Chapter 5

Euclidean Distance Matrix

These results [(1068)] *were obtained by Schoenberg (1935), a surprisingly late date for such a fundamental property of Euclidean geometry.*

– John Clifford Gower [190, §3]

By itself, distance information between many points in Euclidean space is lacking. We might want to know more; such as, relative or absolute position or dimension of some hull. A question naturally arising in some fields (*e.g*, geodesy, economics, genetics, psychology, biochemistry, engineering) [117] asks what facts can be deduced given only distance information. What can we know about the underlying points that the distance information purports to describe? We also ask what it means when given distance information is incomplete; or suppose the distance information is not reliable, available, or specified only by certain tolerances (affine inequalities). These questions motivate a study of interpoint distance, well represented in any spatial dimension by a simple matrix from linear algebra.[5.1] In what follows, we will answer some of these questions via Euclidean distance matrices.

5.1 EDM

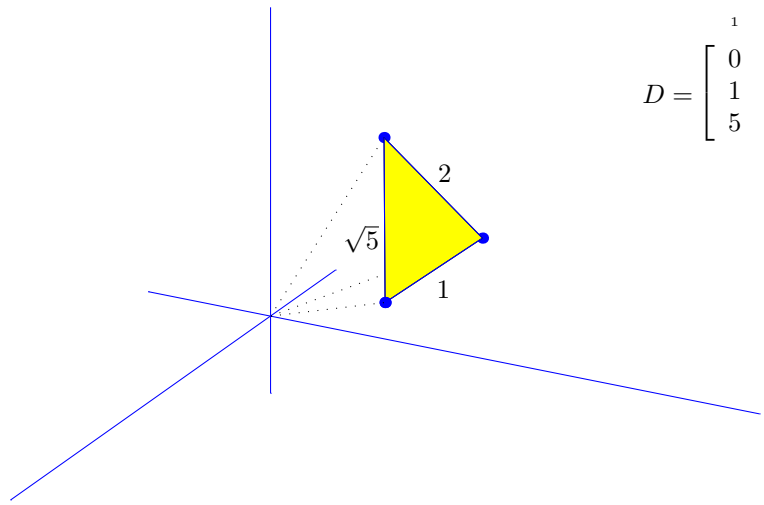
Euclidean space $\mathbb{R}^n$ is a finite-dimensional real vector space having an inner product defined on it, inducing a *metric*. [259, §3.1] A Euclidean distance matrix, an EDM in $\mathbb{R}_+^{N\times N}$, is an exhaustive table of distance-square d_{ij} between points taken by pair from a list of N points $\{x_\ell\ ,\ \ell=1\dots N\}$ in $\mathbb{R}^n$; the squared metric, the measure of distance-square:

$$d_{ij} \;=\; \|x_i - x_j\|_2^2 \;\triangleq\; \langle x_i - x_j\ ,\ x_i - x_j\rangle \tag{1037}$$

Each point is labelled ordinally, hence the row or column index of an EDM, i or $j=1\dots N$, individually addresses all the points in the list.

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

[5.1] *e.g*, $\sqrt[\circ]{D}\in\mathbb{R}^{N\times N}$, a classical two-dimensional matrix representation of absolute interpoint distance because its entries (in ordered rows and columns) can be written neatly on a piece of paper. Matrix D will be reserved throughout to hold distance-square.



$$D = \begin{array}{c c} \begin{array}{ccc} 1 & 2 & 3 \end{array} & \\ \begin{bmatrix} 0 & 1 & 5 \\ 1 & 0 & 4 \\ 5 & 4 & 0 \end{bmatrix} & \begin{array}{c} 1 \\ 2 \\ 3 \end{array} \end{array}$$

Figure 142: Convex hull of three points ($N=3$) is shaded in $\mathbb{R}^{\mathbf{3}}$ ($n=3$). Dotted lines are imagined vectors to points whose affine dimension is 2.

$$D = [d_{ij}] = \begin{bmatrix} d_{11} & d_{12} & d_{13} \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{bmatrix} = \begin{bmatrix} 0 & d_{12} & d_{13} \\ d_{12} & 0 & d_{23} \\ d_{13} & d_{23} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 5 \\ 1 & 0 & 4 \\ 5 & 4 & 0 \end{bmatrix} \tag{1038}$$

Matrix D has N^2 entries but only $N(N-1)/2$ pieces of information. In Figure **142** are shown three points in $\mathbb{R}^{\mathbf{3}}$ that can be arranged in a list to correspond to D in (1038). But such a list is not unique because any rotation, reflection, or translation (§5.5) of those points would produce the same EDM D.

5.2 First metric properties

For $i,j=1\dots N$, absolute distance between points x_i and x_j must satisfy the defining requirements imposed upon any *metric space*: [259, §1.1] [294, §1.7] namely, for Euclidean metric $\sqrt{d_{ij}}$ (§5.4) in $\mathbb{R}^n$

1. $\sqrt{d_{ij}} \geq 0\,,\quad i \neq j$ — nonnegativity
2. $\sqrt{d_{ij}} = 0 \;\Leftrightarrow\; x_i = x_j$ — selfdistance
3. $\sqrt{d_{ij}} = \sqrt{d_{ji}}$ — symmetry
4. $\sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}\;,\quad i \neq j \neq k$ — triangle inequality

Then all entries of an EDM must be in concord with these Euclidean metric properties: specifically, each entry must be nonnegative,[5.2] the main diagonal must be $\mathbf{0}$,[5.3] and an EDM must be symmetric. The fourth property provides upper and lower bounds for each entry. Property 4 is true more generally when there are no restrictions on indices i,j,k, but furnishes no new information.

[5.2] Implicit from the terminology, $\sqrt{d_{ij}} \geq 0 \Leftrightarrow d_{ij} \geq 0$ is always assumed.

[5.3] What we call selfdistance, Marsden calls *nondegeneracy*. [294, §1.6] Kreyszig calls these first metric properties *axioms of the metric*; [259, p.4] Blumenthal refers to them as *postulates*. [55, p.15]

5.3 ∃ fifth Euclidean metric property

The four properties of the Euclidean metric provide information insufficient to certify that a bounded convex polyhedron more complicated than a triangle has a Euclidean realization. [190, §2] Yet any list of points or the vertices of any bounded convex polyhedron must conform to the properties.

5.3.0.0.1 Example. *Triangle.*
Consider the EDM in (1038), but missing one of its entries:

$$D = \begin{bmatrix} 0 & 1 & d_{13} \\ 1 & 0 & 4 \\ d_{31} & 4 & 0 \end{bmatrix} \tag{1039}$$

Can we determine unknown entries of D by applying the metric properties? Property 1 demands $\sqrt{d_{13}}, \sqrt{d_{31}} \geq 0$, property 2 requires the main diagonal be $\mathbf{0}$, while property 3 makes $\sqrt{d_{31}} = \sqrt{d_{13}}$. The fourth property tells us

$$1 \leq \sqrt{d_{13}} \leq 3 \tag{1040}$$

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

5.3.0.0.2 Example. *Small completion problem,* I.
Now consider the polyhedron in Figure **143**b formed from an unknown list $\{x_1, x_2, x_3, x_4\}$. The corresponding EDM less one critical piece of information, d_{14}, is given by

$$D = \begin{bmatrix} 0 & 1 & 5 & d_{14} \\ 1 & 0 & 4 & 1 \\ 5 & 4 & 0 & 1 \\ d_{14} & 1 & 1 & 0 \end{bmatrix} \tag{1041}$$

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

$$\sqrt{5}-1 \;\leq\; \sqrt{d_{14}} \;\leq\; 2 \tag{1042}$$

We cannot further narrow those bounds on $\sqrt{d_{14}}$ using only the four metric properties (§5.8.3.1.1). Yet there is only one possible choice for $\sqrt{d_{14}}$ because points x_2, x_3, x_4 must be collinear. All other values of $\sqrt{d_{14}}$ in the interval $[\sqrt{5}-1, 2]$ specify impossible distances in any dimension; *id est*, in this particular example the triangle inequality does not yield an interval for $\sqrt{d_{14}}$ over which a family of convex polyhedra can be reconstructed. □

We will return to this simple Example 5.3.0.0.2 to illustrate more elegant methods of solution in §5.8.3.1.1, §5.9.2.0.1, and §5.14.4.1.1. Until then, we can deduce some general principles from the foregoing examples:

- Unknown d_{ij} of an EDM are not necessarily uniquely determinable.
- The triangle inequality does not produce necessarily tight bounds.[5.4]
- Four Euclidean metric properties are insufficient for reconstruction.

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

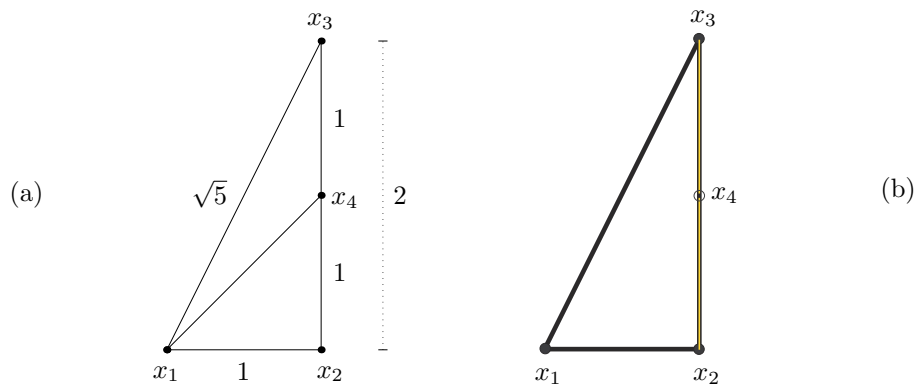


Figure 143: **(a)** Complete dimensionless *EDM graph.* **(b)** Emphasizing obscured segments $\overline{x_2x_4}$, $\overline{x_4x_3}$, and $\overline{x_2x_3}$, now only five $(2N-3)$ absolute distances are specified. EDM so represented is incomplete, missing d_{14} as in (1041), yet the isometric reconstruction (§5.4.2.2.10) is unique as proved in §5.9.2.0.1 and §5.14.4.1.1. First four properties of Euclidean metric are not a recipe for reconstruction of this polyhedron.

5.3.1 lookahead

There must exist at least one requirement more than the four properties of the Euclidean metric that makes them altogether necessary and sufficient to certify realizability of bounded convex polyhedra. Indeed, there are infinitely many more; there are precisely $N+1$ necessary and sufficient Euclidean metric requirements for N points constituting a generating list (§2.3.2). Here is the fifth requirement:

5.3.1.0.1 Fifth Euclidean metric property. *Relative-angle inequality.* (*confer* §5.14.2.1.1) Augmenting the four fundamental properties of the Euclidean metric in $\mathbb{R}^n$, for all $i,j,\ell \neq k \in \{1\dots N\}$, $i<j<\ell$, and for $N \geq 4$ distinct points $\{x_k\}$, the inequalities

$$\begin{gathered}\cos(\theta_{ik\ell}+\theta_{\ell kj}) \;\leq\; \cos\theta_{ikj} \;\leq\; \cos(\theta_{ik\ell}-\theta_{\ell kj}) \\ 0 \leq \theta_{ik\ell}\,,\theta_{\ell kj}\,,\theta_{ikj} \leq \pi\end{gathered} \tag{1043}$$

where $\theta_{ikj}=\theta_{jki}$ represents angle between vectors at vertex x_k (1115) (Figure **144**), must be satisfied at each point x_k regardless of affine dimension. ◇

We will explore this in §5.14. One of our early goals is to determine matrix criteria that subsume all the Euclidean metric properties and any further requirements. Looking ahead, we will find (1394) (1068) (1072)

$$\left.\begin{array}{r} -z^{\mathrm{T}}Dz \geq 0 \\ \mathbf{1}^{\mathrm{T}}z = 0 \\ (\forall\,\|z\|=1) \\ D \in \mathbb{S}_h^N \end{array}\right\} \;\Leftrightarrow\; D \in \mathbb{EDM}^N \tag{1044}$$

where the convex cone of Euclidean distance matrices $\mathbb{EDM}^N \subseteq \mathbb{S}_h^N$ belongs to the subspace of symmetric hollow[5.5] matrices (§2.2.3.0.1). (Numerical test `isedm()` is provided on

[5.5] $\mathbf{0}$ main diagonal.

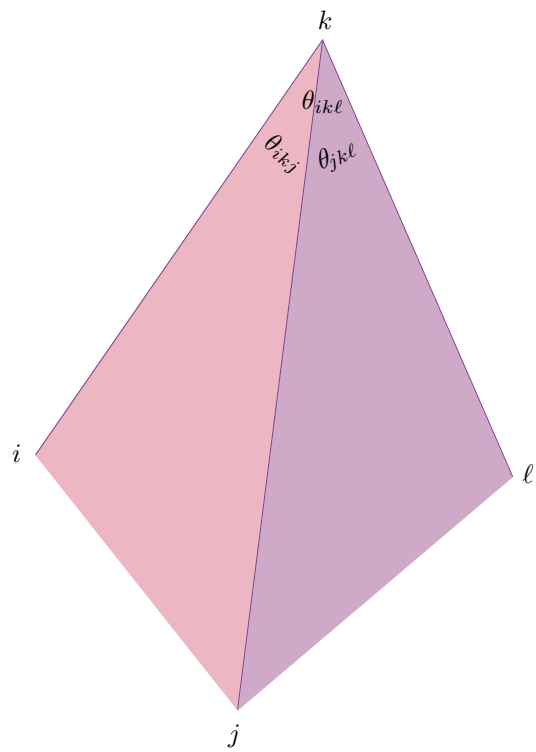


Figure 144: Fifth Euclidean metric property nomenclature. Each angle θ is made by a vector pair at vertex k while i, j, k, ℓ index four points at the vertices of a generally irregular tetrahedron. The fifth property is necessary for realization of four or more points; a reckoning by three angles in any dimension. Together with the first four Euclidean metric properties, this fifth property is necessary and sufficient for realization of four points.

