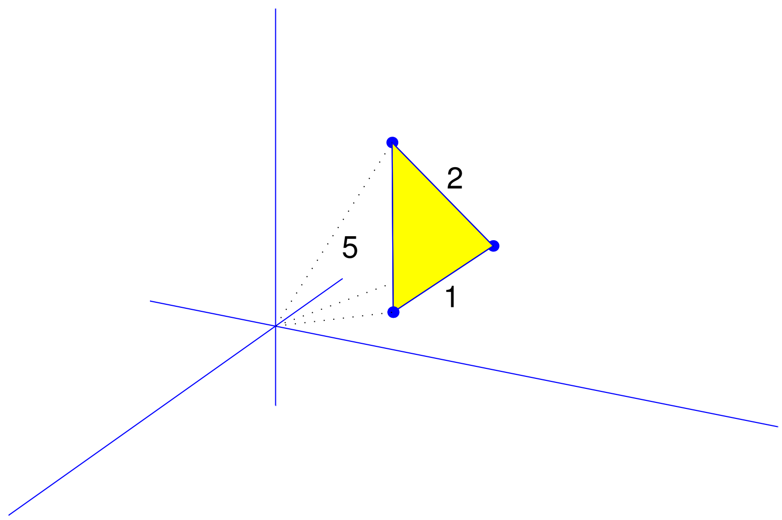

Figure 1: Convex hull of three points ($N = 3$) in $\mathbb{R}^n$ ($n = 3$) is shaded. The small $\times$ denotes the geometric center.

1 Euclidean Distance Matrix

We may intuitively understand a Euclidean distance matrix, an EDM $D \in \mathbb{R}^{N \times N}$, to be an exhaustive table of distance-squared between points from a list of N points in some Euclidean space $\mathbb{R}^n$. Each point is labelled ordinally, hence the row or column index of an EDM, i or $j \in \{1 \ldots N\}$, individually addresses all the points in the list.

Consider the following example of an EDM for the case $N = 3$.

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

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

1.1 Metric space requirements

If by d_{ij} we denote the i, j^{th} entry of the EDM D, then the distances-squared $\{d_{ij},\ i, j = 1 \dots N\}$ must satisfy the requirements imposed by any metric space:

1. $\sqrt{d_{ij}} \geq 0,\ \ i \neq j$ (positivity)
2. $d_{ij} = 0,\ \ i = j$ (self-distance)
3. $d_{ij} = d_{ji}$ (symmetry)
4. $\sqrt{d_{ik}} + \sqrt{d_{kj}} \ \geq\ \sqrt{d_{ij}}$ (triangle inequality)

where $\sqrt{d_{ij}}$ is the Euclidean distance metric in $\mathbb{R}^n$. Hence an EDM must be symmetric $D = D^T$ and its main diagonal zero, $\delta(D) = 0$. If we assume the points in $\mathbb{R}^n$ are distinct, then entries off the main diagonal must be strictly positive $\{\sqrt{d_{ij}} > 0,\ i \neq j\}$. The last three metric space requirements together imply nonnegativity of the $\{\sqrt{d_{ij}}\}$, not strict positivity, [6] but prohibit D from having otherwise arbitrary symmetric entries off the main diagonal. To enforce strict positivity we introduce another matrix criterion.

1.1.1 Strict positivity

The strict positivity criterion comes about when we require each x_l to be distinct; meaning, no entries of D except those along the main diagonal $\delta(D)$ are zero. We claim that *strict* positivity $\{d_{ij} > 0,\ i \neq j\}$ is controlled by the *strict* matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$, symmetry $D^T = D$, and the self-distance criterion $\delta(D) = 0$.[1]

To support our claim, we introduce a full-rank skinny matrix $V_{\mathcal{N}}$ having the attribute $\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$;

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

[1] Nonnegativity is controlled by relaxing the strict inequality.

If any square matrix A is positive definite, then its main diagonal $\delta(A)$ must have all strictly positive elements. [4] For any $D = D^T$ and $\delta(D) = 0$, it follows that

$$-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \;\Rightarrow\; \delta(-V_{\mathcal{N}}^T D V_{\mathcal{N}}) = \begin{bmatrix} d_{12} \\ d_{13} \\ \vdots \\ d_{1N} \end{bmatrix} \succ 0 \tag{3}$$

