\mathbf{2}} \to \mathbb{R}$ *versus* $x$ on some open disc in $\mathbb{R}^{\mathbf{2}}$. Plane slice $\partial\mathcal{H}$ is perpendicular to domain. Intersection of slice with domain connotes slice direction $y$ in domain. Slope of tangent $\mathcal{T}$ at point $(g(\alpha), \alpha)$ is value of directional derivative at $\alpha$ in slice direction; equivalent to $\nabla_x g(\alpha)^T y$ (693). Recall the gradient always belongs to domain of $g$, while the negative gradient is direction of steepest descent [105]. When vector entry $\upsilon_3$ denotes half the directional derivative in direction of the gradient at $\alpha$, and $[\upsilon_1 \ \upsilon_2]^T \triangleq \nabla_x g(\alpha)$, then $-\upsilon \in \mathbb{R}^{\mathbf{3}}$ points directly toward bottom of bowl.

in $t$ is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X+tY)$ as in (664). So the directional derivative of $g(X)$ in direction $Y$ evaluated at $X \in \operatorname{dom} g$ becomes

$$\overset{\to Y}{dg}(X) = \left.\frac{d}{dt}\right|_{t=0} g(X+tY) \in \mathbb{R}^{M\times N} \tag{668}$$

[73, §2.1, §5.4.5] [4, §6.3.1] which is simplest. The derivative with respect to $t$ makes the directional derivative (668) resemble ordinary calculus (§F.2); *e.g.*, when $g(X)$ is linear, $\overset{\to Y}{dg}(X) = g(Y)$. [5, §7.2]

In the case of a real function $g(X): \mathbb{R}^{K\times L} \to \mathbb{R}$, the directional derivative of $g(X)$ at $X$ in direction $Y$ yields the slope of $g$ along the line $X+tY$ through its domain, parameterized by $t$, evaluated at $t=0$. Figure 33, for example, shows a plane slice of a real convex bowl-shaped function $g(x)$ along a line $\alpha + ty$ through its domain. The slice reveals a one-dimensional real function of $t$; $g(\alpha+ty)$. The directional derivative at $x=\alpha$ in direction $y$ is the slope of $g(\alpha+ty)$ with respect to $t$ at $t=0$. For more cases, see §F.1.6.

**Example.** *Simple bowl (Figure 33).* Bowl function

$$g(x): \mathbb{R}^K \to \mathbb{R} \triangleq (x-a)^T(x-a) - b \tag{669}$$

has function offset $-b \in \mathbb{R}$, axis of revolution at $x=a$, and positive definite Hessian (642) everywhere in its domain (an open *hyperdisc* in $\mathbb{R}^K$); *id est*, strictly convex quadratic $g(x)$ has global minimum equal to $-b$ at $x=a$. A vector $-\upsilon$ based anywhere in $\operatorname{dom} g \times \mathbb{R}$ pointing toward the unique bowl bottom is specified:

$$\upsilon \propto \begin{bmatrix} x-a \\ g(x)+b \end{bmatrix} \in \mathbb{R}^K \times \mathbb{R} \tag{670}$$

Such a vector is

$$\upsilon \triangleq \begin{bmatrix} \nabla_x g(x) \\ \frac{1}{2}\overset{\to \nabla_x g(x)}{dg}(x) \end{bmatrix} \tag{671}$$

since the gradient is

$$\nabla_x g(x) = 2(x-a) \tag{672}$$

and the directional derivative in the direction of the gradient is (693)

$$\overset{\to\nabla_x g(x)}{dg(x)} \;=\; \nabla_x g(x)^T \nabla_x g(x) \;=\; 4(x-a)^T(x-a) \;=\; 4(g(x)+b) \tag{673}$$

Solutions to $g(x)=0$ identify the boundary of a hyperdisc $\partial\mathcal{O}_b$; the intersection of the bowl in $\operatorname{dom} g \times \mathbb{R}$ with $\operatorname{dom} g$. The intersection is nonempty when $u > b \geq 0$ where $u$ is some upper bound;

$$\partial\mathcal{O}_b = (\operatorname{dom} g\,,\, g(\operatorname{dom} g)) \cap \operatorname{dom} g = \begin{cases} \{x \mid g(x)=0\} \;=\; \{y+a \mid \|y\|^2 = b\}\,, & u > b \geq 0 \\ \emptyset\,, & \text{otherwise} \end{cases} \tag{674}$$