Wikimization [439].) Having found equivalent matrix criteria, we will see there is a bridge from bounded convex polyhedra to EDMs in §5.9.[5.6]

Now we develop some invaluable concepts, moving toward a link of the Euclidean metric properties to matrix criteria.

5.4 EDM definition

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

$$X = [\, x_1 \ \cdots \ x_N \,] \in \mathbb{R}^{n\times N} \qquad (79)$$

where N is regarded as *cardinality* of list X. When matrix $D = [d_{ij}]$ is an EDM, its entries must be related to those points constituting the list by the Euclidean distance-square: for $i, j = 1 \dots N$ (§A.1.1 *no.*36)

$$\begin{aligned} d_{ij} &= \|x_i - x_j\|^2 = (x_i - x_j)^{\mathrm{T}}(x_i - x_j) = \|x_i\|^2 + \|x_j\|^2 - 2x_i^{\mathrm{T}}x_j \\ &= \begin{bmatrix} x_i^{\mathrm{T}} & x_j^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} I & -I \\ -I & I \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} \\ &= \operatorname{vec}(X)^{\mathrm{T}}(\Phi_{ij} \otimes I) \operatorname{vec} X = \langle \Phi_{ij} \ , \ X^{\mathrm{T}}X \rangle \end{aligned} \qquad (1045)$$

where

$$\operatorname{vec} X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^{nN} \qquad (1046)$$

and where $\otimes$ signifies Kronecker product (§D.1.2.1). $\Phi_{ij} \otimes I$ is positive semidefinite (1652) having $I \in \mathbb{S}^n$ in its ii^{th} and jj^{th} block of entries while $-I \in \mathbb{S}^n$ fills its ij^{th} and ji^{th} block; *id est*,

$$\begin{aligned} \Phi_{ij} &\triangleq \delta\big((e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})\mathbf{1}\big) - (e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}}) \in \mathbb{S}_+^N \\ &= e_i e_i^{\mathrm{T}} + e_j e_j^{\mathrm{T}} - e_i e_j^{\mathrm{T}} - e_j e_i^{\mathrm{T}} \\ &= (e_i - e_j)(e_i - e_j)^{\mathrm{T}} \end{aligned} \qquad (1047)$$

where $\{e_i \in \mathbb{R}^N,\ i = 1 \dots N\}$ is the set of standard basis vectors. Thus each entry d_{ij} is a convex quadratic function (§A.4.0.0.2) of $\operatorname{vec} X$ (39). [349, §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* (§6, Figure **179** p.459);

$$\mathbf{0} \in \mathbb{EDM}^N \subseteq \mathbb{S}_h^N \cap \mathbb{R}_+^{N\times N} \subset \mathbb{S}^N \qquad (1048)$$

An EDM D must be expressible as a function of some list X; *id est*, it must have the form

$$\mathbf{D}(X) \triangleq \delta(X^{\mathrm{T}}X)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\delta(X^{\mathrm{T}}X)^{\mathrm{T}} - 2X^{\mathrm{T}}X \in \mathbb{EDM}^N \qquad (1049)$$

$$= [\operatorname{vec}(X)^{\mathrm{T}}(\Phi_{ij} \otimes I) \operatorname{vec} X \ , \quad i, j = 1 \dots N] \qquad (1050)$$

Function $\mathbf{D}(X)$ will make an EDM given any $X \in \mathbb{R}^{n\times N}$, conversely, but $\mathbf{D}(X)$ is not a convex function of X (§5.4.1). Now the EDM cone may be described:

$$\mathbb{EDM}^N = \left\{ \mathbf{D}(X) \mid X \in \mathbb{R}^{N-1\times N} \right\} \qquad (1051)$$

[5.6] From an EDM, a generating list (§2.3.2, §2.12.2) for a polyhedron can be found (§5.12) correct to within a rotation, reflection, and translation (§5.5).

Expression $\mathbf{D}(X)$ is a matrix definition of EDM and so conforms to the Euclidean metric properties:

Nonnegativity of EDM entries (property 1, §5.2) is obvious from the distance-square definition (1045), so holds for any D expressible in the form $\mathbf{D}(X)$ in (1049).

When we say D is an EDM, reading from (1049), it implicitly means the main diagonal must be $\mathbf{0}$ (property 2, selfdistance) and D must be symmetric (property 3); $\delta(D)=\mathbf{0}$ and $D^{\mathrm{T}}=D$ or, equivalently, $D\in\mathbb{S}_h^N$ are necessary matrix criteria.

5.4.0.1 homogeneity

Function $\mathbf{D}(X)$ is homogeneous in the sense, for $\zeta\in\mathbb{R}$

$$\sqrt[\circ]{\mathbf{D}(\zeta X)}=|\zeta|\sqrt[\circ]{\mathbf{D}(X)} \tag{1052}$$

where the positive square root is entrywise ($^\circ$).

Any nonnegatively scaled EDM remains an EDM; *id est*, the matrix class EDM is invariant to nonnegative scaling $(\alpha\,\mathbf{D}(X)$ for $\alpha\geq 0)$ because all EDMs of dimension N constitute a convex cone $\mathbb{EDM}^N$ (§6, Figure **171**).

5.4.1 $-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(X)V_{\mathcal{N}}$ convexity

We saw that EDM entries $d_{ij}\left(\begin{bmatrix}x_i\\x_j\end{bmatrix}\right)$ are convex quadratic functions. Yet $-\mathbf{D}(X)$ (1049) is not a quasiconvex function of matrix $X\in\mathbb{R}^{n\times N}$ because the second directional derivative (§3.14)

$$-\frac{d^2}{dt^2}\bigg|_{t=0}\mathbf{D}(X+tY)=2\big(-\delta(Y^{\mathrm{T}}Y)\mathbf{1}^{\mathrm{T}}-\mathbf{1}\,\delta(Y^{\mathrm{T}}Y)^{\mathrm{T}}+2\,Y^{\mathrm{T}}Y\big) \tag{1053}$$

is indefinite for any $Y\in\mathbb{R}^{n\times N}$ since its main diagonal is $\mathbf{0}$. [185, §4.2.8] [233, §7.1 prob.2] Hence $-\mathbf{D}(X)$ can neither be convex in X.

The outcome is different when instead we consider

$$-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(X)V_{\mathcal{N}}=2V_{\mathcal{N}}^{\mathrm{T}}X^{\mathrm{T}}XV_{\mathcal{N}} \tag{1054}$$

where we introduce the full-rank thin *Schoenberg auxiliary matrix* (§B.4.2)

$$V_{\mathcal{N}}\;\triangleq\;\frac{1}{\sqrt{2}}\begin{bmatrix}-1&-1&\cdots&-1\\1&&&\mathbf{0}\\&1&&\\&&\ddots&\\\mathbf{0}&&&1\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix}-\mathbf{1}^{\mathrm{T}}\\I\end{bmatrix}\in\mathbb{R}^{N\times N-1} \tag{1055}$$

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

$$\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^{\mathrm{T}})\;,\quad V_{\mathcal{N}}^{\mathrm{T}}\mathbf{1}=\mathbf{0} \tag{1056}$$

Matrix-valued function (1054) meets the criterion for convexity in §3.13.0.0.2 over its domain that is all of $\mathbb{R}^{n\times N}$; *videlicet*, for any $Y\in\mathbb{R}^{n\times N}$

$$-\frac{d^2}{dt^2}\,V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(X+tY)V_{\mathcal{N}}\;=\;4V_{\mathcal{N}}^{\mathrm{T}}Y^{\mathrm{T}}YV_{\mathcal{N}}\;\succeq\;0 \tag{1057}$$

Quadratic matrix-valued function $-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(X)V_{\mathcal{N}}$ is therefore convex in X achieving its minimum, with respect to a positive semidefinite cone (§2.7.2.2), at $X=\mathbf{0}$. When the penultimate number of points exceeds the dimension of the space $n<N-1$, strict convexity of the quadratic (1054) becomes impossible because (1057) could not then be positive definite.

5.4.2 Gram-form EDM definition

Positive semidefinite matrix $X^{\mathrm{T}}X$ in (1049), formed from inner product of list $X\in\mathbb{R}^{n\times N}$, is known as a *Gram matrix*; [285, §3.6]

$$G \triangleq X^{\mathrm{T}}X = \begin{bmatrix} x_1^{\mathrm{T}} \\ \vdots \\ x_N^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} x_1 & \cdots & x_N \end{bmatrix} = \begin{bmatrix} \|x_1\|^2 & x_1^{\mathrm{T}}x_2 & x_1^{\mathrm{T}}x_3 & \cdots & x_1^{\mathrm{T}}x_N \\ x_2^{\mathrm{T}}x_1 & \|x_2\|^2 & x_2^{\mathrm{T}}x_3 & \cdots & x_2^{\mathrm{T}}x_N \\ x_3^{\mathrm{T}}x_1 & x_3^{\mathrm{T}}x_2 & \|x_3\|^2 & \ddots & x_3^{\mathrm{T}}x_N \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ x_N^{\mathrm{T}}x_1 & x_N^{\mathrm{T}}x_2 & x_N^{\mathrm{T}}x_3 & \cdots & \|x_N\|^2 \end{bmatrix} \in \mathbb{S}_+^N$$

$$= \delta\left(\begin{bmatrix} \|x_1\| \\ \|x_2\| \\ \vdots \\ \|x_N\| \end{bmatrix}\right) \begin{bmatrix} 1 & \cos\psi_{12} & \cos\psi_{13} & \cdots & \cos\psi_{1N} \\ \cos\psi_{12} & 1 & \cos\psi_{23} & \cdots & \cos\psi_{2N} \\ \cos\psi_{13} & \cos\psi_{23} & 1 & \ddots & \cos\psi_{3N} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \cos\psi_{1N} & \cos\psi_{2N} & \cos\psi_{3N} & \cdots & 1 \end{bmatrix} \delta\left(\begin{bmatrix} \|x_1\| \\ \|x_2\| \\ \vdots \\ \|x_N\| \end{bmatrix}\right) \tag{1058}$$

$$\triangleq \sqrt{\delta^2(G)}\,\Psi\sqrt{\delta^2(G)}$$

where ψ_{ij} (1077) is angle between vectors x_i and x_j, and where δ^2 denotes a diagonal matrix in this case. Positive semidefiniteness of *interpoint angle matrix* Ψ implies positive semidefiniteness of Gram matrix G;

$$G \succeq 0 \;\Leftarrow\; \Psi \succeq 0 \tag{1059}$$

When $\delta^2(G)$ is nonsingular, then $G\succeq 0 \;\Leftrightarrow\; \Psi\succeq 0$. (§A.3.1.0.5)

Distance-square d_{ij} (1045) is related to Gram matrix entries $G^{\mathrm{T}}=G\triangleq[g_{ij}]$

$$\begin{aligned} d_{ij} &= g_{ii}+g_{jj}-2g_{ij} \\ &= \langle \Phi_{ij}\,,\,G\rangle \end{aligned} \tag{1060}$$

where Φ_{ij} is defined in (1047). Hence the linear EDM definition

$$\left.\begin{aligned} \mathbf{D}(G) &\triangleq \delta(G)\mathbf{1}^{\mathrm{T}}+\mathbf{1}\,\delta(G)^{\mathrm{T}}-2G \;\in \mathbb{EDM}^N \\ &= [\langle \Phi_{ij}\,,\,G\rangle\,,\; i,j=1\ldots N] \end{aligned}\right\} \;\Leftarrow\; G\succeq 0 \tag{1061}$$

The EDM cone may be described, (*confer* (1150)(1156))

$$\mathbb{EDM}^N = \left\{\mathbf{D}(G) \mid G\in\mathbb{S}_+^N\right\} \tag{1062}$$

5.4.2.1 First point at origin

Assume the first point x_1 in an unknown list $X\in\mathbb{R}^{n\times N}$ resides at the origin;

$$Xe_1=\mathbf{0} \;\Leftrightarrow\; Ge_1=\mathbf{0} \tag{1063}$$

Consider the symmetric translation $(I-\mathbf{1}e_1^{\mathrm{T}})\mathbf{D}(G)(I-e_1\mathbf{1}^{\mathrm{T}})$ that shifts the first row and column of $\mathbf{D}(G)$ to the origin; setting Gram-form EDM operator $\mathbf{D}(G)=D$ for convenience,

$$-\big(D-(De_1\mathbf{1}^{\mathrm{T}}+\mathbf{1}e_1^{\mathrm{T}}D)+\mathbf{1}e_1^{\mathrm{T}}De_1\mathbf{1}^{\mathrm{T}}\big)\tfrac{1}{2} = G-(Ge_1\mathbf{1}^{\mathrm{T}}+\mathbf{1}e_1^{\mathrm{T}}G)+\mathbf{1}e_1^{\mathrm{T}}Ge_1\mathbf{1}^{\mathrm{T}} \tag{1064}$$

where

$$e_1 \triangleq \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{1065}$$

is the first vector from the standard basis. Then it follows, for $D \in \mathbb{S}_h^N$

$$\begin{aligned} G &= -\big(D - (De_1\mathbf{1}^{\mathrm{T}} + \mathbf{1}e_1^{\mathrm{T}}D)\big)\tfrac{1}{2}\,, \qquad x_1 = \mathbf{0} \\ &= -\begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix}^{\mathrm{T}} D \begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix}\tfrac{1}{2} \\ &= \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \end{bmatrix} \\ V_{\mathcal{N}}^{\mathrm{T}}GV_{\mathcal{N}} &= -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\tfrac{1}{2} \qquad \forall\, X \end{aligned} \tag{1066}$$

where

$$I - e_1\mathbf{1}^{\mathrm{T}} = \begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix} \tag{1067}$$

is a projector (§B.4.2 *no.*7) nonorthogonally projecting (§E.1, §E.8) on subspace

$$\begin{aligned} \mathbb{S}_{\mathbf{0}}^N &= \{G \in \mathbb{S}^N \mid Ge_1 = \mathbf{0}\} \\ &= \left\{\begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix}^{\mathrm{T}} Y \begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix} \mid Y \in \mathbb{S}^N\right\} \end{aligned} \tag{2220}$$

in the Euclidean sense. From (1066) we get sufficiency of the first matrix criterion for an EDM proved by Schoenberg in 1935; [355][5.7]

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \begin{cases} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \in \mathbb{S}_+^{N-1} \\ D \in \mathbb{S}_h^N \end{cases} \tag{1068}$$

We provide a rigorous complete more geometric proof of this fundamental *Schoenberg criterion* in §5.9.1.0.4. [439, `isedm()`]

By substituting $G = \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \end{bmatrix}$ (1066) into $\mathbf{D}(G)$ (1061),

$$D = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big) \end{bmatrix}\mathbf{1}^{\mathrm{T}} + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)^{\mathrm{T}} \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \end{bmatrix} \tag{1170}$$

assuming $x_1 = \mathbf{0}$. Details of this bijection are provided in §5.6.2.