Multiplication of $V_{\mathcal{N}}$ by any permutation matrix Ξ has null effect on its range. 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*, $\mathcal{R}(\Xi V_{\mathcal{N}}) = \mathcal{R}(V_{\mathcal{N}}\Xi) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^T)$. Hence, the matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$ implies $-V_{\mathcal{N}}^T \Xi^T D \Xi V_{\mathcal{N}} \succ 0$ (and $-\Xi^T V_{\mathcal{N}}^T D V_{\mathcal{N}} \Xi \succ 0$). Various permutation matrices will sift the remaining d_{ij} similarly to (3) thereby proving their strict positivity.[2] $\diamondsuit$

1.2 EDM definition

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

$$X = [x_1 \;\cdots\; x_N] \in \mathbb{R}^{n \times N} \tag{4}$$

The entries of D are related to the points constituting the list like so:

$$d_{ij} \;=\; \|x_i - x_j\|^2 \;=\; \|x_i\|^2 + \|x_j\|^2 - 2x_i^T x_j \tag{5}$$

For D to be EDM it must be expressible in terms of some X,

$$\mathcal{D}(X) = \delta(X^T X)\mathbf{1}^T + \mathbf{1}\delta^T(X^T X) - 2X^T X \tag{6}$$

where $\delta(A)$ means the column vector formed from the main diagonal of the matrix A. When we say D is EDM, reading directly from (6), it implicitly means $D = D^T$ and $\delta(D) = 0$ are matrix criteria (but we already knew that). If each x_l is distinct, then $\{d_{ij} > 0,\ i \neq j\}$; in matrix terms, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$. Otherwise, $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ when each x_l is not distinct.

[2] The rule of thumb is: if $\Xi(i,1) = 1$, then $\delta(-V_{\mathcal{N}}^T \Xi^T D \Xi V_{\mathcal{N}})$ is some permutation of the nonzero elements from the i^{th} row or column of D.

1.3 Embedding Dimension

The *convex hull* of any list (or set) of points in Euclidean space forms a closed (or *solid*) polyhedron whose vertices are the points constituting the list; [2]

$$\text{conv}\{x_l,\, l = 1 \ldots N\} \;=\; \{Xa \mid a^T\mathbf{1} = 1,\, a \succeq 0\} \tag{7}$$

The boundary and relative interior of that polyhedron constitute the convex hull. The convex hull is the smallest convex set that contains the list. For the particular example in Figure 1, the convex hull is the closed triangle while its three vertices constitute the list.

The lower bound on Euclidean dimension consistent with an EDM D is called the *embedding* (or *affine*) dimension, r. The embedding dimension r is the dimension of the smallest hyperplane in $\mathbb{R}^n$ that contains the convex hull of the list in X. Dimension r is the same as the dimension of the convex hull of the list X contains, but r is not necessarily equal to the rank of X.[3] The fact $r \leq \min\{n, N-1\}$ can be visualized from the example in Figure 1. There we imagine a vector from the origin to each point in the list. Those three vectors are linearly independent in $\mathbb{R}^3$, but the embedding dimension r equals 2 because the three points lie in a plane (the unique plane in which the points are embedded; the plane that contains their convex hull), the *embedding plane* (or *affine hull*). In other words, the three points are linearly independent with respect to $\mathbb{R}^3$, but *de*pendent with respect to the embedding plane.

Embedding dimension is important because we lose any offset component common to all the x_l in $\mathbb{R}^n$ when determining position given only distance information. To calculate the embedding dimension, we first eliminate any offset that serves to increase the dimensionality of the subspace required to contain the convex hull; subtracting *any* point in the embedding plane from every list member will work. We choose the *geometric center*[4] of the $\{x_l\}$;

$$c_g = \frac{1}{N} X\mathbf{1} \;\in\; \mathbb{R}^n \tag{8}$$

Subtracting the geometric center from all the points like so, $X - c_g\mathbf{1}^T$, translates their geometric center to the origin in $\mathbb{R}^n$. The embedding dimension

[3] $\text{rank}(X) \leq \min\{n, N\}$

[4] If we were to associate a point-mass m_l with each of the points x_l in a list, then their *center of mass* (or *gravity*) would be $c = (\sum x_l\, m_l)/\sum m_l$. The geometric center is the same as the center of mass under the assumption of uniform mass density across points. [5] The geometric center always lies in the convex hull.

is then $r = \text{rank}(X - c_g \mathbf{1}^T)$. In general, we say that the $\{x_l \in \mathbb{R}^n\}$ and their convex hull are *embedded* in some hyperplane, the embedding hyperplane whose dimension is r. It is equally accurate to say that the $\{x_l - c_g\}$ and their convex hull are embedded in some subspace of $\mathbb{R}^n$ whose dimension is r.