$\square$

### F.1.5 Second directional derivative

By similar argument, it turns out that the second directional derivative is equally simple. Given $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}^{M\times N}$,

$$\nabla \frac{\partial g_{mn}(X)}{\partial X_{kl}} = \frac{\partial \nabla g_{mn}(X)}{\partial X_{kl}} \triangleq \begin{bmatrix} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{11}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{12}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{1L}} \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{21}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{22}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{K1}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{K2}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L} \tag{675}$$

$$\begin{aligned} \nabla^2 g_{mn}(X) &\triangleq \begin{bmatrix} \nabla\frac{\partial g_{mn}(X)}{\partial X_{11}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g_{mn}(X)}{\partial X_{21}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g_{mn}(X)}{\partial X_{K1}} & \nabla\frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L} \\ &= \begin{bmatrix} \frac{\partial\nabla g_{mn}(X)}{\partial X_{11}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial\nabla g_{mn}(X)}{\partial X_{21}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial\nabla g_{mn}(X)}{\partial X_{K1}} & \frac{\partial\nabla g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial\nabla g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \end{aligned} \tag{676}$$

Rotating our perspective, we get several views of the second-order gradient.[105]

$$\nabla^2 g(X) = \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M\times N\times K\times L\times K\times L}$$

$$= \begin{bmatrix} \nabla\frac{\partial g(X)}{\partial X_{11}} & \nabla\frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{1L}} \\ \nabla\frac{\partial g(X)}{\partial X_{21}} & \nabla\frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla\frac{\partial g(X)}{\partial X_{K1}} & \nabla\frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla\frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times M\times N\times K\times L} \tag{677}$$

$$= \begin{bmatrix} \frac{\partial \nabla g(X)}{\partial X_{11}} & \frac{\partial \nabla g(X)}{\partial X_{12}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g(X)}{\partial X_{21}} & \frac{\partial \nabla g(X)}{\partial X_{22}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g(X)}{\partial X_{K1}} & \frac{\partial \nabla g(X)}{\partial X_{K2}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K\times L\times K\times L\times M\times N}$$

Assuming that the limits exist, we may state the partial derivative of the $mn^{\text{th}}$ entry of $g$ with respect to the $kl^{\text{th}}$ and $ij^{\text{th}}$ entries of $X$ ;

$$\frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} = \tag{678}$$

$$\lim_{\Delta\tau,\Delta t\to 0} \frac{g_{mn}(X + \Delta t\, e_k e_l^T + \Delta\tau\, e_i e_j^T) - g_{mn}(X + \Delta t\, e_k e_l^T) - \big(g_{mn}(X + \Delta\tau\, e_i e_j^T) - g_{mn}(X)\big)}{\Delta\tau\, \Delta t}$$

Differentiating (660) and then scaling by $Y_{ij}$ ,

$$\frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} \;=\; \lim_{\Delta t\to 0} \frac{\partial g_{mn}(X + \Delta t\, Y_{kl}\, e_k e_l^T) - \partial g_{mn}(X)}{\partial X_{ij}\, \Delta t} Y_{ij} \tag{679}$$

[105] When $M=N=L=1$, the second-order gradient is called the Hessian.

$$= \lim_{\Delta\tau,\Delta t\to 0} \frac{g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T + \Delta\tau\, Y_{ij}\, e_i e_j^T) - g_{mn}(X+\Delta t\, Y_{kl}\, e_k e_l^T) - \big(g_{mn}(X+\Delta\tau\, Y_{ij}\, e_i e_j^T) - g_{mn}(X)\big)}{\Delta\tau\,\Delta t}$$

that can be proved by substitution of variables in (678). The $mn^{\text{th}}$ second-order total differential due to $Y$ is

$$\begin{aligned} d^2 g_{mn}(X)|_{dX\to Y} &= \sum_{i,j}\sum_{k,l} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} = \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g_{mn}(X)^T Y\big)^T Y\Big) &(680)\\ &= \sum_{i,j} \lim_{\Delta t\to 0} \frac{\partial g_{mn}(X+\Delta t\, Y) - \partial g_{mn}(X)}{\partial X_{ij}\,\Delta t} Y_{ij} &(681)\\ &= \lim_{\Delta t\to 0} \frac{g_{mn}(X+2\Delta t\, Y) - 2g_{mn}(X+\Delta t\, Y) + g_{mn}(X)}{\Delta t^2} &(682)\\ &= \left.\frac{d^2}{dt^2}\right|_{t=0} g_{mn}(X+t\,Y) &(683)\end{aligned}$$