5.4.2.2 0 geometric center

Assume the *geometric center* (§5.5.1.0.1) of an unknown list $X \in \mathbb{R}^{n\times N}$ to be the origin;

$$X\mathbf{1} = \mathbf{0} \;\Leftrightarrow\; G\mathbf{1} = \mathbf{0} \tag{1069}$$

Now consider the calculation $(I - \frac{1}{N}\mathbf{1}\mathbf{1}^{\mathrm{T}})\mathbf{D}(G)(I - \frac{1}{N}\mathbf{1}\mathbf{1}^{\mathrm{T}})$, a geometric centering or projection operation. (§E.7.2.0.2) Setting $\mathbf{D}(G) = D$ for convenience as in §5.4.2.1,

$$\begin{aligned} G &= -\big(D - \tfrac{1}{N}(D\mathbf{1}\mathbf{1}^{\mathrm{T}} + \mathbf{1}\mathbf{1}^{\mathrm{T}}D) + \tfrac{1}{N^2}\mathbf{1}\mathbf{1}^{\mathrm{T}}D\mathbf{1}\mathbf{1}^{\mathrm{T}}\big)\tfrac{1}{2}\,, \quad X\mathbf{1} = \mathbf{0} \\ &= -VDV\tfrac{1}{2} \\ VGV &= -VDV\tfrac{1}{2} \qquad \forall\, X \end{aligned} \tag{1070}$$

[5.7] From (1056) we know $\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^{\mathrm{T}})$, so (1068) is the same as (1044). In fact, any matrix V in place of $V_{\mathcal{N}}$ will satisfy (1068) whenever $\mathcal{R}(V) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^{\mathrm{T}})$. But $V_{\mathcal{N}}$ is the matrix implicit in Schoenberg's seminal exposition.

where more properties of the auxiliary (*geometric centering,* projection) matrix

$$V \triangleq I - \frac{1}{N}\mathbf{1}\mathbf{1}^{\mathrm{T}} \in \mathbb{S}^N \tag{1071}$$

are found in §B.4. From (1070) and the assumption $D \in \mathbb{S}_h^N$ we get sufficiency of the more popular form of Schoenberg criterion:

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \left\{ \begin{array}{c} -VDV \in \mathbb{S}_+^N \\ D \in \mathbb{S}_h^N \end{array} \right. \tag{1072}$$

Of particular utility when $D \in \mathbb{EDM}^N$ is the fact, (§B.4.2 *no.*20) (1045)

$$\begin{aligned} \operatorname{tr}\big(-VDV\tfrac{1}{2}\big) &= \tfrac{1}{2N}\sum_{i,j} d_{ij} &&= \tfrac{1}{2N}\operatorname{vec}(X)^{\mathrm{T}}\left(\sum_{i,j}\Phi_{ij}\otimes I\right)\operatorname{vec}X \\ &= \operatorname{tr}(VGV)\;, \quad G \succeq 0 \\ &= \operatorname{tr} G &&= \sum_{\ell=1}^{N}\|x_\ell\|^2 = \|X\|_{\mathrm{F}}^2 \;, \qquad X\mathbf{1}=\mathbf{0} \end{aligned} \tag{1073}$$

where $\sum \Phi_{ij} \in \mathbb{S}_+^N$ (1047), therefore convex in $\operatorname{vec} X$. We will find this trace useful as a heuristic to minimize affine dimension of an unknown list arranged columnar in X (§7.2.2), but it tends to facilitate reconstruction of a list configuration having least energy; *id est*, it compacts a reconstructed list by minimizing total norm-square of the vertices.

By substituting $G = -VDV\frac{1}{2}$ (1070) into $\mathbf{D}(G)$ (1061), assuming $X\mathbf{1}=\mathbf{0}$

$$D = \delta\big(-VDV\tfrac{1}{2}\big)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\delta\big(-VDV\tfrac{1}{2}\big)^{\mathrm{T}} - 2\big(-VDV\tfrac{1}{2}\big) \tag{1160}$$

Details of this bijection can be found in §5.6.1.1.

5.4.2.2.1 Example. *Hypersphere.*

These foregoing relationships allow combination of distance and Gram constraints in any optimization problem we might pose:

- Interpoint angle Ψ can be constrained by fixing all individual point lengths $\sqrt[\circ]{\delta(G)}$; then
$$\Psi = -\sqrt{\delta^2(G)}^{\,-1} VDV\tfrac{1}{2}\sqrt{\delta^2(G)}^{\,-1}, \qquad X\mathbf{1}=\mathbf{0} \tag{1074}$$

- (*confer* §5.9.1.0.3, (1259) (1403)) Constraining all main diagonal entries g_{ii} of a Gram matrix to 1, for example, is equivalent to the constraint that all points lie on a hypersphere of radius 1 centered at the origin.
$$D = 2(g_{11}\mathbf{1}\mathbf{1}^{\mathrm{T}} - G) \in \mathbb{EDM}^N \tag{1075}$$
Requiring $\mathbf{0}$ geometric center then becomes equivalent to the constraint: $D\mathbf{1} = 2N\mathbf{1}$. [98, p.116] Any further constraint on that Gram matrix applies only to interpoint angle matrix $\Psi = G$.

Because any point list may be constrained to lie on a hypersphere boundary whose affine dimension exceeds that of the list, a Gram matrix may always be constrained to have equal positive values along its main diagonal. (Laura Klanfer 1933 [355, §3]) This observation renewed interest in the elliptope (§5.9.1.0.1). □

5.4.2.2.2 Example. *List-member constraints via Gram matrix.*
Capitalizing on identity (1070) relating Gram and EDM D matrices, a constraint set such as

$$\left.\begin{aligned} \operatorname{tr}\big(-\tfrac{1}{2}VDVe_ie_i^{\mathrm{T}}\big) &= \|x_i\|^2 \\ \operatorname{tr}\big(-\tfrac{1}{2}VDV(e_ie_j^{\mathrm{T}}+e_je_i^{\mathrm{T}})\tfrac{1}{2}\big) &= x_i^{\mathrm{T}}x_j \\ \operatorname{tr}\big(-\tfrac{1}{2}VDVe_je_j^{\mathrm{T}}\big) &= \|x_j\|^2 \end{aligned}\right\} \tag{1076}$$

relates list member x_i to x_j to within an isometry through inner-product identity (35) [450, §1-7]

$$\cos\psi_{ij} = \frac{x_i^{\mathrm{T}}x_j}{\|x_i\|\,\|x_j\|} \tag{1077}$$

where ψ_{ij} is angle between the two vectors as in (1058). For M list members, there total $M(M+1)/2$ such constraints. Angle constraints are incorporated in Example 5.4.2.2.5 and Example 5.4.2.2.13. □

5.4.2.2.3 Example. *Gram matrix as optimization problem.*
Consider the academic problem of finding a Gram matrix (1070) subject to constraints on each and every entry of the corresponding EDM:

$$\begin{aligned} \underset{D\in\mathbb{S}_h^N}{\text{find}} \quad & -VDV\tfrac{1}{2} \in \mathbb{S}^N \\ \text{subject to} \quad & \big\langle D\,,\,(e_ie_j^{\mathrm{T}}+e_je_i^{\mathrm{T}})\tfrac{1}{2}\big\rangle = \check{d}_{ij}\ , \quad i,j=1\ldots N\,, \quad i<j \\ & -VDV \succeq 0 \end{aligned} \tag{1078}$$

where the $\check{d}_{ij}$ are given nonnegative constants. EDM D can, of course, be replaced with the equivalent Gram-form (1061). Requiring only the selfadjointness property (1588) of the main-diagonal linear operator δ we get, for $A\in\mathbb{S}^N$

$$\langle D\,,\,A\rangle \;=\; \big\langle \delta(G)\mathbf{1}^{\mathrm{T}}+\mathbf{1}\,\delta(G)^{\mathrm{T}}-2G\,,\,A\big\rangle \;=\; 2\,\langle G\,,\,\delta(A\mathbf{1})-A\rangle \tag{1079}$$

Then the problem equivalent to (1078) becomes, for $G\in\mathbb{S}_c^N \Leftrightarrow G\mathbf{1}=\mathbf{0}$

$$\begin{aligned} \underset{G\in\mathbb{S}_c^N}{\text{find}} \quad & G \in \mathbb{S}^N \\ \text{subject to} \quad & \Big\langle G\,,\,\delta\big((e_ie_j^{\mathrm{T}}+e_je_i^{\mathrm{T}})\mathbf{1}\big)-(e_ie_j^{\mathrm{T}}+e_je_i^{\mathrm{T}})\Big\rangle = \check{d}_{ij}\ , \quad i,j=1\ldots N\,, \quad i<j \\ & G \succeq 0 \end{aligned} \tag{1080}$$

Barvinok's Proposition 2.9.3.0.1 predicts existence for either formulation (1078) or (1080) such that implicit equality constraints (induced by subspace membership) are ignored

$$\operatorname{rank}G\ ,\ \operatorname{rank}VDV \le \left\lfloor \frac{\sqrt{8\big(N(N-1)/2\big)+1}-1}{2} \right\rfloor = N-1 \tag{1081}$$

because, in each case, the Gram matrix is confined to a face of positive semidefinite cone $\mathbb{S}_+^N$ isomorphic with $\mathbb{S}_+^{N-1}$ (§6.6.1). (§E.7.2.0.2) This bound is tight (§5.7.1.1) and is the greatest upper bound.[5.8] □

5.4.2.2.4 Example. *First duality.*
Kuhn reports that the first dual optimization problem[5.9] to be recorded in the literature

[5.8] $-VDV|_{N\leftarrow 1}=0$ (§B.4.1)

[5.9] By *dual problem* is meant, in the strongest sense: the optimal objective achieved by a maximization problem, dual to a given (primal) minimization problem, is always equal to the optimal objective achieved by the minimization. (Figure **64** Example 2.13.1.1.2) A dual problem is always convex when derived from a primal via Lagrangian function.

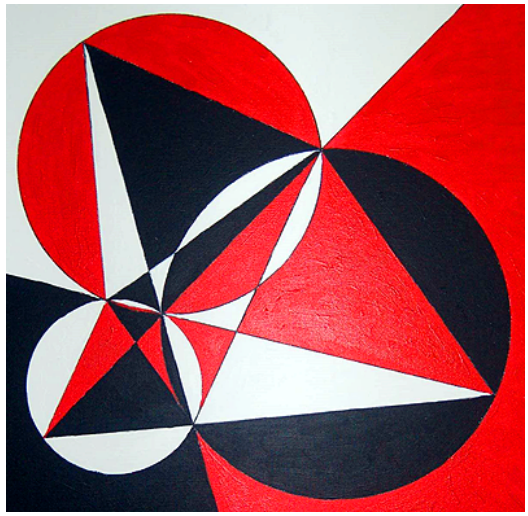


Figure 145: Rendering of *Fermat point* in acrylic on canvas by Suman Vaze. Three circles intersect at Fermat point of minimum total distance from three vertices of (and interior to) red/black/white triangle.

dates back to 1755. [426] Perhaps more intriguing is the fact: this earliest instance of duality is a two-dimensional Euclidean distance geometry problem known as *Fermat point* (Figure **145**) named after the French mathematician. Given N distinct points in the plane $\{x_i \in \mathbb{R}^{\mathbf{2}},\, i=1\dots N\}$, the Fermat point y is an optimal solution to

$$\underset{y}{\text{minimize}} \quad \sum_{i=1}^{N} \|y - x_i\| \tag{1082}$$

a convex minimization of total distance. The historically first dual problem formulation asks for the smallest equilateral triangle encompassing ($N=3$) three points x_i. Another problem dual to (1082) (Kuhn 1967)

$$\begin{array}{ll} \underset{\{z_i\}}{\text{maximize}} & \sum_{i=1}^{N} \langle z_i\,,\, x_i\rangle \\ \text{subject to} & \sum_{i=1}^{N} z_i = \mathbf{0} \\ & \|z_i\| \le 1 \quad \forall\, i \end{array} \tag{1083}$$

has interpretation as minimization of work required to balance potential energy in an N-way tug-of-war between equally matched opponents situated at $\{x_i\}$. [445]

It is not so straightforward to write the Fermat point problem (1082) equivalently in terms of a Gram matrix from this section. Squaring instead

$$\underset{\alpha}{\text{minimize}} \sum_{i=1}^{N} \|\alpha - x_i\|^2 \;\equiv\; \begin{array}{ll} \underset{D\in\mathbb{S}^{N+1}}{\text{minimize}} & \langle -V\,,\, D\rangle \\ \text{subject to} & \langle D\,,\, e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}}\rangle \frac{1}{2} = \check{d}_{ij} \quad \forall (i,j)\in\mathcal{I} \\ & -V D V \succeq 0 \end{array} \tag{1084}$$

yields an inequivalent convex geometric centering problem whose equality constraints comprise EDM D main-diagonal zeros and known distances-square.[5.10] Going the other