It will become convenient to define a matrix V that arises naturally as a consequence of translating the geometric center to the origin. Instead of $X - c_g \mathbf{1}^T$ we may write XV; *viz.*,

$$X - c_g \mathbf{1}^T \;=\; X - \frac{1}{N} X \mathbf{1}\mathbf{1}^T \;=\; X(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T) \;=\; XV \in \mathbb{R}^{n \times N} \tag{9}$$

Obviously,

$$V = V^T = I - \frac{1}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{R}^{N \times N} \tag{10}$$

so we may write the embedding dimension r more simply;

$$\begin{aligned} r &= \dim\text{conv}\{x_l,\, l = 1 \ldots N\} \\ &= \text{rank}(X - c_g \mathbf{1}^T) \\ &= \text{rank}(XV) \end{aligned} \tag{11}$$

where V is an elementary matrix and a projection matrix.[5]

$$\begin{gathered} r \leq \min\{n, N-1\} \\ \Leftrightarrow \\ r \leq n \quad \text{and} \quad r < N \end{gathered} \tag{12}$$

[5]A matrix of the form $E = I - \alpha u v^T$ where α is a scalar and u and v are vectors of the same dimension, is called an *elementary* matrix, or a *rank-one modification of the identity.* [3] Any elementary matrix in $\mathbb{R}^{N \times N}$ has $N-1$ eigenvalues equal to 1. For the particular elementary matrix V, the remaining eigenvalue equals 0. Because $V = V^T$ is diagonalizable, the number of zero eigenvalues must be equal to $\dim \mathcal{N}(V^T) = 1$, and because $V^T\mathbf{1} = 0$, then $\mathcal{N}(V^T) = \mathcal{R}(\mathbf{1})$. Because $V = V^T$ and $V^2 = V$, the elementary matrix V is a projection matrix onto its range $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$ having dimension $N-1$.

1.4 Rotation, Reflection, Offset

When D is EDM, there exist an infinite number of corresponding N-point lists in Euclidean space. All those lists are related by rotation, reflection, and offset (translation).

If there were a common offset among all the x_l, it would be cancelled in the formation of each d_{ij}. Knowing that offset in advance, call it $c \in \mathbb{R}^n$, we might remove it from X by subtracting $c\mathbf{1}^T$. Then by definition (6) of an EDM, it stands to reason for any fixed offset c,

$$\mathcal{D}(X - c\mathbf{1}^T) = \mathcal{D}(X) \tag{13}$$

When $c = c_g$ we get

$$\mathcal{D}(X - c_g\mathbf{1}^T) \;=\; \mathcal{D}(XV) \;=\; \mathcal{D}(X) \tag{14}$$

In words, inter-point distances are unaffected by offset.

Rotation about some arbitrary point or reflection through some hyperplane can be easily accomplished using an orthogonal matrix, call it Q. [9] Again, inter-point distances are unaffected by rotation and reflection. We rightfully expect that

$$\mathcal{D}(QX - c\mathbf{1}^T) = \mathcal{D}(Q(X - c\mathbf{1}^T)) = \mathcal{D}(QXV) = \mathcal{D}(QX) = \mathcal{D}(XV) \tag{15}$$

So in the formation of the EDM D, any rotation, reflection, or offset information is lost and there is no hope of recovering it. Reconstruction of point position X can be guaranteed correct, therefore, only in the embedding dimension r; *id est*, in relative position.

Because $\mathcal{D}(X)$ is insensitive to offset, we may safely ignore it and consider only the impact of matrices that pre-multiply X; as in $\mathcal{D}(Q_oX)$. The class of pre-multiplying matrices for which inter-point distances are unaffected is somewhat more broad than orthogonal matrices. Looking at definition (6), it appears that any matrix Q_o such that

$$X^TQ_o^TQ_oX = X^TX \tag{16}$$

will have the property $\mathcal{D}(Q_oX) = \mathcal{D}(X)$. That class includes skinny Q_o having orthonormal columns. Fat Q_o are conceivable as long as (16) is satisfied.

2 EDM criteria

Given some arbitrary candidate matrix D, fundamental questions are: What are the criteria for the entries of D sufficient to belong to an EDM, and what is the minimum dimension r of the Euclidean space implied by EDM D?

2.1 Geometric condition

We continue considering the criteria necessary for a candidate matrix to be EDM. We provide an intuitive geometric condition based upon the fact that the convex hull of any list (or set) of points in Euclidean space $\mathbb{R}^n$ is a closed polyhedron.