Hence[106] the second directional derivative,

$$\overset{\to Y}{dg^2}(X) \triangleq \left.\begin{bmatrix} d^2 g_{11}(X) & d^2 g_{12}(X) & \cdots & d^2 g_{1N}(X)\\ d^2 g_{21}(X) & d^2 g_{22}(X) & \cdots & d^2 g_{2N}(X)\\ \vdots & \vdots & & \vdots\\ d^2 g_{M1}(X) & d^2 g_{M2}(X) & \cdots & d^2 g_{MN}(X)\end{bmatrix}\right|_{dX\to Y} \in \mathbb{R}^{M\times N}$$

$$= \begin{bmatrix} \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{11}(X)^T Y\big)^T Y\Big) & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{12}(X)^T Y\big)^T Y\Big) & \cdots & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{1N}(X)^T Y\big)^T Y\Big)\\ \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{21}(X)^T Y\big)^T Y\Big) & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{22}(X)^T Y\big)^T Y\Big) & \cdots & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{2N}(X)^T Y\big)^T Y\Big)\\ \vdots & \vdots & & \vdots\\ \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{M1}(X)^T Y\big)^T Y\Big) & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{M2}(X)^T Y\big)^T Y\Big) & \cdots & \operatorname{tr}\Big(\nabla \operatorname{tr}\big(\nabla g_{MN}(X)^T Y\big)^T Y\Big)\end{bmatrix}$$

$$= \begin{bmatrix} \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{11}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{12}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{1N}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij}\\ \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{21}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{22}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{2N}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij}\\ \vdots & \vdots & & \vdots\\ \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{M1}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{M2}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum\limits_{i,j}\sum\limits_{k,l} \frac{\partial^2 g_{MN}(X)}{\partial X_{kl}\,\partial X_{ij}} Y_{kl} Y_{ij}\end{bmatrix} \tag{684}$$

[106] Equality of (680) to (682) the second-order Gateaux differential (*confer* (663)) is algebraically verifiable. *Mathematica* is capable of symbolic partial differentiation and limiting operations on a specified $g$. [106]

from which it follows

$$\overset{\to Y}{dg}{}^2(X)=\sum_{i,j}\sum_{k,l}\frac{\partial^2 g(X)}{\partial X_{kl}\,\partial X_{ij}}Y_{kl}Y_{ij}=\sum_{i,j}\frac{\partial}{\partial X_{ij}}\overset{\to Y}{dg}(X)\,Y_{ij} \tag{685}$$

Yet for all $X\in\operatorname{dom}g$, any $Y\in\mathbb{R}^{K\times L}$, and some open interval of $t\in\mathbb{R}$,

$$g(X+t\,Y)=g(X)\;+\;t\,\overset{\to Y}{dg}(X)\;+\;\frac{1}{2!}t^2\,\overset{\to Y}{dg}{}^2(X)\;+\;o(t^3) \tag{686}$$

which is the second-order Taylor expansion about $X$. [10, §0.4.2] [32, §18.4] [61, §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 (683). So the second directional derivative becomes

$$\overset{\to Y}{dg}{}^2(X)=\left.\frac{d^2}{dt^2}\right|_{t=0} g(X+t\,Y)\;\in\mathbb{R}^{M\times N} \tag{687}$$

[73, §2.1, §5.4.5] [4, §6.3.1] which is again simplest. (*confer* (668))

### F.1.6 Taylor series

Series expansions of the differentiable matrix-valued function $g(X)$, of matrix argument, were given earlier in (667) and (686). The *mean value theorem* of calculus insures a finite number of terms in the series. [32] Assuming $g(X)$ has continuous first, second, and third-order gradients over the open set $\operatorname{dom} g$, then for all $X \in \operatorname{dom} g$ and any $Y \in \mathbb{R}^{K\times L}$ on some open interval of $\mu \in \mathbb{R}$ the complete Taylor series is expressed,

$$g(X+\mu Y) = g(X) + \mu \overset{\to Y}{dg}(X) + \frac{1}{2!}\mu^2 \overset{\to Y}{dg^2}(X) + \frac{1}{3!}\mu^3 \overset{\to Y}{dg^3}(X) + o(\mu^4) \tag{688}$$

or on some open interval of $\|Y\|$ [39, App.A.5],

$$g(Y) = g(X) \;+\; \overset{\to Y-X}{dg}(X) \;+\; \frac{1}{2!}\overset{\to Y-X}{dg^2}(X) \;+\; \frac{1}{3!}\overset{\to Y-X}{dg^3}(X) \;+\; o(\|Y\|^4) \tag{689}$$

which are third-order expansions about $X$.