[5.10] $\alpha^\star$ is geometric center of points x_i (1134). For three points, $\mathcal{I}=\{1,2,3\}$; optimal affine dimension

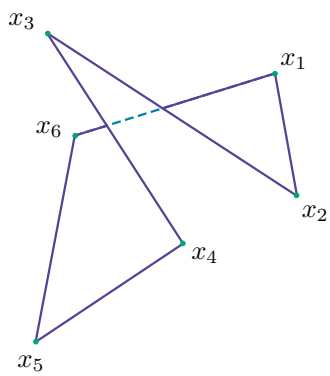


Figure 146: Arbitrary hexagon in $\mathbb{R}^{\mathbf{3}}$ whose vertices are labelled clockwise.

way, a problem dual to total distance-square maximization (Example 6.7.0.0.1) is a penultimate minimum eigenvalue problem having application to *PageRank* calculation by search engines [264, §4]. [383]

Fermat function (1082) is empirically compared with (1084) in [66, §8.7.3], but for multiple unknowns in $\mathbb{R}^{\mathbf{2}}$, where propensity of (1082) for producing zero distance between unknowns is revealed. An optimal solution to (1082) gravitates toward gradient discontinuities (§D.2.1), as in Figure **77**, whereas optimal solution to (1084) is less compact in the unknowns.[5.11] □

5.4.2.2.5 Example. *Hexagon.*
Barvinok [27, §2.6] poses a problem in *geometric realizability* of an arbitrary hexagon (Figure **146**) having:

1. prescribed (one-dimensional) face-lengths l
2. prescribed angles φ between the three pairs of opposing faces
3. a constraint on the sum of norm-square of each and every vertex x;

ten affine equality constraints in all on a Gram matrix $G \in \mathbb{S}^{\mathbf{6}}$ (1070). Let's realize this as a convex feasibility problem (with constraints written in the same order) also assuming $\mathbf{0}$ geometric center (1069):

$$\begin{array}{rll} \underset{D\in\mathbb{S}^{\mathbf{6}}_h}{\text{find}} & -VDV\frac{1}{2} \in \mathbb{S}^{\mathbf{6}} & \\ \text{subject to} & \operatorname{tr}\big(D(e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})\frac{1}{2}\big) = l_{ij}^2 \;, & j-1 = (i = 1\ldots 6) \bmod 6 \\ & \operatorname{tr}\big(-\frac{1}{2}VDV(A_i + A_i^{\mathrm{T}})\frac{1}{2}\big) = \cos\varphi_i \;, & i = 1,2,3 \\ & \operatorname{tr}(-\frac{1}{2}VDV) = 1 & \\ & -VDV \succeq 0 & \end{array} \tag{1085}$$

where, for $A_i \in \mathbb{R}^{\mathbf{6}\times\mathbf{6}}$ (1077)

$$\begin{aligned} A_1 &= (e_1 - e_6)(e_3 - e_4)^{\mathrm{T}}/(l_{61}l_{34}) \\ A_2 &= (e_2 - e_1)(e_4 - e_5)^{\mathrm{T}}/(l_{12}l_{45}) \\ A_3 &= (e_3 - e_2)(e_5 - e_6)^{\mathrm{T}}/(l_{23}l_{56}) \end{aligned} \tag{1086}$$

(§5.7) must be 2 because a third dimension can only increase total distance. Minimization of $\langle -V, D\rangle$ is a heuristic for rank minimization. (§7.2.2)

[5.11] Optimal solution to (1082) has mechanical interpretation in terms of interconnecting springs with constant force when distance is nonzero; otherwise, 0 force. Problem (1084) is interpreted instead using linear springs.

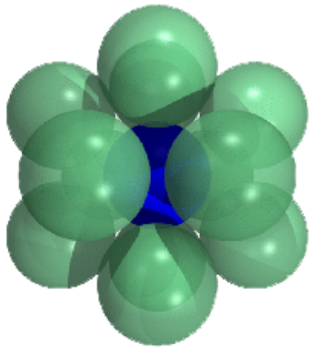


Figure 147: Sphere-packing illustration from [444, *kissing number*]. Translucent balls illustrated all have the same diameter.

and where the first constraint on length-square l_{ij}^2 can be equivalently written as a constraint on the Gram matrix $-VDV\frac{1}{2}$ via (1079). We show how to numerically solve such a problem by *alternating projection* in §E.10.2.1.1. Barvinok's Proposition 2.9.3.0.1 asserts existence of a list, corresponding to Gram matrix G solving this feasibility problem, whose affine dimension (§5.7.1.1) does not exceed 3 because the convex feasible set is bounded by the third constraint $\operatorname{tr}(-\frac{1}{2}VDV)=1$ (1073). □

5.4.2.2.6 Example. *Kissing number of sphere packing.*
Two nonoverlapping Euclidean balls are said to *kiss* if they touch. An elementary geometrical problem can be posed: *Given hyperspheres, each having the same diameter* 1 , *how many hyperspheres can simultaneously kiss one central hypersphere*? [465] Noncentral hyperspheres are allowed, but not required, to kiss.

As posed, the problem seeks the maximal number of spheres K kissing a central sphere in a particular dimension. The total number of spheres is $N=K+1$. In one dimension, the answer to this kissing problem is 2. In two dimensions, 6. (Figure **9**)

The question was presented, in three dimensions, to Isaac Newton by David Gregory in the context of celestial mechanics. And so was born a controversy between the two scholars on the campus of Trinity College Cambridge in 1694. Newton correctly identified the kissing number as 12 (Figure **147**) while Gregory argued for 13. Their dispute was finally resolved in 1953 by Schütte & van der Waerden. [340] In 2003, Oleg Musin tightened the upper bound on kissing number K in four dimensions from 25 to $K=24$ by refining a method of Philippe Delsarte from 1973. Delsarte's method provides an infinite number [18] of linear inequalities necessary for converting a rank-constrained semidefinite program[5.12] to a linear program.[5.13] [310]

There are no proofs known for kissing number in higher dimension excepting dimensions eight and twenty four. Interest persists [93] because sphere packing has found application to error correcting codes from the fields of communications and information theory; specifically to quantum computing. [101]

Translating this problem to an *EDM graph* realization (Figure **143**, Figure **148**) is suggested by Pfender & Ziegler. Imagine the center of each sphere to be connected to

[5.12] whose feasible set belongs to that subset of an elliptope (§5.9.1.0.1) bounded above by some desired rank.

[5.13] Simplex-method solvers for linear programs produce numerically better results than contemporary log-barrier (interior-point method) solvers, for semidefinite programs, by about 7 orders of magnitude; they are far more predisposed to vertex solutions [104, p.158].

every other by line segments. Then distance between centers must obey simple criteria: Each sphere touching the central sphere has a line segment of length exactly 1 joining its center to the central sphere's center. All spheres, excepting the central sphere, must have centers separated by a distance of at least 1.

From this perspective, the kissing problem can be posed as a semidefinite program. Assign index 1 to the central sphere assuming a total of N spheres:

$$\begin{array}{lll} \underset{D\in\mathbb{S}^N}{\text{minimize}} & -\operatorname{tr}(W V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}) & \\ \text{subject to} & D_{1j}=1\,, & j=2\dots N \\ & D_{ij}\geq 1\,, & 2\leq i<j=3\dots N \\ & D\in\mathbb{EDM}^N & \end{array} \tag{1087}$$

Then kissing number

$$K = N_{\max} - 1 \tag{1088}$$

is found from the maximal number N of spheres that solve this semidefinite program in a given affine dimension r whose realization is assured by 0 optimal objective. Matrix W is constant, in this program, determined by a method disclosed in §4.5.1. Matrix $W\in\mathbb{S}_+^{N-1}$ can be interpreted as direction of search through the positive semidefinite cone for a rank-r optimal solution $-V_{\mathcal{N}}^{\mathrm{T}} D^\star V_{\mathcal{N}}\in\mathbb{S}_+^{N-1}$: In one dimension, optimal direction matrix $W^\star$ has rank $= K-r = 2-1 = 1$;

$$W^\star = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\frac{1}{2} \tag{1089}$$

In two dimensions, optimal $W^\star$ has rank $= K-r = 6-2 = 4$;

$$W^\star = \begin{bmatrix} 4 & 1 & 2 & -1 & -1 & 1 \\ 1 & 4 & -1 & -1 & 2 & 1 \\ 2 & -1 & 4 & 1 & 1 & -1 \\ -1 & -1 & 1 & 4 & 1 & 2 \\ -1 & 2 & 1 & 1 & 4 & -1 \\ 1 & 1 & -1 & 2 & -1 & 4 \end{bmatrix}\frac{1}{6} \tag{1090}$$

In three dimensions, we leave it an exercise to find a rational optimal direction matrix $W^\star$ having rank $= K-r = 12-3 = 9$. Here is a full-rank rational optimal direction matrix:

$$W^\star = \begin{bmatrix} 9 & 1 & -2 & -1 & 3 & -1 & -1 & 1 & 2 & 1 & -2 & 1 \\ 1 & 9 & 3 & -1 & -1 & 1 & 1 & -2 & 1 & 2 & -1 & -1 \\ -2 & 3 & 9 & 1 & 2 & -1 & -1 & 2 & -1 & -1 & 1 & 2 \\ -1 & -1 & 1 & 9 & 1 & -1 & 1 & -1 & 3 & 2 & -1 & 1 \\ 3 & -1 & 2 & 1 & 9 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 9 & 2 & -1 & 2 & -1 & 2 & 3 \\ -1 & 1 & -1 & 1 & 1 & 2 & 9 & 3 & -1 & 1 & -2 & -1 \\ 1 & -2 & 2 & -1 & -1 & -1 & 3 & 9 & 2 & -1 & 1 & 1 \\ 2 & 1 & -1 & 3 & -1 & 2 & -1 & 2 & 9 & -1 & 1 & -1 \\ 1 & 2 & -1 & 2 & -1 & -1 & 1 & -1 & -1 & 9 & 3 & 1 \\ -2 & -1 & 1 & -1 & 1 & 2 & -2 & 1 & 1 & 3 & 9 & -1 \\ 1 & -1 & 2 & 1 & -1 & 3 & -1 & 1 & -1 & 1 & -1 & 9 \end{bmatrix}\frac{1}{12} \tag{1091}$$

A four-dimensional solution also has rational optimal direction matrix $W^\star$ having rank $= K-r = 24-4 = 20$;

$$
W^{\star} = \left[\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrr}
20 & -2 & 2 & -2 & 0 & 0 & -2 & 2 & 2 & -2 & 2 & 0 & 2 & 4 & 2 & 2 & 0 & -2 & -2 & -2 & 2 & 0 & 0 & -2 \\
-2 & 20 & 2 & 0 & 2 & -2 & -2 & 0 & 2 & 0 & 2 & -2 & 0 & 2 & -2 & 4 & 2 & -2 & 2 & 0 & 0 & -2 & 2 & -2 \\
2 & 2 & 20 & 2 & 2 & 2 & 0 & 2 & 0 & -2 & 0 & 2 & -2 & -2 & 0 & -2 & -2 & 0 & 0 & 2 & -2 & -2 & -2 & 4 \\
-2 & 0 & 2 & 20 & -2 & 2 & -2 & 0 & -2 & 0 & 2 & -2 & 4 & 2 & 2 & 0 & -2 & 2 & -2 & 0 & 0 & 2 & 2 & -2 \\
0 & 2 & 2 & -2 & 20 & 0 & 2 & -2 & -2 & 2 & -2 & 0 & 2 & 0 & 2 & -2 & 0 & 2 & -2 & -2 & 2 & 4 & 0 & -2 \\
0 & -2 & 2 & 2 & 0 & 20 & 2 & -2 & 2 & 2 & -2 & 0 & -2 & 0 & -2 & 2 & 4 & -2 & 2 & -2 & 2 & 0 & 0 & -2 \\
-2 & -2 & 0 & -2 & 2 & 2 & 20 & 2 & 0 & -2 & 4 & -2 & 2 & 2 & 0 & 2 & -2 & 0 & 0 & 2 & -2 & -2 & 2 & 0 \\
2 & 0 & 2 & 0 & -2 & -2 & 2 & 20 & -2 & 4 & -2 & -2 & 0 & -2 & -2 & 0 & 2 & 2 & 2 & 0 & 0 & 2 & 2 & -2 \\
2 & 2 & 0 & -2 & -2 & 2 & 0 & -2 & 20 & 2 & 0 & -2 & 2 & -2 & 0 & -2 & -2 & 4 & 0 & 2 & -2 & 2 & 2 & 0 \\
-2 & 0 & -2 & 0 & 2 & 2 & -2 & 4 & 2 & 20 & 2 & 2 & 0 & 2 & 2 & 0 & -2 & -2 & -2 & 0 & 0 & -2 & -2 & 2 \\
2 & 2 & 0 & 2 & -2 & -2 & 4 & -2 & 0 & 2 & 20 & 2 & -2 & -2 & 0 & -2 & 2 & 0 & 0 & -2 & 2 & 2 & -2 & 0 \\
0 & -2 & 2 & -2 & 0 & 0 & -2 & -2 & -2 & 2 & 2 & 20 & 2 & 0 & -2 & 2 & 0 & 2 & 2 & 2 & -2 & 0 & 4 & -2 \\
2 & 0 & -2 & 4 & 2 & -2 & 2 & 0 & 2 & 0 & -2 & 2 & 20 & -2 & -2 & 0 & 2 & -2 & 2 & 0 & 0 & -2 & -2 & 2 \\
4 & 2 & -2 & 2 & 0 & 0 & 2 & -2 & -2 & 2 & -2 & 0 & -2 & 20 & -2 & -2 & 0 & 2 & 2 & 2 & -2 & 0 & 0 & 2 \\
2 & -2 & 0 & 2 & 2 & -2 & 0 & -2 & 0 & 2 & 0 & -2 & -2 & -2 & 20 & 2 & 2 & 0 & 4 & 2 & -2 & -2 & 2 & 0 \\
2 & 4 & -2 & 0 & -2 & 2 & 2 & 0 & -2 & 0 & -2 & 2 & 0 & -2 & 2 & 20 & -2 & 2 & -2 & 0 & 0 & 2 & -2 & 2 \\
0 & 2 & -2 & -2 & 0 & 4 & -2 & 2 & -2 & -2 & 2 & 0 & 2 & 0 & 2 & -2 & 20 & 2 & -2 & 2 & -2 & 0 & 0 & 2 \\
-2 & -2 & 0 & 2 & 2 & -2 & 0 & 2 & 4 & -2 & 0 & 2 & -2 & 2 & 0 & 2 & 2 & 20 & 0 & -2 & 2 & -2 & -2 & 0 \\
-2 & 2 & 0 & -2 & -2 & 2 & 0 & 2 & 0 & -2 & 0 & 2 & 2 & 2 & 4 & -2 & -2 & 0 & 20 & -2 & 2 & 2 & -2 & 0 \\
-2 & 0 & 2 & 0 & -2 & -2 & 2 & 0 & 2 & 0 & -2 & 2 & 0 & 2 & 2 & 0 & 2 & -2 & -2 & 20 & 4 & 2 & -2 & -2 \\
2 & 0 & -2 & 0 & 2 & 2 & -2 & 0 & -2 & 0 & 2 & -2 & 0 & -2 & -2 & 0 & -2 & 2 & 2 & 4 & 20 & -2 & 2 & 2 \\
0 & -2 & -2 & 2 & 4 & 0 & -2 & 2 & 2 & -2 & 2 & 0 & -2 & 0 & -2 & 2 & 0 & -2 & 2 & 2 & -2 & 20 & 0 & 2 \\
0 & 2 & -2 & 2 & 0 & 0 & 2 & 2 & 2 & -2 & -2 & 4 & -2 & 0 & 2 & -2 & 0 & -2 & -2 & -2 & 2 & 0 & 20 & 2 \\
-2 & -2 & 4 & -2 & -2 & -2 & 0 & -2 & 0 & 2 & 0 & -2 & 2 & 2 & 0 & 2 & 2 & 0 & 0 & -2 & 2 & 2 & 2 & 20
\end{array}\right] \frac{1}{24} \tag{1092}
$$