We assert that $D \in \mathbb{R}^{N\times N}$ is a Euclidean distance matrix if and only if distances-squared from the origin

$$\{\|p\|^2 = -\frac{1}{2}a^T V^T D V a \mid a^T\mathbf{1} = 1,\ a \succeq 0\} \tag{17}$$

are consistent with a point $p \in \mathbb{R}^n$ in some closed polyhedron that is embedded in a subspace of $\mathbb{R}^n$ and has zero geometric center. (V as in (10).)

It is straightforward to show that the assertion is true in the forward direction. We assume that D is indeed an EDM; *id est*, D comes from a list of N unknown vertices in Euclidean space $\mathbb{R}^n$; $D = \mathcal{D}(X)$ as in (6). Now shift the geometric center of those unknown vertices to the origin, as in (9), and then take any point p in their convex hull, as in (7);

$$\{p \;=\; (X - c_g\mathbf{1}^T)a \;=\; XVa \mid a^T\mathbf{1} = 1,\ a \succeq 0\} \tag{18}$$

Then any distance to the polyhedral convex hull can be formulated as

$$\{p^T p \;=\; \|p\|^2 \;=\; a^T V^T X^T X V a \mid a^T\mathbf{1} = 1,\ a \succeq 0\} \tag{19}$$

Rearranging (6), $X^T X$ may be expressed

$$X^T X = \frac{1}{2}(\delta(X^T X)\mathbf{1}^T + \mathbf{1}\delta^T(X^T X) - D) \tag{20}$$

Substituting (20) into (19) yields (17) because $V^T\mathbf{1} = 0$.

To validate the assertion in the reverse direction, we must demonstrate that if all distances-squared from the origin described by (17) are consistent with a point p in some embedded polyhedron, then D is EDM. To show that,

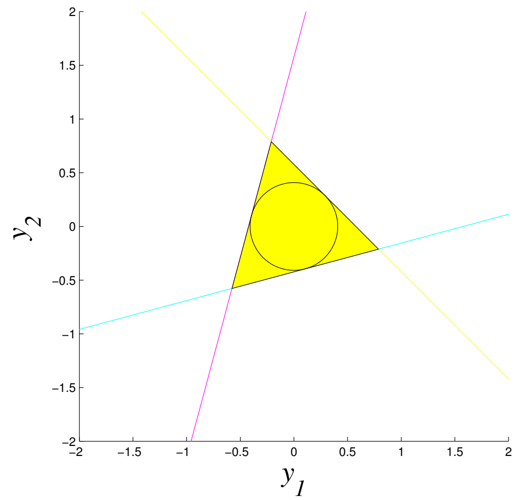

Figure 2: Illustrated is a portion of the semi-infinite closed slab $Vy \succeq -\frac{1}{N}\mathbf{1}$ for $N = 2$ showing the inscribed ball of radius $\frac{1}{\sqrt{N!}}$.

we must first derive an expression equivalent to (17). The condition $a^T\mathbf{1} = 1$ is equivalent to $a = \frac{1}{N}\mathbf{1} + Vy$, where $y \in \mathbb{R}^N$, because $\mathcal{R}(V) = \mathcal{N}(\mathbf{1}^T)$. Substituting a into (17),

$$\{\|p\|^2 = -\frac{1}{2}y^TV^TDVy \mid Vy \succeq -\frac{1}{N}\mathbf{1},\ -V^TDV \succeq 0\} \tag{21}$$

because $V^2 = V$. Because the solutions to $Vy \succeq -\frac{1}{N}\mathbf{1}$ constitute a semi-infinite closed slab about the origin in $\mathbb{R}^N$(Figure 2), a ball of radius $1/\sqrt{N!}$ centered at the origin can be fit into the interior. [10] Obviously it follows that $-V^TDV$ must be positive semidefinite (PSD).[6] We may assume $-\frac{1}{2}V^TDV$ is symmetric[7] hence diagonalizable as $Q\Lambda Q^T \in \mathbb{R}^{N\times N}$. So, equivalent to (17) is

$$\{\|p\|^2 = a^TQ\Lambda Q^Ta \mid a^T\mathbf{1} = 1,\ a \succeq 0,\ \Lambda \succeq 0\} \tag{22}$$

consistent with an embedded polyhedron by assumption. It remains to show that D is EDM. Corresponding points $\{p = \Lambda^{1/2}Q^Ta \mid a^T\mathbf{1} = 1,\ a \succeq 0,\ \Lambda \succeq 0\}$ $\in \mathbb{R}^N(n = N)$[8] describe a polyhedron as in (7). Identify vertices $XV =$

[6] $\|p\|^2 \geq 0$ in *all* directions y, but that is not a sufficient condition for $\|p\|^2$ to be consistent with a polyhedron.