In the case of a real function $g(X) : \mathbb{R}^{K\times L} \to \mathbb{R}$, all the directional derivatives are in $\mathbb{R}$:

$$\overset{\to Y}{dg}(X) = \operatorname{tr}\big(\nabla g(X)^T Y\big) \tag{690}$$

$$\overset{\to Y}{dg^2}(X) = \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g(X)^T Y\big)^T Y\Big) = \operatorname{tr}\left(\nabla_X \overset{\to Y}{dg}(X)^T Y\right) \tag{691}$$

$$\overset{\to Y}{dg^3}(X) = \operatorname{tr}\left(\nabla_X \operatorname{tr}\Big(\nabla_X \operatorname{tr}\big(\nabla g(X)^T Y\big)^T Y\Big)^T Y\right) = \operatorname{tr}\left(\nabla_X \overset{\to Y}{dg^2}(X)^T Y\right) \tag{692}$$

In the case $g(X) : \mathbb{R}^K \to \mathbb{R}$ has vector argument, they further simplify:

$$\overset{\to Y}{dg}(X) = \nabla g(X)^T Y \tag{693}$$

$$\overset{\to Y}{dg^2}(X) = Y^T \nabla^2 g(X) Y \tag{694}$$

$$\overset{\to Y}{dg^3}(X) = \nabla_X \big(Y^T \nabla^2 g(X) Y\big)^T Y \tag{695}$$

and so on, where the symmetric second-order gradient matrix $\nabla^2 g(X)$ is the Hessian (642) while its transpose is known as the *Jacobian*.

### F.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 $t$:

#### first order

Removing from (668) the evaluation at $t=0$,[107] we find an expression for the directional derivative of $g(X)$ in the direction $Y$ evaluated anywhere along a line $X+t\,Y$ intersecting $\operatorname{dom} g$, parameterized by $t$;

$$\overset{\to Y}{dg}(X+t\,Y)=\frac{d}{dt}g(X+t\,Y) \tag{696}$$

In the general case $g(X):\mathbb{R}^{K\times L}\to\mathbb{R}^{M\times N}$, from (661) and (664) we find,

$$\operatorname{tr}\big(\nabla_X\, g_{mn}(X+t\,Y)^T Y\big)=\frac{d}{dt}g_{mn}(X+t\,Y) \tag{697}$$

which is valid at $t=0$, of course, when $X\in\operatorname{dom} g$. In the important case of a real function $g(X):\mathbb{R}^{K\times L}\to\mathbb{R}$, from (690) we have simply,

$$\operatorname{tr}\big(\nabla_X\, g(X+t\,Y)^T Y\big)=\frac{d}{dt}g(X+t\,Y) \tag{698}$$

When, additionally, $g(X):\mathbb{R}^{K}\to\mathbb{R}$ has vector argument,

$$\nabla_X\, g(X+t\,Y)^T Y=\frac{d}{dt}g(X+t\,Y) \tag{699}$$

**Example.** *Gradient.* $g(X)=w^TX^TXw$, $X\in\mathbb{R}^{K\times L}$, $w\in\mathbb{R}^L$. Using the tables in §F.2,

$$\begin{aligned}\operatorname{tr}\big(\nabla_X\, g(X+t\,Y)^T Y\big) &= \operatorname{tr}\big(2ww^T(X^T+t\,Y^T)Y\big) &(700)\\ &= 2w^T(X^TY+t\,Y^TY)w &(701)\end{aligned}$$

[107] Justified by replacing $X$ with $X+t\,Y$ in (661)-(663); beginning,

$$dg_{mn}(X+t\,Y)|_{dX\to Y}=\sum_{k,l}\frac{\partial g_{mn}(X+t\,Y)}{\partial X_{kl}}Y_{kl}$$

Applying the equivalence (698),

$$\begin{aligned}\frac{d}{dt}g(X+t\,Y) &= \frac{d}{dt}w^T(X+t\,Y)^T(X+t\,Y)w &(702)\\ &= w^T\left(X^TY+Y^TX+2t\,Y^TY\right)w &(703)\\ &= 2w^T(X^TY+t\,Y^TY)w &(704)\end{aligned}$$

which is the same as (701); hence, the equivalence is demonstrated.

It is easy to extract $\nabla g(X)$ from (704) knowing only (698):

$$\begin{aligned}\operatorname{tr}\left(\nabla_X\, g(X+t\,Y)^TY\right) &= 2w^T(X^TY+t\,Y^TY)w &(705)\\ &= 2\operatorname{tr}\left(ww^T(X^T+t\,Y^T)Y\right) &(706)\\ \operatorname{tr}\left(\nabla_X\, g(X)^TY\right) &= 2\operatorname{tr}\left(ww^TX^TY\right) &(707)\\ &\Leftrightarrow &(708)\\ \nabla_X\, g(X) &= 2Xww^T &(709)\end{aligned}$$