but these direction matrices are not unique and their precision not critical. Here is an optimal four-dimensional point list,[5.14] in MATLAB output format, reconstructed by a method in §5.12:

```
Columns 1 through 6
X =     0   -0.1983   -0.4584    0.1657    0.9399    0.7416
        0    0.6863    0.2936    0.6239   -0.2936    0.3927
        0   -0.4835    0.8146   -0.6448    0.0611   -0.4224
        0    0.5059    0.2004   -0.4093   -0.1632    0.3427
Columns 7 through 12
 -0.4815   -0.9399   -0.7416    0.1983    0.4584   -0.2832
        0    0.2936   -0.3927   -0.6863   -0.2936   -0.6863
 -0.8756   -0.0611    0.4224    0.4835   -0.8146   -0.3922
 -0.0372    0.1632   -0.3427   -0.5059   -0.2004   -0.5431
Columns 13 through 18
  0.2832   -0.2926   -0.6473    0.0943    0.3640   -0.3640
  0.6863    0.9176   -0.6239   -0.2313   -0.0624    0.0624
  0.3922    0.1698   -0.2309   -0.6533   -0.1613    0.1613
  0.5431   -0.2088    0.3721    0.7147   -0.9152    0.9152
Columns 19 through 25
 -0.0943    0.6473   -0.1657    0.2926   -0.5759    0.5759    0.4815
  0.2313    0.6239   -0.6239   -0.9176    0.2313   -0.2313         0
  0.6533    0.2309    0.6448   -0.1698   -0.2224    0.2224    0.8756
 -0.7147   -0.3721    0.4093    0.2088   -0.7520    0.7520    0.0372
```

The r nonzero optimal eigenvalues of $-V_{\mathcal{N}}^{\mathrm{T}} D^{\star} V_{\mathcal{N}}$ are equal; remaining eigenvalues are zero as per $-\operatorname{tr}(W^{\star} V_{\mathcal{N}}^{\mathrm{T}} D^{\star} V_{\mathcal{N}}) = 0$ (815). Numerical problems begin to arise with matrices of this size due to interior-point methods of solution to (1087). By eliminating some equality constraints from the kissing number problem, matrix size can be reduced: From

[5.14] An optimal five-dimensional point list is known: *The answer was known at least 175 years ago. I believe Gauss knew it. Moreover, Korkine & Zolotarev proved in 1882 that* D_5 *is the densest lattice in five dimensions. So they proved that if a kissing arrangement in five dimensions can be extended to some lattice, then* $k(5)=40$. *Of course, the conjecture in the general case also is:* $k(5)=40$. *You would like to see coordinates? Easily. Let* $\mathrm{A}=\sqrt{2}$. *Then* $p(1)=(\mathrm{A},\mathrm{A},0,0,0)$, $p(2)=(-\mathrm{A},\mathrm{A},0,0,0)$, $p(3)=(\mathrm{A},-\mathrm{A},0,0,0)$, $\ldots$ $p(40)=(0,0,0,-\mathrm{A},-\mathrm{A})$; i.e, *we are considering points with coordinates that have two* A *and three* 0 *with any choice of signs and any ordering of the coordinates; the same coordinates-expression in dimensions* 3 *and* 4.

The first miracle happens in dimension 6. *There are better packings than* D_6 (*Conjecture:* $k(6)=72$). *It's a real miracle how dense the packing is in eight dimensions* (E_8 = *Korkine & Zolotarev packing that was discovered in 1880s*) *and especially in dimension* 24, *that is the so-called* Leech lattice.

Actually, people in coding theory have conjectures on the kissing numbers for dimensions up to 32 (*or even greater?*). *However, sometimes they found better lower bounds. I know that Ericson & Zinoviev a few years ago discovered* (*by hand, no computer*) *in dimensions* 13 *and* 14 *better kissing arrangements than were known before.* —Oleg Musin

§5.8.3 we have

$$-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} = \mathbf{1}\mathbf{1}^{\mathrm{T}} - [\,\mathbf{0} \quad I\,]\, D \begin{bmatrix} \mathbf{0}^{\mathrm{T}} \\ I \end{bmatrix} \tfrac{1}{2} \tag{1093}$$

(which does not hold more generally) where Identity matrix $I \in \mathbb{S}^{N-1}$ has one less dimension than EDM D. By defining an EDM principal submatrix

$$\hat{D} \triangleq [\,\mathbf{0} \quad I\,]\, D \begin{bmatrix} \mathbf{0}^{\mathrm{T}} \\ I \end{bmatrix} \in \mathbb{S}_h^{N-1} \tag{1094}$$

so that

$$-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} = \mathbf{1}\mathbf{1}^{\mathrm{T}} - \hat{D}\tfrac{1}{2} \tag{1095}$$

we get a convex problem equivalent to (1087)

$$\begin{array}{ll} \underset{\hat{D}\in\mathbb{S}^K}{\text{minimize}} & -\operatorname{tr}(W\hat{D}) \\ \text{subject to} & \hat{D}_{ij} \geq 1\,, \qquad 1 \leq i < j = 2\ldots K \\ & \mathbf{1}\mathbf{1}^{\mathrm{T}} - \hat{D}\tfrac{1}{2} \succeq 0 \\ & \delta(\hat{D}) = \mathbf{0} \end{array} \tag{1096}$$

Any feasible solution $\mathbf{1}\mathbf{1}^{\mathrm{T}} - \hat{D}\frac{1}{2}$ belongs to an elliptope (§5.9.1.0.1). □

5.4.2.2.7 Exercise. *Rational optimal kissing direction matrix $W^\star$.*
Replace (1091) with a rational $W^\star$ having rank $= K - r = 12 - 3 = 9$, main diagonal 9, and common denominator 12. ▼

This next example shows how finding the common point of intersection for three circles in a plane, a nonlinear problem, has convex expression.

5.4.2.2.8 Example. *Trilateration in wireless sensor network.* [189]
Given three known absolute point positions in $\mathbb{R}^{\mathbf{2}}$ (three anchors $\check{x}_2, \check{x}_3, \check{x}_4$) and only one unknown point (one sensor x_1), the sensor's absolute position is determined from its noiseless measured distance-square $\check{d}_{i1}$ to each of three anchors (Figure 4, Figure 148a). This trilateration can be expressed as a convex optimization problem in terms of list $X \triangleq [\,x_1 \;\; \check{x}_2 \;\; \check{x}_3 \;\; \check{x}_4\,] \in \mathbb{R}^{\mathbf{2}\times\mathbf{4}}$ and Gram matrix $G \in \mathbb{S}^{\mathbf{4}}$ (1058):

$$\begin{array}{lll} \underset{G\in\mathbb{S}^{\mathbf{4}},\; X\in\mathbb{R}^{\mathbf{2}\times\mathbf{4}}}{\text{minimize}} & \operatorname{tr} G & \\ \text{subject to} & \operatorname{tr}(G\Phi_{i1}) = \check{d}_{i1}\,, & i = 2,3,4 \\ & \operatorname{tr}\big(G e_i e_i^{\mathrm{T}}\big) = \|\check{x}_i\|^2\,, & i = 2,3,4 \\ & \operatorname{tr}(G(e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})/2) = \check{x}_i^{\mathrm{T}}\check{x}_j\,, & 2 \leq i < j = 3,4 \\ & X(:,2{:}4) = [\,\check{x}_2 \;\; \check{x}_3 \;\; \check{x}_4\,] & \\ & \begin{bmatrix} I & X \\ X^{\mathrm{T}} & G \end{bmatrix} \succeq 0 & \end{array} \tag{1097}$$

where

$$\Phi_{ij} = (e_i - e_j)(e_i - e_j)^{\mathrm{T}} \in \mathbb{S}_+^N \qquad (1047)$$

and where the constraint on distance-square $\check{d}_{i1}$ is equivalently written as a constraint on the Gram matrix via (1060). There are 9 linearly independent affine equality constraints on that Gram matrix while the sensor is constrained, only by dimensioning, to lie in $\mathbb{R}^{\mathbf{2}}$. Although the objective $\operatorname{tr} G$ of minimization[5.15] insures a solution on the boundary of positive semidefinite cone $\mathbb{S}_+^{\mathbf{4}}$, for this problem,

[5.15] Trace ($\operatorname{tr} G = \langle I, G\rangle$) minimization is a heuristic for rank minimization. (§7.2.2.1) It may be interpreted as squashing G which is bounded below by $X^{\mathrm{T}}X$ as in (1098); *id est*, $G - X^{\mathrm{T}}X \succeq 0 \Rightarrow \operatorname{tr} G \geq \operatorname{tr} X^{\mathrm{T}}X$ (1659). $\delta(G - X^{\mathrm{T}}X) = \mathbf{0} \Leftrightarrow G = X^{\mathrm{T}}X$ (§A.7.2) $\Rightarrow \operatorname{tr} G = \operatorname{tr} X^{\mathrm{T}}X$ which is a condition necessary for equality.