[7] The antisymmetric part $(-\frac{1}{2}V^TDV - (-\frac{1}{2}V^TDV)^T)/2$ of $-\frac{1}{2}V^TDV$ is benign in $\|p\|^2$.

[8] From (12) $r < N$, so we may always choose n equal to N when X is unknown.

$\Lambda^{1/2}Q^T \in \mathbb{R}^{N\times N}$($X$ not unique, Section 1.4). Then D is EDM because it can be expressed in the form of (6) by using the vertices we found. Applying (14),

$$D \;=\; \mathcal{D}(X) \;=\; \mathcal{D}(XV) \;=\; \mathcal{D}(\Lambda^{1/2}Q^T) \tag{23}$$

$\diamondsuit$

2.2 Matrix criteria

In Section 2.1 we showed

$$\begin{array}{c} D \text{ EDM} \\ \Leftrightarrow \\ \{\|p\|^2 = -\tfrac{1}{2}a^T V^T D V a \mid a^T \mathbf{1} = 1,\, a \succeq 0\}\ (17) \\ \text{is consistent with some embedded polyhedron} \\ \Rightarrow \\ -V^T D V \succeq 0 \end{array} \tag{24}$$

while in Section 1.1.1 we learned that a strict matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$

$$\begin{array}{c} \{d_{ij} > 0,\, i \neq j\}, \quad -V^T D V \succeq 0 \\ \Leftarrow \\ D = D^T, \quad \delta(D) = 0, \quad -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \end{array} \tag{25}$$

yields distinction. Here we establish the necessary and sufficient conditions for candidate D to be EDM; namely,

$$\begin{array}{c} D \text{ EDM} \\ \Leftrightarrow \\ D = D^T, \quad \delta(D) = 0, \quad -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0 \end{array} \tag{26}$$

We then consider the minimum dimension r of the Euclidean space implied by EDM D.

Given $D = D^T$, $\delta(D) = 0$, and $-V^T D V \succ 0$, then by (24) and (25) it is sufficient to show that (17) is consistent with some closed polyhedron that is embedded in an r-dimensional subspace of $\mathbb{R}^n$ and has zero geometric center. Since $-\frac{1}{2}V^T D V$ is assumed symmetric, it is diagonalizable as $Q\Lambda Q^T$ where $Q \in \mathbb{R}^{N\times N}$,

$$\Lambda = \begin{bmatrix} \Lambda_r & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{N\times N} \tag{27}$$

and where Λ_r holds r strictly positive eigenvalues. As implied by (10), $\mathbf{1} \in \mathcal{N}(-\frac{1}{2}V^T D V) \Rightarrow r < N$ like in (12),[9] so Λ must always have at least one 0 eigenvalue. Since $-\frac{1}{2}V^T D V$ is also assumed PSD, it is factorable;

$$-\frac{1}{2}V^T D V = Q\Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} Q^T \tag{28}$$

where $Q_o \in \mathbb{R}^{n\times N}$ is unknown as is its dimension n. Q_o is constrained, however, such that its first r columns are orthonormal. Its remaining columns are arbitrary. We may then rewrite (17):

$$\{p^T p = a^T Q\Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} Q^T a \mid a^T\mathbf{1} = 1,\ a \succeq 0,\ \Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} = \Lambda \succeq 0\} \tag{29}$$

Then $\{p = Q_o \Lambda^{1/2} Q^T a \mid a^T\mathbf{1} = 1,\ a \succeq 0,\ \Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} = \Lambda \succeq 0\} \in \mathbb{R}^n$ describes a polyhedron as in (7) having vertices

$$XV = Q_o \Lambda^{1/2} Q^T \in \mathbb{R}^{n\times N} \tag{30}$$

whose geometric center $\frac{1}{N} Q_o \Lambda^{1/2} Q^T \mathbf{1}$ is the origin.[10] If we like, we may choose n to be $\operatorname{rank}(Q_o \Lambda^{1/2} Q^T) = \operatorname{rank}(\Lambda) = r$ which is the smallest n possible.[11]

$\diamondsuit$

[9] For any square matrix A, the number of 0 eigenvalues is at least equal to $\dim\mathcal{N}(A)$. For any diagonalizable matrix A, the number of 0 eigenvalues is exactly equal to $\dim\mathcal{N}(A)$.