□

**second order**

Likewise removing the evaluation at $t=0$ from (687),

$$\overset{\to Y}{dg^2}(X+t\,Y) = \frac{d^2}{dt^2}g(X+t\,Y) \tag{710}$$

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 (680) and (683),

$$\operatorname{tr}\left(\nabla_X \operatorname{tr}\left(\nabla_X\, g_{mn}(X+t\,Y)^TY\right)^TY\right) = \frac{d^2}{dt^2}g_{mn}(X+t\,Y) \tag{711}$$

In the case of a real function $g(X):\mathbb{R}^{K\times L}\to\mathbb{R}$, we have, of course,

$$\operatorname{tr}\left(\nabla_X \operatorname{tr}\left(\nabla_X\, g(X+t\,Y)^TY\right)^TY\right) = \frac{d^2}{dt^2}g(X+t\,Y) \tag{712}$$

From (694), the simpler case, where the real function $g(X):\mathbb{R}^K\to\mathbb{R}$ has vector argument,

$$Y^T\nabla_X^2 g(X+t\,Y)Y = \frac{d^2}{dt^2}g(X+t\,Y) \tag{713}$$

**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 §F.2,

$$h(X) \triangleq \nabla g(X) = X^{-1} \in \operatorname{int} \mathbb{S}_+^K \tag{714}$$

so $\nabla^2 g(X) = \nabla h(X)$. By (697) and (667), for $Y \in \mathbb{S}^K$,

$$\begin{aligned}
\operatorname{tr}\big(\nabla h_{mn}(X)^T Y\big) &= \left.\frac{d}{dt}\right|_{t=0} h_{mn}(X + t\,Y) && (715)\\
&= \left(\left.\frac{d}{dt}\right|_{t=0} h(X + t\,Y)\right)_{mn} && (716)\\
&= \left(\left.\frac{d}{dt}\right|_{t=0} (X + t\,Y)^{-1}\right)_{mn} && (717)\\
&= -\big(X^{-1} Y X^{-1}\big)_{mn} && (718)
\end{aligned}$$

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 (7), we find

$$\nabla^2 g(X)_{mnkl} = \operatorname{tr}\big(\nabla h_{mn}(X)^T E_{kl}\big) = \nabla h_{mn}(X)_{kl} = -\,(X^{-1} E_{kl}\, X^{-1})_{mn} \tag{719}$$

$$\nabla^2 g(X)_{kl} = \nabla h(X)_{kl} = -\big(X^{-1} E_{kl}\, X^{-1}\big) \in \mathbb{R}^{K\times K} \tag{720}$$

$\square$

From all these first and second-order expressions, we may generate new ones by evaluating both sides at arbitrary $t$, on some open interval, but only after the differentiation.

## F.2 Tables of gradients and derivatives

- [20] [107] 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.

- $x^\mu$ means $\delta(\delta(x)^\mu)$ for $\mu\in\mathbb{R}$; *id est*, entry-wise exponentiation. $\delta$ is the main-diagonal operator (180) (§C.5). $x^0 \triangleq \mathbf{1}$, $X^0 \triangleq I$.

- $\frac{d}{dx} \triangleq \begin{bmatrix} \frac{d}{dx_1} \\ \vdots \\ \frac{d}{dx_k} \end{bmatrix}$, $\overset{\rightarrow y}{dg}(x)$, $\overset{\rightarrow y}{dg^2}(x)$ (directional derivatives §F.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.*, (§C.5)

$$\frac{d}{dx}x^{-1} \triangleq \nabla_x\,\mathbf{1}^T\delta(x)^{-1}\mathbf{1} \tag{721}$$

- Given $g(x,y) : \mathcal{X}\times\mathcal{Y}\to\mathbb{R}$ defined on arbitrary sets $\mathcal{X}$ and $\mathcal{Y}$, [10, §0.1.2]

$$\inf_{x\in\mathcal{X},\,y\in\mathcal{Y}} g(x,y) \;=\; \inf_{x\in\mathcal{X}}\,\inf_{y\in\mathcal{Y}} g(x,y) \;=\; \inf_{y\in\mathcal{Y}}\,\inf_{x\in\mathcal{X}} g(x,y) \tag{722}$$

- 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 [108, §3.6]

$$e^A = \sum_{k=0}^{\infty}\frac{1}{k!}A^k \tag{723}$$

Further, [19, §5.4]

$$e^A \succ 0\,, \qquad \forall A\in\mathbb{S}^m \tag{724}$$

- For all square $A$ and integer $k$,

$$\det^k A = \det A^k \tag{725}$$

Try to generalize 2X2 cases...
Find product rule for trace; *e.g.*, trace(f(X)g(X))...