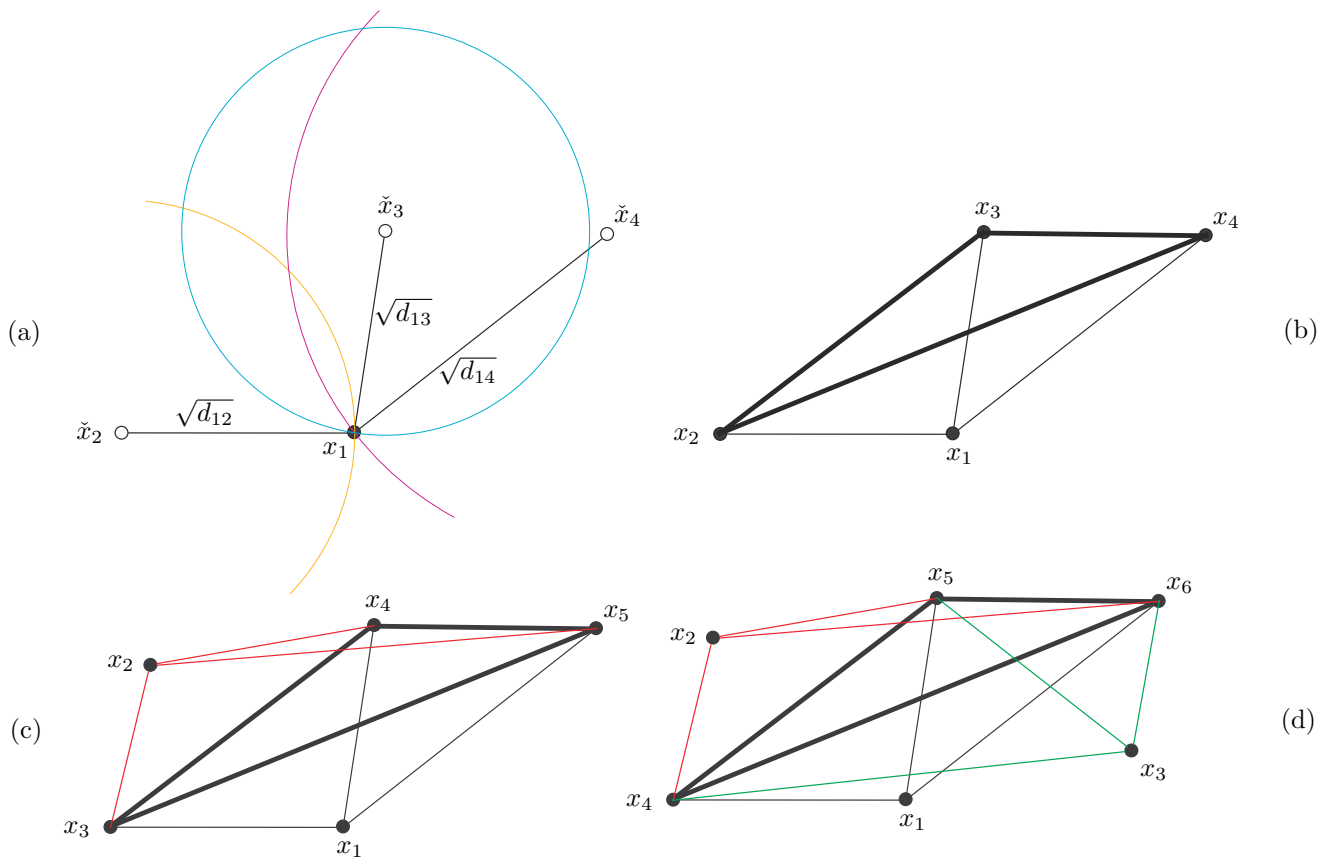


Figure 148: **(a)** Given three distances indicated with absolute point positions $\check{x}_2, \check{x}_3, \check{x}_4$ known and noncollinear, absolute position of x_1 in $\mathbb{R}^{\mathbf{2}}$ can be precisely and uniquely determined by *trilateration*; solution to a system of nonlinear equations. Dimensionless EDM graphs **(b)** **(c)** **(d)** represent EDMs in various states of completion. Line segments represent known absolute distances and may cross without vertex at intersection. **(b)** Four-point list must always be embeddable in affine subset having dimension $\operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ not exceeding 3. To determine relative position of x_2, x_3, x_4, triangle inequality is necessary and sufficient (§5.14.1). Knowing all distance information, then (by injectivity of $\mathbf{D}$ (§5.6)) point position x_1 is uniquely determined to within an isometry in any dimension. **(c)** When fifth point is introduced, only distances to x_3, x_4, x_5 are required to determine relative position of x_2 in $\mathbb{R}^{\mathbf{2}}$. Graph represents first instance of missing distance information; $\sqrt{d_{12}}$. **(d)** Three distances are absent ($\sqrt{d_{12}}$, $\sqrt{d_{13}}$, $\sqrt{d_{23}}$) from complete set of interpoint distances, yet unique isometric reconstruction (§5.4.2.2.10) of six points in $\mathbb{R}^{\mathbf{2}}$ is certain.

- we claim that the set of feasible Gram matrices forms a line, (§2.5.1.1) in isomorphic $\mathbb{R}^{\mathbf{10}}$, tangent (§2.1.7.1.2) to the positive semidefinite cone boundary. (§5.4.2.2.9, *confer* §4.2.1.3)

By Schur complement (§A.4, §2.9.1.0.1), any feasible G and X provide

$$G \succeq X^{\mathrm{T}} X \tag{1098}$$

which is a convex relaxation of the desired (nonconvex) equality constraint

$$\begin{bmatrix} I & X \\ X^{\mathrm{T}} & G \end{bmatrix} = \begin{bmatrix} I \\ X^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} I & X \end{bmatrix} \tag{1099}$$

expected positive semidefinite rank-2 under noiseless conditions. But, by (1661), the relaxation admits

$$(3 \geq) \operatorname{rank} G \geq \operatorname{rank} X \tag{1100}$$

(a third dimension corresponding to an intersection of three spheres, not circles, were there noise). If rank of an optimal solution equals 2,

$$\operatorname{rank} \begin{bmatrix} I & X^{\star} \\ X^{\star\mathrm{T}} & G^{\star} \end{bmatrix} = 2 \tag{1101}$$

then $G^{\star} = X^{\star\mathrm{T}} X^{\star}$ by Theorem A.4.0.1.3.

As posed, this *localization* problem does not require affinely independent (Figure **30**, three noncollinear) anchors. Assuming the anchors exhibit no rotational or reflective symmetry in their affine hull (§5.5.2) and assuming the sensor x_1 lies in that affine hull, then sensor position solution $x_1^{\star} = X^{\star}(:,1)$ is unique under noiseless measurement. [363]

□

This preceding transformation of trilateration to a semidefinite program works all the time ((1101) holds) despite relaxation (1098) because the optimal solution set is a unique point.

5.4.2.2.9 Proof (sketch). Only the sensor location x_1 is unknown. The objective function together with the equality constraints make a linear system of equations in Gram matrix variable G

$$\begin{aligned} \operatorname{tr} G &= \|x_1\|^2 + \|\check{x}_2\|^2 + \|\check{x}_3\|^2 + \|\check{x}_4\|^2 \\ \operatorname{tr}(G\Phi_{i1}) &= \check{d}_{i1}\ , && i = 2,3,4 \\ \operatorname{tr}\big(G e_i e_i^{\mathrm{T}}\big) &= \|\check{x}_i\|^2\ , && i = 2,3,4 \\ \operatorname{tr}(G(e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})/2) &= \check{x}_i^{\mathrm{T}} \check{x}_j\ , && 2 \leq i < j = 3,4 \end{aligned} \tag{1102}$$

which is invertible:

$$\operatorname{svec} G = \begin{bmatrix} \operatorname{svec}(I)^{\mathrm{T}} \\ \operatorname{svec}(\Phi_{21})^{\mathrm{T}} \\ \operatorname{svec}(\Phi_{31})^{\mathrm{T}} \\ \operatorname{svec}(\Phi_{41})^{\mathrm{T}} \\ \operatorname{svec}(e_2 e_2^{\mathrm{T}})^{\mathrm{T}} \\ \operatorname{svec}(e_3 e_3^{\mathrm{T}})^{\mathrm{T}} \\ \operatorname{svec}(e_4 e_4^{\mathrm{T}})^{\mathrm{T}} \\ \operatorname{svec}\big((e_2 e_3^{\mathrm{T}} + e_3 e_2^{\mathrm{T}})/2\big)^{\mathrm{T}} \\ \operatorname{svec}\big((e_2 e_4^{\mathrm{T}} + e_4 e_2^{\mathrm{T}})/2\big)^{\mathrm{T}} \\ \operatorname{svec}\big((e_3 e_4^{\mathrm{T}} + e_4 e_3^{\mathrm{T}})/2\big)^{\mathrm{T}} \end{bmatrix}^{-1} \begin{bmatrix} \|x_1\|^2 + \|\check{x}_2\|^2 + \|\check{x}_3\|^2 + \|\check{x}_4\|^2 \\ \check{d}_{21} \\ \check{d}_{31} \\ \check{d}_{41} \\ \|\check{x}_2\|^2 \\ \|\check{x}_3\|^2 \\ \|\check{x}_4\|^2 \\ \check{x}_2^{\mathrm{T}} \check{x}_3 \\ \check{x}_2^{\mathrm{T}} \check{x}_4 \\ \check{x}_3^{\mathrm{T}} \check{x}_4 \end{bmatrix} \tag{1103}$$

That line in the ambient space $\mathbb{S}^4$ of G, claimed on page 361, is traced by $\|x_1\|^2 \in \mathbb{R}$ on the right side, as it turns out. One must show this line to be tangential (§2.1.7.1.2) to $\mathbb{S}^4_+$ in order to prove uniqueness. Tangency is possible for affine dimension 1 or 2 while its occurrence depends completely on the known measurement data. ■

But as soon as significant noise is introduced or whenever distance data is incomplete, such problems can remain convex although the set of all optimal solutions generally becomes a convex set bigger than a single point (and still containing the noiseless solution).

5.4.2.2.10 Definition. *Isometric reconstruction.* (*confer* §5.5.3)
Isometric reconstruction from an EDM means building a list X correct to within a rotation, reflection, and translation; in other terms, reconstruction of relative position, unique to within an isometry, correct to within a rigid transformation. △

How much distance information is needed to uniquely localize a sensor (to recover actual relative position)? The narrative in Figure **148** helps dispel any notion of distance data proliferation in *low affine dimension* ($r < N-2$).[5.16] Huang, Liang, and Pardalos [237, §4.2] claim $\mathrm{O}(2N)$ distances is a least lower bound (independent of affine dimension r) for unique isometric reconstruction; achievable under certain noiseless conditions on graph connectivity and point position. Alfakih shows how to ascertain uniqueness over all affine dimensions via *Gale matrix.* [10] [5] [6] Figure **143**b (p.346, from *small completion problem* Example 5.3.0.0.2) is an example in $\mathbb{R}^2$ requiring only $2N-3=5$ known symmetric entries for unique isometric reconstruction, although the four-point example in Figure **148**b will not yield a unique reconstruction when any one of the distances is left unspecified.

The list represented by the particular dimensionless *EDM graph* in Figure **149**, having only $2N-3=9$ absolute distances specified, has only one realization in $\mathbb{R}^2$ but has more realizations in higher dimensions. Unique r-dimensional isometric reconstruction by semidefinite relaxation like (1098) occurs iff realization in $\mathbb{R}^r$ is unique and there exist no nontrivial higher-dimensional realizations. [363] For sake of reference, we provide the complete corresponding EDM:

$$D = \begin{bmatrix} 0 & 50641 & 56129 & 8245 & 18457 & 26645 \\ 50641 & 0 & 49300 & 25994 & 8810 & 20612 \\ 56129 & 49300 & 0 & 24202 & 31330 & 9160 \\ 8245 & 25994 & 24202 & 0 & 4680 & 5290 \\ 18457 & 8810 & 31330 & 4680 & 0 & 6658 \\ 26645 & 20612 & 9160 & 5290 & 6658 & 0 \end{bmatrix} \tag{1104}$$

We consider paucity of distance information in this next example which shows it is possible to recover exact relative position given incomplete noiseless distance information. An *ad hoc* method for recovery of the least-rank optimal solution under noiseless conditions is introduced:

[5.16] When affine dimension r reaches $N-2$, then all distances-square in the EDM must be known for unique isometric reconstruction in $\mathbb{R}^r$; going the other way, when $r=1$ then the condition that the dimensionless EDM graph be connected is necessary and sufficient. [218, §2.2]

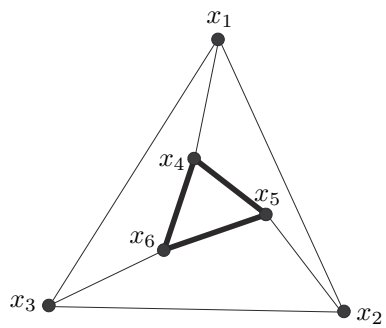


Figure 149: (*confer* (1104)) Incomplete EDM corresponding to this dimensionless EDM graph (drawn freehand; no symmetry intended) provides unique isometric reconstruction in $\mathbb{R}^{\mathbf{2}}$.

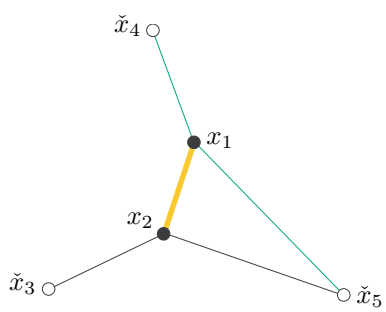


Figure 150: (Ye) Two sensors $\bullet$ and three anchors $\circ$ in $\mathbb{R}^{\mathbf{2}}$. Connecting line-segments denote known absolute distances. Incomplete EDM corresponding to this dimensionless EDM graph provides unique isometric reconstruction in $\mathbb{R}^{\mathbf{2}}$.

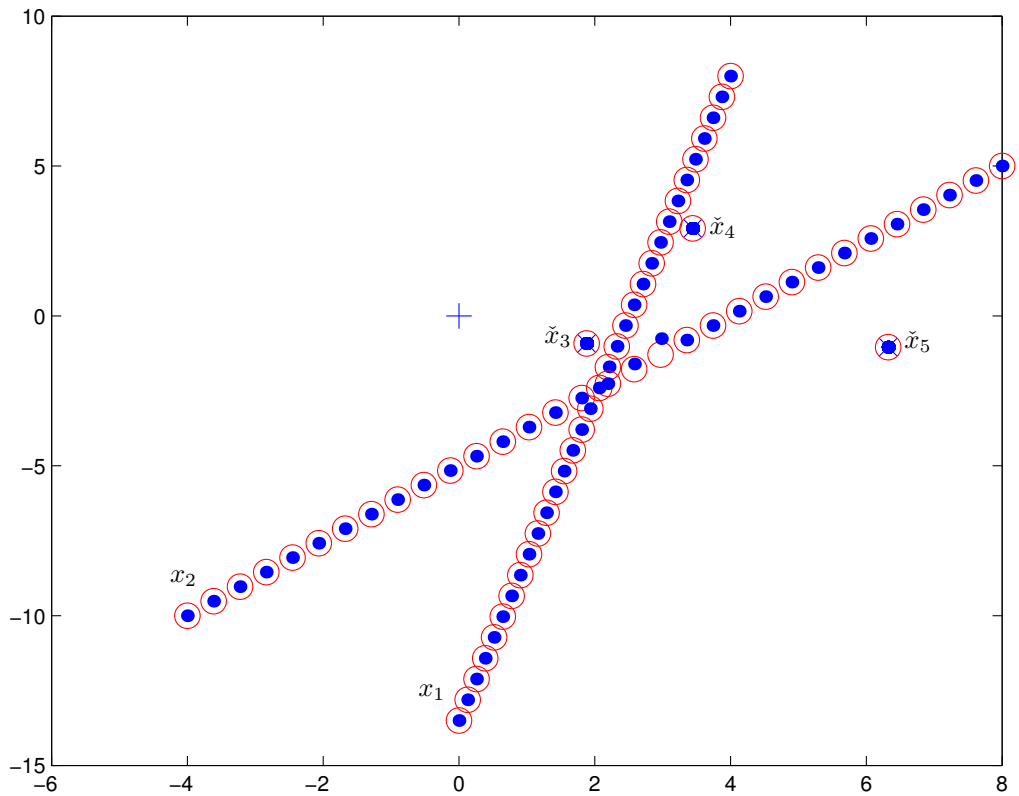


Figure 151: Given in red ○ are two discrete linear trajectories of sensors x_1 and x_2 in $\mathbb{R}^2$ localized by algorithm (1105) as indicated by blue bullets •. Anchors $\check{x}_3$, $\check{x}_4$, $\check{x}_5$, corresponding to Figure **150**, are indicated by ⊗. When targets ○ and bullets • coincide under these noiseless conditions, localization is successful. On this run, two visible localization errors are due to rank-3 Gram optimal solutions. These errors can be corrected by choosing a different normal in objective of minimization.