[10] For any A, $\mathcal{N}(A^T A) = \mathcal{N}(A)$. [9] In our case, $\mathcal{N}(-\frac{1}{2}V^T D V) = \mathcal{N}(Q\Lambda Q^T) = \mathcal{N}(Q\Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} Q^T) = \mathcal{N}(Q_o \Lambda^{1/2} Q^T) = \mathcal{N}(XV)$.

[11] If we write $Q^T = \begin{bmatrix} q_1^T \\ \vdots \\ q_N^T \end{bmatrix}$ in terms of row vectors, $\Lambda = \begin{bmatrix} \lambda_1 & & & 0 \\ & \ddots & & \\ & & \lambda_r & \\ 0 & & & 0 \end{bmatrix}$ in terms of eigenvalues, and $Q_o = [q_{o_1} \cdots q_{o_N}]$ in terms of column vectors, then $Q_o \Lambda^{1/2} Q^T = \sum_{i=1}^{r} \lambda_i^{1/2} q_{o_i} q_i^T$ is a sum of r linearly independent rank-one matrices. Hence the result has rank r.

Recall from (12), $r < N$ and $r \leq n$. n is finite but otherwise unbounded above. Given an EDM D, then for any valid choice of n, there is an $X \in \mathbb{R}^{n\times N}$ and a $Q_o \in \mathbb{R}^{n\times N}$ having the property $\Lambda^{1/2} Q_o^T Q_o \Lambda^{1/2} = \Lambda$, such that

$$D \;=\; \mathcal{D}(X) \;=\; \mathcal{D}(XV) \;=\; \mathcal{D}(Q_o \Lambda^{1/2} Q^T) \;=\; \mathcal{D}(\Lambda^{1/2} Q^T) \tag{31}$$

2.2.1 Metric space requirements vs. matrix criteria

In Section 1.1.1 we demonstrated that the strict matrix inequality $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succ 0$ replaces the strict positivity criterion $\{d_{ij} > 0,\ i \neq j\}$. Comparing the three criteria in (26) to the three requirements imposed by any metric space, enumerated in Section 1.1, it appears that the strict matrix inequality is simultaneously the matrix analog to the triangle inequality. Because the criteria for the existence of an EDM must be identical to the requirements imposed by a Euclidean metric space, we may conclude that the three criteria in (26) are equivalent to the metric space requirements. So we have the analogous criteria for an EDM:

1. $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ (positivity)
2. $\delta(D) = 0$ (self-distance)
3. $D^T = D$ (symmetry)
4. $-V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ (triangle inequality)

If we replace the inequality with its strict version, then duplicate x_l are not allowed.

2.3 Cone of EDM

3 Map of the USA

Beyond fundamental questions regarding the characteristics of an EDM, a more intriguing question is whether or not it is possible to reconstruct relative point position given only an EDM.

The validation of our assertion is constructive. The embedding dimension r may be determined by counting the number of nonzero eigenvalues. Certainly from (11) we know that $\dim \mathcal{R}(XV) = r$, which means some rows of X found by way of (**??**) can always be truncated.

We may want to test our results thus far.

4 Spectral Analysis

The discrete Fourier transform (DFT) is a staple of the digital signal processing community. [7] In essence, the DFT is a correlation of a windowed *sequence* (or *discrete signal*) with exponentials whose frequencies are equally spaced on the unit circle.[12] The DFT of the sequence $\{f(i) \in \mathbb{R}, i = 0 \ldots n-1\}$ is, in traditional form,[13]

$$F(k) = \sum_{i=0}^{n-1} f(i)\, e^{-ji2\pi k/n} \tag{32}$$

for $k = 0 \ldots n-1$ and $j = \sqrt{-1}$. The implicit window on $f(i)$ in (32) is rectangular. The values $\{F(k) \in \mathbb{C},\ k = 0 \ldots n-1\}$ are considered a spectral analysis of the sequence $f(i)$; *id est*, the $F(k)$ are amplitudes of exponentials which when combined, give back the original sequence,

$$f(i) = \frac{1}{n} \sum_{k=0}^{n-1} F(k)\, e^{ji2\pi k/n} \tag{33}$$

The argument of F, the index k, corresponds to the discrete frequencies $2\pi k/n$ of the exponentials $e^{ji2\pi k/n}$ in the synthesis equation (33).