### F.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) |
| $\nabla_x (Ax - b) = A^T$ | |
| $\nabla_x \big(x^TA - b^T\big) = A$ | |
| $\nabla_x (Ax-b)^T(Ax-b) = 2A^T(Ax-b)$ | |
| $\nabla_x^2 (Ax-b)^T(Ax-b) = 2A^TA$ | |
| $\nabla_x \big(x^TAx + 2x^TBy + y^TCy\big) = (A+A^T)x + 2By$ | |
| $\nabla_x^2 \big(x^TAx + 2x^TBy + y^TCy\big) = A + A^T$ | |
| | $\nabla_X\, a^TXb \;=\nabla_X\, b^TX^Ta \;=\; ab^T$ |
| | $\nabla_X\, a^TX^2b = X^Tab^T + ab^TX^T$ |
| | $\nabla_X\, a^TX^{-1}b = -X^{-T}ab^TX^{-T}$ |
| | $\nabla_X (X^{-1})_{kl} = \dfrac{\partial X^{-1}}{\partial X_{kl}} = -X^{-1}E_{kl}\,X^{-1}\,,\quad$ *confer* (659)(720) |
| $\nabla_x\, a^Tx^Txb = 2xa^Tb$ | $\nabla_X\, a^TX^TXb = X(ab^T + ba^T)$ |
| $\nabla_x\, a^Txx^Tb = (ab^T + ba^T)x$ | $\nabla_X\, a^TXX^Tb = (ab^T + ba^T)X$ |
| $\nabla_x\, a^Tx^Txa = 2xa^Ta$ | $\nabla_X\, a^TX^TXa = 2Xaa^T$ |
| $\nabla_x\, a^Txx^Ta = 2aa^Tx$ | $\nabla_X\, a^TXX^Ta = 2aa^TX$ |
| $\nabla_x\, a^Tyx^Tb = ba^Ty$ | $\nabla_X\, a^TYX^Tb = ba^TY$ |
| $\nabla_x\, a^Ty^Txb = yb^Ta$ | $\nabla_X\, a^TY^TXb = Yab^T$ |
| $\nabla_x\, a^Txy^Tb = ab^Ty$ | $\nabla_X\, a^TXY^Tb = ab^TY$ |
| $\nabla_x\, a^Tx^Tyb = ya^Tb$ | $\nabla_X\, a^TX^TYb = Yba^T$ |

#### F.2.1.1 **Algebraic** cont.

$$\frac{d}{dt}(X + t\,Y) = Y$$

$$\frac{d}{dt}B^T(X + t\,Y)^{-1}A = -B^T(X + t\,Y)^{-1}Y(X + t\,Y)^{-1}A$$
$$\frac{d}{dt}B^T(X + t\,Y)^{-T}A = -B^T(X + t\,Y)^{-T}Y^T(X + t\,Y)^{-T}A$$

$$\frac{d^2}{dt^2}B^T(X + t\,Y)^{-1}A = 2B^T(X + t\,Y)^{-1}Y(X + t\,Y)^{-1}Y(X + t\,Y)^{-1}A$$