5.4.2.2.11 Example. *Tandem trilateration in wireless sensor network.*
Given three known absolute point-positions in $\mathbb{R}^2$ (three anchors $\check{x}_3, \check{x}_4, \check{x}_5$), two unknown sensors $x_1, x_2 \in \mathbb{R}^2$ have absolute position determinable from their noiseless distances-square (as indicated in Figure **150**) assuming the anchors exhibit no rotational or reflective symmetry in their affine hull (§5.5.2). This example differs from Example 5.4.2.2.8 insofar as trilateration of each sensor is now in terms of one unknown position: the other sensor. We express this localization as a convex optimization problem (a semidefinite program, §4.1) in terms of list $X \triangleq [\, x_1 \;\; x_2 \;\; \check{x}_3 \;\; \check{x}_4 \;\; \check{x}_5 \,] \in \mathbb{R}^{2\times 5}$ and Gram matrix $G \in \mathbb{S}^5$ (1058) via relaxation (1098):

$$\begin{array}{lll} \underset{G\in\mathbb{S}^5,\; X\in\mathbb{R}^{2\times 5}}{\text{minimize}} & \operatorname{tr} G & \\ \text{subject to} & \operatorname{tr}(G\Phi_{i1}) & = \check{d}_{i1}\;, \qquad i=2,4,5 \\ & \operatorname{tr}(G\Phi_{i2}) & = \check{d}_{i2}\;, \qquad i=3,5 \\ & \operatorname{tr}\big(G e_i e_i^{\mathrm{T}}\big) & = \|\check{x}_i\|^2\;, \qquad i=3,4,5 \\ & \operatorname{tr}(G(e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})/2) & = \check{x}_i^{\mathrm{T}}\check{x}_j\;, \qquad 3\le i<j=4,5 \\ & X(:,3{:}5) & = [\, \check{x}_3 \;\; \check{x}_4 \;\; \check{x}_5 \,] \\ & \begin{bmatrix} I & X \\ X^{\mathrm{T}} & G \end{bmatrix} & \succeq 0 \end{array} \tag{1105}$$

where

$$\Phi_{ij} = (e_i - e_j)(e_i - e_j)^{\mathrm{T}} \in \mathbb{S}_+^N \tag{1047}$$

This problem realization is fragile because of the unknown distances between sensors and anchors. Yet there is no more information we may include beyond the 11 independent equality constraints on the Gram matrix (nonredundant constraints not antithetical) to reduce the feasible set.[5.17]

Exhibited in Figure **151** are two mistakes in solution $X^\star(:,1{:}2)$ due to a rank-3 optimal Gram matrix $G^\star$. The trace objective is a heuristic minimizing convex envelope of quasiconcave function[5.18] $\operatorname{rank} G$. (§2.9.2.9.2, §7.2.2.1) A rank-2 optimal Gram matrix can be found and the errors corrected by choosing a different normal for the linear objective function, now implicitly the Identity matrix I; *id est*,

$$\operatorname{tr} G = \langle G\,,\, I\rangle \;\leftarrow\; \langle G\,,\, \delta(u)\rangle \tag{1106}$$

where vector $u \in \mathbb{R}^5$ is randomly selected. A random search for a good normal $\delta(u)$ in only a few iterations is quite easy and effective because: the problem is small, an optimal solution is known *a priori* to exist in two dimensions, a good normal direction is not necessarily unique, and (we speculate) because the feasible affine-subset slices the positive semidefinite cone thinly in the Euclidean sense.[5.19] □

We explore ramifications of noise and incomplete data throughout; their individual effect being to expand the optimal solution set, introducing more solutions and higher-rank solutions. Hence our focus shifts in §4.5 to discovery of a reliable means for diminishing the optimal solution set by introduction of a rank constraint.

Now we illustrate how a problem in distance geometry can be solved without equality constraints representing measured distance; instead, we have only upper and lower bounds on distances measured:

[5.17] By virtue of their dimensioning, the sensors are already constrained to $\mathbb{R}^2$ the affine hull of the anchors.
[5.18] Projection on that nonconvex subset of all $N\times N$-dimensional positive semidefinite matrices, in an affine subset, whose rank does not exceed 2 is a problem considered difficult to solve. [400, §4]
[5.19] The $\log\det$ rank-heuristic from §7.2.2.4 does not work here because it chooses the wrong normal. Rank reduction (§4.1.2.1) is unsuccessful here because Barvinok's upper bound (§2.9.3.0.1) on rank of $G^\star$ is 4.

5.4.2.2.12 Example. *Wireless location in a cellular telephone network.*
Utilizing measurements of distance, time of flight, angle of arrival, or signal power in the context of wireless telephony, *multilateration* is the process of localizing (determining absolute position of) a radio signal source $\bullet$ by inferring geometry relative to multiple fixed *base stations* $\circ$ whose locations are known.

We consider localization of a cellular telephone by distance geometry, so we assume distance to any particular base station can be inferred from received signal power. On a large open flat expanse of terrain, signal-power measurement corresponds well with inverse distance. But it is not uncommon for measurement of signal power to suffer 20 decibels in loss caused by factors such as *multipath* interference (signal reflections), mountainous terrain, man-made structures, turning one's head, or rolling the windows up in an automobile. Consequently, contours of equal signal power are no longer circular; their geometry is irregular and would more aptly be approximated by translated ellipsoids of graduated orientation and eccentricity as in Figure **153**.

Depicted in Figure **152** is one cell phone x_1 whose signal power is automatically and repeatedly measured by 6 base stations $\circ$ nearby.[5.20] Those signal power measurements are transmitted from that cell phone to base station $\check{x}_2$ who decides whether to transfer (*hand-off* or *hand-over*) responsibility for that call should the user roam outside its cell.[5.21]

Due to noise, at least one distance measurement more than the minimum number of measurements is required for reliable localization in practice; 3 measurements are minimum in two dimensions, 4 in three.[5.22] Existence of noise precludes measured distance from the input data. We instead assign measured distance to a range estimate specified by individual upper and lower bounds: $\overline{d_{i1}}$ is the upper bound on distance-square from the cell phone to i^{th} base station, while $\underline{d_{i1}}$ is the lower bound. These bounds become the input data. Each measurement range is presumed different from the others.

Then convex problem (1097) takes the form:

$$\begin{array}{lll}
\underset{G\in\mathbb{S}^7,\ X\in\mathbb{R}^{2\times 7}}{\text{minimize}} & \operatorname{tr} G & \\
\text{subject to} & \underline{d_{i1}} \le \operatorname{tr}(G\Phi_{i1}) \le \overline{d_{i1}}\ , & i=2\dots 7 \\
& \operatorname{tr}\big(G e_i e_i^{\mathrm{T}}\big) = \|\check{x}_i\|^2\ , & i=2\dots 7 \\
& \operatorname{tr}(G(e_i e_j^{\mathrm{T}} + e_j e_i^{\mathrm{T}})/2) = \check{x}_i^{\mathrm{T}}\check{x}_j\ , & 2\le i<j=3\dots 7 \\
& X(:,2{:}7) = [\,\check{x}_2\ \check{x}_3\ \check{x}_4\ \check{x}_5\ \check{x}_6\ \check{x}_7\,] & \\
& \begin{bmatrix} I & X \\ X^{\mathrm{T}} & G \end{bmatrix} \succeq 0 & \qquad (1107)
\end{array}$$

where

$$\Phi_{ij} = (e_i - e_j)(e_i - e_j)^{\mathrm{T}} \in \mathbb{S}_+^N \qquad (1047)$$

This semidefinite program realizes the wireless location problem illustrated in Figure **152**. Location $X^\star(:,1)$ is taken as solution, although measurement noise will often cause $\operatorname{rank} G^\star$ to exceed 2. Randomized search for a rank-2 optimal solution is not so easy here as in Example 5.4.2.2.11. We introduce a method in §4.5 for enforcing the stronger rank-constraint (1101). To formulate this same problem in three dimensions, point list X is simply redimensioned in the semidefinite program. $\square$

[5.20] Cell phone signal power is typically encoded logarithmically with 1-decibel increment and 64-decibel dynamic range.

[5.21] Because distance to base station is quite difficult to infer from signal power measurements in an urban environment, localization of a particular cell phone $\bullet$ by distance geometry would be far easier were the whole cellular system instead conceived so cell phone x_1 also transmits (to base station $\check{x}_2$) its signal power as received by all other cell phones within range.

[5.22] In Example 4.5.1.2.4, we explore how this convex optimization algorithm fares in the face of measurement noise.

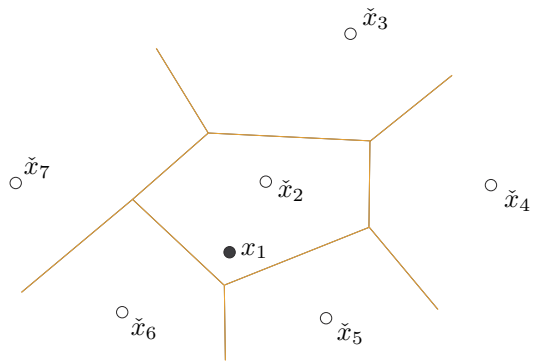


Figure 152: Regions of coverage by base stations $\circ$ in a cellular telephone network. The term *cellular* arises from packing of regions best covered by neighboring base stations. Illustrated is a pentagonal *cell* best covered by base station $\check{x}_2$. Like a Voronoi diagram, cell geometry depends on base-station arrangement. In some US urban environments, it is not unusual to find base stations spaced approximately 1 mile apart. There can be as many as 20 base-station antennae capable of receiving signal from any given cell phone $\bullet$; practically, that number is closer to 6.

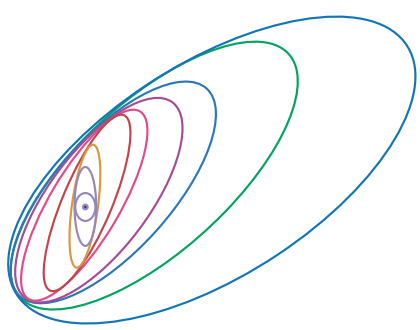


Figure 153: Some fitted contours of equal signal power in $\mathbb{R}^2$ transmitted from a commercial cellular telephone $\bullet$ over about 1 mile suburban terrain outside San Francisco in 2005. (Data by courtesy of Polaris Wireless.)

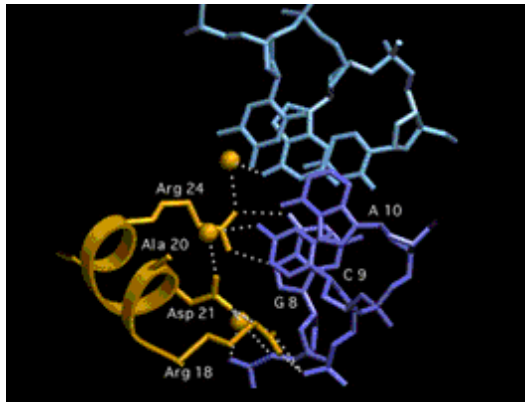


Figure 154: A depiction of molecular conformation. [135]

5.4.2.2.13 Example. (Biswas, Nigam, Ye) *Molecular Conformation.*
The subatomic measurement technique called *nuclear magnetic resonance spectroscopy* (NMR) is employed to ascertain physical conformation of molecules; *e.g*, Figure **5**, Figure **154**. From this technique, distance, angle, and dihedral angle measurements can be obtained. Dihedral angles arise consequent to a phenomenon where atom subsets are physically constrained to Euclidean planes.

> *In the* rigid covalent geometry *approximation, the bond lengths and angles are treated as completely fixed, so that a given spatial structure can be described very compactly indeed by a list of torsion angles alone... These are the dihedral angles between the planes spanned by the two consecutive triples in a chain of four covalently bonded atoms.*
>
> −G. M. Crippen & T. F. Havel, 1988 [97, §1.1]

Crippen & Havel recommend working exclusively with distance data because they consider angle data to be mathematically cumbersome. The present example shows instead how inclusion of dihedral angle data into a problem statement can be made elegant and convex.