The DFT (32) is separable in the real and the imaginary part; meaning, the analysis exhibits no dependency between the two parts when the sequence is real; *viz.*,

$$F(k) = \sum_{i=0}^{n-1} f(i)\ \cos(i2\pi k/n) - j \sum_{i=0}^{n-1} f(i)\ \sin(i2\pi k/n) \tag{34}$$

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 of polyhedral vertices $\{x_l \in \mathbb{R}^n,\ l = 1 \ldots N\}$ will be the new imaginary list $\{y_l \in \mathbb{R}^n,\ l = 1 \ldots N\}$, where

$$\begin{aligned} x_1 &= [f(i),\ i = 0 \ldots n-1] \\ y_1 &= [f(i),\ i = 0 \ldots n-1] \\ x_l &= [\ \ \cos(i2\pi(l-2)/n),\ i = 0 \ldots n-1], \quad l = 2 \ldots N \\ y_l &= [-\sin(i2\pi(l-2)/n),\ i = 0 \ldots n-1], \quad l = 2 \ldots N \end{aligned} \tag{35}$$

[12] the unit circle in the z plane; $z = e^{sT}$ where $s = \sigma + j\omega$ is the traditional Laplace frequency, ω is the Fourier frequency in radians $2\pi f$, while T is the sample period.

[13] The convention is lowercase for the sequence and uppercase for its transform.

where $N = n+1$, and where the [ ] bracket notation means a vector made from a sequence. The row-1 elements (columns $l = 2 \ldots N$) of EDM D^x are

$$\begin{aligned}
d^x_{1l} &= \sum_{i=0}^{n-1} (x_l - x_1)^2 \\
&= \sum_{i=0}^{n-1} (\cos(i2\pi(l-2)/n) \ - \ f(i))^2 \\
&= \sum_{i=0}^{n-1} \cos^2(i2\pi(l-2)/n) \ + \ f^2(i) \ - \ 2f(i)\cos(i2\pi(l-2)/n) \\
&= \tfrac{1}{4}(2n+1+\tfrac{\sin(2\pi(l(2n-1)+2)/n)}{\sin(2\pi(l-2)/n)}) \ + \ \tfrac{1}{n}\sum_{k=0}^{n-1}|F(k)|^2 \ - \ 2\,\Re F(l-2)
\end{aligned} \tag{36}$$

where $\Re$ takes the real part of its argument, and where the Fourier summation is from the Parseval relation for the DFT.[14] [7] For the imaginary vertices we have a separate EDM D^y whose row-1 elements (columns $l = 2 \ldots N$) are

$$\begin{aligned}
d^y_{1l} &= \sum_{i=0}^{n-1} (y_l - y_1)^2 \\
&= \sum_{i=0}^{n-1} (\sin(i2\pi(l-2)/n) \ + \ f(i))^2 \\
&= \sum_{i=0}^{n-1} \sin^2(i2\pi(l-2)/n) \ + \ f^2(i) \ + \ 2f(i)\sin(i2\pi(l-2)/n) \\
&= \tfrac{1}{4}(2n-1-\tfrac{\sin(2\pi(l(2n-1)+2)/n)}{\sin(2\pi(l-2)/n)}) \ + \ \tfrac{1}{n}\sum_{k=0}^{n-1}|F(k)|^2 \ - \ 2\,\Im F(l-2)
\end{aligned} \tag{37}$$

where $\Im$ takes the imaginary part of its argument. In the remaining rows ($m = 2 \ldots N,\ m < l$) of these two EDMs, D^x and D^y, we have[15]

$$\begin{aligned}
d^x_{ml} &= \sum_{i=0}^{n-1} (\cos(i2\pi(l-2)/n) \ - \ \cos(i2\pi(m-2)/n))^2 \\
&= \tfrac{1}{4}(4n+2+\tfrac{\sin(2\pi(l(2n-1)+2)/n)}{\sin(2\pi(l-2)/n)}+\tfrac{\sin(2\pi(m(2n-1)+2)/n)}{\sin(2\pi(m-2)/n)}) \\
d^y_{ml} &= \sum_{i=0}^{n-1} (\sin(i2\pi(l-2)/n) \ - \ \sin(i2\pi(m-2)/n))^2 \\
&= \tfrac{1}{4}(4n-2-\tfrac{\sin(2\pi(l(2n-1)+2)/n)}{\sin(2\pi(l-2)/n)}-\tfrac{\sin(2\pi(m(2n-1)+2)/n)}{\sin(2\pi(m-2)/n)})
\end{aligned} \tag{38}$$

[14] 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. [11]

[15] $\lim\limits_{i\to 2} \frac{\sin(2\pi(i(2n-1)+2)/n)}{\sin(2\pi(i-2)/n)} = 2n-1$

We observe from these distance-squared equations that only the first row and column of the EDM depends upon the sequence itself. The remainder of the EDM depends only upon the sequence length n.