$$\frac{d}{dt}\Big((X + t\,Y)^TA(X + t\,Y)\Big) = Y^TAX + X^TAY + 2\,t\,Y^TAY$$

$$\frac{d^2}{dt^2}\Big((X + t\,Y)^TA(X + t\,Y)\Big) = 2\,Y^TAY$$

$$\frac{d}{dt}((X + t\,Y)A(X + t\,Y)) = YAX + XAY + 2\,t\,YAY$$

$$\frac{d^2}{dt^2}((X + t\,Y)A(X + t\,Y)) = 2\,YAY$$

### F.2.2 Trace

| | |
|---|---|
| $\nabla_x\, \mu\, x = \mu I$ | $\nabla_X \operatorname{tr} \mu X = \nabla_X\, \mu \operatorname{tr} X = \mu I$ |
| $\nabla_x\, \mathbf{1}^T \delta(x)^{-1} \mathbf{1} = \frac{d}{dx} x^{-1} = -x^{-2}$<br>$\nabla_x\, \mathbf{1}^T \delta(x)^{-1} y = -\delta(x)^{-2} y$ (§C.5) | $\nabla_X \operatorname{tr} X^{-1} = -X^{-2T}$<br>$\nabla_X \operatorname{tr}(X^{-1}Y) = \nabla_X \operatorname{tr}(YX^{-1}) = -X^{-T}Y^TX^{-T}$ |
| $\frac{d}{dx} x^\mu = \mu x^{\mu-1}$ | $\nabla_X \operatorname{tr} X^\mu = \mu X^{(\mu-1)T}\,, \qquad X \in \mathbb{R}^{\mathbf{2\times2}}$ |
| | $\nabla_X \operatorname{tr} X^k = kX^{(k-1)T}$ |
| $\nabla_x (b - a^Tx)^{-1} = (b - a^Tx)^{-2} a$ | $\nabla_X \operatorname{tr}((B - AX)^{-1}) = \left((B - AX)^{-2} A\right)^T$ |
| $\nabla_x (b - a^Tx)^\mu = -\mu (b - a^Tx)^{\mu-1} a$ | |
| $\nabla_x\, x^Ty = \nabla_x\, y^Tx = y$ | $\nabla_X \operatorname{tr}(X^TY) = \nabla_X \operatorname{tr}(YX^T) = \nabla_X \operatorname{tr}(Y^TX) = \nabla_X \operatorname{tr}(XY^T) = Y$ |
| | $\nabla_X \operatorname{tr}(AXBX^T) = \nabla_X \operatorname{tr}(XBX^TA) = A^TXB^T + AXB$<br>$\nabla_X \operatorname{tr}(AXBX) = \nabla_X \operatorname{tr}(XBXA) = A^TX^TB^T + B^TX^TA^T$ |
| | $\nabla_X \operatorname{tr}(AXAXAX) = \nabla_X \operatorname{tr}(XAXAXA) = 3(AXAXA)^T$ |
| | $\nabla_X \operatorname{tr}(YX^j) = \sum_{i=0}^{j-1} \left(X^iYX^{j-1-i}\right)^T$ |
| | $\nabla_X \operatorname{tr}(Y^TXX^TY) = \nabla_X \operatorname{tr}(X^TYY^TX) = 2\,YY^TX$<br>$\nabla_X \operatorname{tr}(Y^TX^TXY) = \nabla_X \operatorname{tr}(XYY^TX^T) = 2XYY^T$ |
| | $\nabla_X \operatorname{tr}\big((X+Y)^T(X+Y)\big) = 2(X+Y)$<br>$\nabla_X \operatorname{tr}((X+Y)(X+Y)) = 2(X+Y)^T$ |
| | $\nabla_X \operatorname{tr}(A^TXB) = \nabla_X \operatorname{tr}(X^TAB^T) = AB^T$<br>$\nabla_X \operatorname{tr}(A^TX^{-1}B) = \nabla_X \operatorname{tr}(X^{-T}AB^T) = -X^{-T}AB^TX^{-T}$ |
| | $\nabla_X\, a^TXb = \nabla_X \operatorname{tr}(ba^TX) = \nabla_X \operatorname{tr}(Xba^T) = ab^T$<br>$\nabla_X\, b^TX^Ta = \nabla_X \operatorname{tr}(X^Tab^T) = \nabla_X \operatorname{tr}(ab^TX^T) = ab^T$<br>$\nabla_X\, a^TX^{-1}b = \nabla_X \operatorname{tr}(X^{-T}ab^T) = -X^{-T}ab^TX^{-T}$<br>$\nabla_X\, a^TX^\mu b =$ |

#### F.2.2.1 **Trace** cont.

$$\tfrac{d}{dt}\operatorname{tr} g(X+t\,Y) = \operatorname{tr}\tfrac{d}{dt}\, g(X+t\,Y)$$

$$\tfrac{d}{dt}\operatorname{tr}(X+t\,Y) = \operatorname{tr} Y$$

$$\tfrac{d}{dt}\operatorname{tr}^j(X+t\,Y) = j\operatorname{tr}^{j-1}(X+t\,Y)\operatorname{tr} Y$$

$$\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)^j) = j\operatorname{tr}((X+t\,Y)^{j-1}\,Y)$$

$$\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)^{-1}) = -\operatorname{tr}((X+t\,Y)^{-1}Y(X+t\,Y)^{-1})$$

$$\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)^j\,Y) =$$

$$\tfrac{d}{dt}\operatorname{tr}((X+t\,Y)^{-1}Y) = -\operatorname{tr}((X+t\,Y)^{-1}Y(X+t\,Y)^{-1}Y)$$

### F.2.3 Log determinant

$x \succ 0$, $\det X > 0$ on some open neighborhood of $X$, $\det(X + t\,Y) > 0$ on some open interval of $t$; otherwise, $\log(\cdot)$ is discontinuous.

| | |
|---|---|
| $\frac{d}{dx}\log x = x^{-1}$ | $\nabla_X \log\det X = X^{-T}$<br>$\nabla_X^2 \log\det(X)_{kl} = \dfrac{\partial X^{-T}}{\partial X_{kl}} = -(X^{-1}E_{kl}X^{-1})^T$, *confer* (676)(720) |
| $\frac{d}{dx}\log x^{-1} = -x^{-1}$ | $\nabla_X \log\det X^{-1} = -X^{-T}$ |
| $\frac{d}{dx}\log x^{\mu} = \mu x^{-1}$ | $\nabla_X \log\det^{\mu} X = \mu X^{-T}$ |
| | $\nabla_X \log\det X^{\mu} = \mu X^{-T}$, $X \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$ |
| | $\nabla_X \log\det X^{k} = \nabla_X \log\det^{k} X = kX^{-T}$ |
| | $\nabla_X \log\det^{\mu}(X + t\,Y) = \mu(X + t\,Y)^{-T}$ |
| | $\nabla_X \log\det(X + t\,Y)^{k} = \nabla_X \log\det^{k}(X + t\,Y) = k(X + t\,Y)^{-T}$ |
| | $\frac{d}{dt}\log\det(X + t\,Y) = \operatorname{tr}((X + t\,Y)^{-1}Y)$ |
| | $\frac{d^2}{dt^2}\log\det(X + t\,Y) = -\operatorname{tr}((X + t\,Y)^{-1}Y(X + t\,Y)^{-1}Y)$ |
| | $\frac{d}{dt}\log\det(X + t\,Y)^{-1} = -\operatorname{tr}((X + t\,Y)^{-1}Y)$ |
| | $\frac{d^2}{dt^2}\log\det(X + t\,Y)^{-1} = \operatorname{tr}((X + t\,Y)^{-1}Y(X + t\,Y)^{-1}Y)$ |

### F.2.4 Determinant

$$\nabla_X \det X = \nabla_X \det X^T = \det(X) X^{-T}$$

$$\nabla_X \det X^{-1} = -\det(X^{-1}) X^{-T} = -\det(X)^{-1} X^{-T}$$

$$\nabla_X \det^\mu X = \mu \det^\mu(X) X^{-T}$$

$$\nabla_X \det X^\mu = \mu \det(X^\mu) X^{-T}\,, \qquad X \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$$

$$\nabla_X \det X^k = k \det^{k-1}(X)\big(\operatorname{tr}(X) I - X^T\big)\,, \qquad X \in \mathbb{R}^{\mathbf{2}\times\mathbf{2}}$$

$$\nabla_X \det X^k = \nabla_X \det^k X = k \det(X^k) X^{-T} = k \det^k(X) X^{-T}$$

$$\nabla_X \det^\mu(X + t\,Y) = \mu \det^\mu(X + t\,Y)(X + t\,Y)^{-T}$$

$$\nabla_X \det(X + t\,Y)^k = \nabla_X \det^k(X + t\,Y) = k \det^k(X + t\,Y)(X + t\,Y)^{-T}$$

$$\tfrac{d}{dt} \det(X + t\,Y) = \det(X + t\,Y) \operatorname{tr}((X + t\,Y)^{-1} Y)$$

$$\tfrac{d^2}{dt^2} \det(X + t\,Y) = \det(X + t\,Y) \left(\operatorname{tr}^2((X + t\,Y)^{-1} Y) - \operatorname{tr}((X + t\,Y)^{-1} Y (X + t\,Y)^{-1} Y)\right)$$

$$\tfrac{d}{dt} \det(X + t\,Y)^{-1} = -\det(X + t\,Y)^{-1} \operatorname{tr}((X + t\,Y)^{-1} Y)$$

$$\tfrac{d^2}{dt^2} \det(X + t\,Y)^{-1} = \det(X + t\,Y)^{-1} (\operatorname{tr}^2((X + t\,Y)^{-1} Y) + \operatorname{tr}((X + t\,Y)^{-1} Y (X + t\,Y)^{-1} Y))$$

$$\tfrac{d}{dt} \det^\mu(X + t\,Y) =$$

### F.2.5 Exponential

[108, §3.6, §4.5] [19, §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[9, new p.60]

$$\tfrac{d^j}{dt^j}e^{\operatorname{tr}(X+\,tY)} = e^{\operatorname{tr}(X+\,tY)}\operatorname{tr}^j(Y)$$

$$\tfrac{d}{dt}e^{tY} = e^{tY}Y = Ye^{tY}$$

$$\tfrac{d}{dt}e^{X+\,tY} = e^{X+\,tY}Y = Ye^{X+\,tY}\,, \qquad XY = YX$$

$$\tfrac{d^2}{dt^2}e^{X+\,tY} = e^{X+\,tY}Y^2 = Ye^{X+\,tY}Y = Y^2e^{X+\,tY}\,, \qquad XY = YX$$

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