To relate the EDMs D^x and D^y to the DFT in a useful way, we consider finding the inverse DFT (IDFT) via either EDM. For reasonable values of N, the number of matrix entries N^2 can become prohibitively large. But the DFT is subject to the same order of computational intensity. The matrix form of the DFT is written

$$F = Wf \tag{39}$$

where $F = [F(k),\, k = 0 \dots n-1]$, $f = [f(i),\, i = 0 \dots n-1]$, and the *DFT matrix* is [8]

$$W = W^T = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & e^{-j2\pi k/n} & e^{-j4\pi k/n} & \cdots & e^{-j(n-1)2\pi k/n} \\ 1 & e^{-j4\pi k/n} & e^{-j8\pi k/n} & \cdots & e^{-j(n-1)4\pi k/n} \\ 1 & e^{-j6\pi k/n} & e^{-j12\pi k/n} & \cdots & e^{-j(n-1)6\pi k/n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & e^{-j(n-1)2\pi k/n} & e^{-j(n-1)4\pi k/n} & \cdots & e^{-j(n-1)^2 2\pi k/n} \end{bmatrix} \tag{40}$$

When presented in this non-traditional way, the size of the DFT matrix $W \in \mathbb{R}^{n\times n}$ becomes apparent. It is obvious that a direct implementation of (39) would require on the order of n^2 operations for large n. Similarly, the IDFT is

$$f = \frac{1}{n} W^H F \tag{41}$$

where we have taken the conjugate transpose of the DFT matrix.

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 $n\log(n)$. [7] It is neither our purpose nor goal to invent a fast algorithm for doing this, we simply present an example of finding the IDFT by way of the EDM. The technique we use was developed in Section 2.1:

1. Diagonalize $-\frac{1}{2}V^TDV$ as $Q\Lambda Q^T \in \mathbb{R}^{N\times N}$.

2. Identify polyhedral vertices $XV = Q_o\Lambda^{1/2}Q^T \in \mathbb{R}^{n\times N}$ where Q_o is an unknown rotation/reflection matrix, and where $\Lambda \succeq 0$ for an EDM.

5 Matrix completion problem

Even more intriguing is whether the positional information can be reconstructed given an incomplete EDM.

A loose ends

$r \;=\; \operatorname{rank}(XV) \;=\; \operatorname{rank}(V^TX^TXV) \;=\; \operatorname{rank}(-V^TDV)$

$-V^TDV \succeq 0 \;\Leftrightarrow\; -z^TDz \geq 0 \quad \text{on } z \in \mathcal{N}(\mathbf{1}^T)$

$\operatorname{tr}(-\tfrac{1}{2}V^TDV) \;=\; \frac{1}{N}\sum_{i,j} d_{ij} \;=\; \frac{1}{2N}\mathbf{1}^TD\mathbf{1}$

$\mathcal{D}(X) = \mathcal{D}(XV)$.

Then substitution of $V^TX^TXV = -\frac{1}{2}V^TDV \Rightarrow$
$D = \delta(-\frac{1}{2}V^TDV)\mathbf{1}^T + \mathbf{1}\delta^T(-\frac{1}{2}V^TDV) + V^TDV$

A.1 V_w

$$V_w = \begin{bmatrix} \frac{-1}{\sqrt{N}} & \frac{-1}{\sqrt{N}} & \cdots & \frac{-1}{\sqrt{N}} \\ 1+\frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & \frac{-1}{N+\sqrt{N}} \\ \frac{-1}{N+\sqrt{N}} & 1+\frac{-1}{N+\sqrt{N}} & \cdots & \frac{-1}{N+\sqrt{N}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-1}{N+\sqrt{N}} & \frac{-1}{N+\sqrt{N}} & \cdots & 1+\frac{-1}{N+\sqrt{N}} \end{bmatrix} \in \mathbb{R}^{N\times N-1} \tag{42}$$

V can be expressed in terms of the full rank matrix V_w; [1]

$$V = V_wV_w^T \tag{43}$$

where $V_w^TV_w = I$. Hence the positive semidefinite criterion can be expressed instead as $-V_w^TDV_w \succeq 0$.[16]

Equivalently, we may simply interpret V in the positive definite criterion to mean any matrix whose range spans $\mathcal{N}(\mathbf{1}^T)$. The fact that V can be expressed as in (43) shows that V is a projection matrix; all projection matrices P can be expressed in the form $P = QQ^T$ where Q is an orthogonal matrix.

[16] This is easily shown because $V_w^TV_w = I$ and $-z^TV^TDVz \geq 0$ must be true for all z including $z = V_wy$.

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