As before, ascribe position information to the matrix

$$X = [\, x_1 \;\cdots\; x_N \,] \in \mathbb{R}^{\mathbf{3}\times N} \qquad (79)$$

and introduce a matrix $\aleph$ holding normals η to planes respecting dihedral angles φ:

$$\aleph \triangleq [\, \eta_1 \;\cdots\; \eta_M \,] \in \mathbb{R}^{\mathbf{3}\times M} \qquad (1108)$$

As in the other examples, we preferentially work with Gram matrices G because of the bridge they provide between other variables; we define

$$\begin{bmatrix} G_\aleph & Z \\ Z^{\mathrm{T}} & G_X \end{bmatrix} \triangleq \begin{bmatrix} \aleph^{\mathrm{T}}\aleph & \aleph^{\mathrm{T}}X \\ X^{\mathrm{T}}\aleph & X^{\mathrm{T}}X \end{bmatrix} = \begin{bmatrix} \aleph^{\mathrm{T}} \\ X^{\mathrm{T}} \end{bmatrix} [\, \aleph \;\; X \,] \in \mathbb{R}^{N+M\times N+M} \qquad (1109)$$

whose rank is 3 by assumption. So our problem's variables are the two Gram matrices G_X and $G_\aleph$ and matrix $Z = \aleph^{\mathrm{T}}X$ of cross products. Then measurements of distance-square d can be expressed as linear constraints on G_X as in (1107), dihedral angle φ measurements can be expressed as linear constraints on $G_\aleph$ by (1077), and normal-vector η conditions can be expressed by vanishing linear constraints on cross-product matrix Z: Consider

three points x labelled $1,2,3$ assumed to lie in the ℓth plane whose normal is η_ℓ. There might occur, for example, the independent constraints

$$\begin{aligned} \eta_\ell^{\mathrm{T}}(x_1 - x_2) &= 0 \\ \eta_\ell^{\mathrm{T}}(x_2 - x_3) &= 0 \end{aligned} \tag{1110}$$

which are expressible in terms of constant matrices $A_k \in \mathbb{R}^{M\times N}$;

$$\begin{aligned} \langle Z\,,\, A_{\ell 12}\rangle &= 0 \\ \langle Z\,,\, A_{\ell 23}\rangle &= 0 \end{aligned} \tag{1111}$$

Although normals η can be constrained exactly to unit length,

$$\delta(G_{\aleph}) = \mathbf{1} \tag{1112}$$

NMR data is noisy; so measurements are given as $\overline{\text{upper}}$ and $\underline{\text{lower}}$ bounds. Given $\overline{\text{bounds}}$ on dihedral angles respecting $0 \le \varphi_j \le \pi$ and $\overline{\text{bounds}}$ on distances d_i and given constant matrices A_k (1111) and symmetric matrices Φ_i (1047) and B_j per (1077), then a molecular conformation problem can be expressed:

$$\begin{array}{lllll} \underset{G_{\aleph}\in\mathbb{S}^M,\ G_X\in\mathbb{S}^N,\ Z\in\mathbb{R}^{M\times N}}{\text{find}} & G_X & & & \\ \text{subject to} & \underline{d_i} \le & \operatorname{tr}(G_X\,\Phi_i) & \le\ \overline{d_i} & \forall\, i\in\mathcal{I}_1 \\ & \underline{\cos\varphi_j} \le & \operatorname{tr}(G_{\aleph}\,B_j) & \le\ \overline{\cos\varphi_j} & \forall\, j\in\mathcal{I}_2 \\ & \langle Z\,,\, A_k\rangle & & =\ 0 & \forall\, k\in\mathcal{I}_3 \\ & G_X\mathbf{1} & & =\ \mathbf{0} & \\ & \delta(G_{\aleph}) & & =\ \mathbf{1} & \\ & \begin{bmatrix} G_{\aleph} & Z \\ Z^{\mathrm{T}} & G_X \end{bmatrix} & & \succeq\ 0 & \\ & \operatorname{rank}\begin{bmatrix} G_{\aleph} & Z \\ Z^{\mathrm{T}} & G_X \end{bmatrix} & & =\ 3 & \end{array} \tag{1113}$$

where $G_X\mathbf{1}=\mathbf{0}$ provides a geometrically centered list X (§5.4.2.2). Ignoring the rank constraint would tend to force cross-product matrix Z to zero. What binds these three variables is the rank constraint; we show how to satisfy it in §4.5. □

5.4.3 Inner-product form EDM definition

> *We might, for example, want to realize a constellation given only interstellar distance* (*or, equivalently, parsecs from our Sun and relative angular measurement; the Sun as vertex to two distant stars*)*; called* stellar cartography... −p.19

Equivalent to (1045) is [450, §1-7] [374, §3.2]

$$\begin{aligned} d_{ij} &= d_{ik} + d_{kj} - 2\sqrt{d_{ik}\,d_{kj}}\cos\theta_{ikj} \\ &= \begin{bmatrix}\sqrt{d_{ik}} & \sqrt{d_{kj}}\end{bmatrix}\begin{bmatrix} 1 & -e^{\imath\theta_{ikj}} \\ -e^{-\imath\theta_{ikj}} & 1 \end{bmatrix}\begin{bmatrix}\sqrt{d_{ik}} \\ \sqrt{d_{kj}}\end{bmatrix} \end{aligned} \tag{1114}$$

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

$$\cos\theta_{ikj} = \frac{\frac{1}{2}(d_{ik} + d_{kj} - d_{ij})}{\sqrt{d_{ik}\,d_{kj}}} = \frac{(x_i - x_k)^{\mathrm{T}}(x_j - x_k)}{\|x_i - x_k\|\,\|x_j - x_k\|} \tag{1115}$$

where the numerator forms an inner product of vectors. Distance-square $d_{ij}\left(\begin{bmatrix}\sqrt{d_{ik}}\\ \sqrt{d_{kj}}\end{bmatrix}\right)$ is a convex quadratic function[5.23] on $\mathbb{R}^{\mathbf{2}}_{+}$ whereas $d_{ij}(\theta_{ikj})$ is quasiconvex (§3.14) minimized over domain $\{-\pi\leq\theta_{ikj}\leq\pi\}$ by $\theta^{\star}_{ikj}=0$, we get the *Pythagorean theorem* when $\theta_{ikj}=\pm\pi/2$, and $d_{ij}(\theta_{ikj})$ is maximized when $\theta^{\star}_{ikj}=\pm\pi$;

$$\begin{aligned} d_{ij} &= \left(\sqrt{d_{ik}}+\sqrt{d_{kj}}\right)^2, & \theta_{ikj} &= \pm\pi \\ d_{ij} &= d_{ik}+d_{kj}\ , & \theta_{ikj} &= \pm\tfrac{\pi}{2} \\ d_{ij} &= \left(\sqrt{d_{ik}}-\sqrt{d_{kj}}\right)^2, & \theta_{ikj} &= \ \ 0 \end{aligned} \tag{1116}$$

so

$$|\sqrt{d_{ik}}-\sqrt{d_{kj}}\,| \ \leq\ \sqrt{d_{ij}}\ \leq\ \sqrt{d_{ik}}+\sqrt{d_{kj}} \tag{1117}$$

Hence the triangle inequality, Euclidean metric property 4, holds for any EDM D.

We may construct an inner-product form of the EDM definition for matrices by evaluating (1114) for $k=1$: By defining

$$\Theta^{\mathrm{T}}\Theta \triangleq \begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214} & \cdots & \sqrt{d_{12}d_{1N}}\cos\theta_{21N} \\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & \cdots & \sqrt{d_{13}d_{1N}}\cos\theta_{31N} \\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14} & \ddots & \sqrt{d_{14}d_{1N}}\cos\theta_{41N} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \sqrt{d_{12}d_{1N}}\cos\theta_{21N} & \sqrt{d_{13}d_{1N}}\cos\theta_{31N} & \sqrt{d_{14}d_{1N}}\cos\theta_{41N} & \cdots & d_{1N} \end{bmatrix} \in \mathbb{S}^{N-1} \tag{1118}$$

then any EDM may be expressed

$$\begin{aligned} \mathbf{D}(\Theta) &\triangleq \begin{bmatrix} 0 \\ \delta(\Theta^{\mathrm{T}}\Theta) \end{bmatrix}\mathbf{1}^{\mathrm{T}} + \mathbf{1}\begin{bmatrix} 0 & \delta(\Theta^{\mathrm{T}}\Theta)^{\mathrm{T}} \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \Theta^{\mathrm{T}}\Theta \end{bmatrix} \in \mathbb{EDM}^N \\ &= \begin{bmatrix} 0 & \delta(\Theta^{\mathrm{T}}\Theta)^{\mathrm{T}} \\ \delta(\Theta^{\mathrm{T}}\Theta) & \delta(\Theta^{\mathrm{T}}\Theta)\mathbf{1}^{\mathrm{T}}+\mathbf{1}\delta(\Theta^{\mathrm{T}}\Theta)^{\mathrm{T}}-2\Theta^{\mathrm{T}}\Theta \end{bmatrix} \end{aligned} \tag{1119}$$

$$\mathbb{EDM}^N = \left\{\mathbf{D}(\Theta)\ |\ \Theta\in\mathbb{R}^{N-1\times N-1}\right\} \tag{1120}$$

for which all Euclidean metric properties hold. Entries of $\Theta^{\mathrm{T}}\Theta$ result from vector inner-products as in (1115); *id est*,

$$\Theta = \begin{bmatrix} x_2-x_1 & x_3-x_1 & \cdots & x_N-x_1 \end{bmatrix} = X\sqrt{2}V_{\mathcal{N}} \in \mathbb{R}^{n\times N-1} \tag{1121}$$

Inner product $\Theta^{\mathrm{T}}\Theta$ is obviously related to a Gram matrix (1058),

$$G = \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \Theta^{\mathrm{T}}\Theta \end{bmatrix}, \qquad x_1 = \mathbf{0} \tag{1122}$$

For $D=\mathbf{D}(\Theta)$ and no condition on the list X (*confer* (1066) (1070))

$$\Theta^{\mathrm{T}}\Theta = -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \ \in \mathbb{R}^{N-1\times N-1} \tag{1123}$$

5.23 $\begin{bmatrix} 1 & -e^{\imath\theta_{ikj}} \\ -e^{-\imath\theta_{ikj}} & 1 \end{bmatrix} \succeq 0$, having eigenvalues $\{0,2\}$.

Minimum is attained for $\begin{bmatrix}\sqrt{d_{ik}}\\ \sqrt{d_{kj}}\end{bmatrix} = \begin{cases} \mu\mathbf{1}, & \mu\geq 0,\ \theta_{ikj}=0 \\ \mathbf{0}, & -\pi\leq\theta_{ikj}\leq\pi\ ,\ \theta_{ikj}\neq 0 \end{cases}$ (§D.2.1, [66, exmp.4.5]).

5.4.3.1 Relative-angle form

The inner-product form EDM definition is not a unique definition of Euclidean distance matrix; there are approximately five flavors distinguished by their argument to operator $\mathbf{D}$. Here is another one:

Like $\mathbf{D}(X)$ (1049), $\mathbf{D}(\Theta)$ will make an EDM given any $\Theta\in\mathbb{R}^{n\times N-1}$, it is neither a convex function of Θ (§5.4.3.2), and it is homogeneous in the sense (1052). Scrutinizing $\Theta^{\mathrm{T}}\Theta$ (1118) we find that because of the arbitrary choice $k=1$, distances therein are all with respect to point x_1. Similarly, relative angles in $\Theta^{\mathrm{T}}\Theta$ are between all vector pairs having vertex x_1. Yet picking arbitrary θ_{i1j} to fill $\Theta^{\mathrm{T}}\Theta$ will not necessarily make an EDM; inner product (1118) must be positive semidefinite.

$$\Theta^{\mathrm{T}}\Theta \;=\; \sqrt{\delta(d)}\,\Omega\,\sqrt{\delta(d)} \;\triangleq$$

$$\begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \begin{bmatrix} 1 & \cos\theta_{213} & \cdots & \cos\theta_{21N} \\ \cos\theta_{213} & 1 & \ddots & \cos\theta_{31N} \\ \vdots & \ddots & \ddots & \vdots \\ \cos\theta_{21N} & \cos\theta_{31N} & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sqrt{d_{12}} & & & \mathbf{0} \\ & \sqrt{d_{13}} & & \\ & & \ddots & \\ \mathbf{0} & & & \sqrt{d_{1N}} \end{bmatrix} \tag{1124}$$

Expression $\mathbf{D}(\Theta)$ defines an EDM for any positive semidefinite *relative-angle matrix*

$$\Omega \;=\; [\cos\theta_{i1j}\;,\;\; i,j=2\ldots N] \in \mathbb{S}^{N-1} \tag{1125}$$

and any nonnegative distance vector

$$d \;=\; [d_{1j}\;,\;\; j=2\ldots N] \;=\; \delta(\Theta^{\mathrm{T}}\Theta) \in \mathbb{R}^{N-1} \tag{1126}$$

because (§A.3.1.0.5)

$$\Omega \succeq 0 \;\Rightarrow\; \Theta^{\mathrm{T}}\Theta \succeq 0 \tag{1127}$$

Decomposition (1124) and the *relative-angle matrix inequality* $\Omega\succeq 0$ lead to a different expression of an inner-product form EDM definition (1119)

$$\begin{aligned} \mathbf{D}(\Omega\,,d) \;&\triangleq\; \begin{bmatrix} 0 \\ d \end{bmatrix}\mathbf{1}^{\mathrm{T}} + \mathbf{1}\begin{bmatrix} 0 & d^{\mathrm{T}} \end{bmatrix} - 2\sqrt{\delta\left(\begin{bmatrix} 0 \\ d \end{bmatrix}\right)}\begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \Omega \end{bmatrix}\sqrt{\delta\left(\begin{bmatrix} 0 \\ d \end{bmatrix}\right)} \\ &=\; \begin{bmatrix} 0 & d^{\mathrm{T}} \\ d & d\mathbf{1}^{\mathrm{T}} + \mathbf{1}d^{\mathrm{T}} - 2\sqrt{\delta(d)}\,\Omega\,\sqrt{\delta(d)} \end{bmatrix} \in \mathbb{EDM}^N \end{aligned} \tag{1128}$$

and another expression of the EDM cone:

$$\mathbb{EDM}^N = \left\{\mathbf{D}(\Omega\,,d) \mid \Omega\succeq 0\,,\; \sqrt{\delta(d)}\succeq 0\right\} \tag{1129}$$

In the particular circumstance $x_1=\mathbf{0}$, we can relate interpoint angle matrix Ψ from the Gram decomposition in (1058) to relative-angle matrix Ω in (1124). Thus,

$$\Psi \;\equiv\; \begin{bmatrix} 1 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \Omega \end{bmatrix}, \qquad x_1 = \mathbf{0} \tag{1130}$$

5.4.3.2 Inner-product form $-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(\Theta)V_{\mathcal{N}}$ convexity

On page 370 we saw that each EDM entry d_{ij} is a convex quadratic function of $\begin{bmatrix} \sqrt{d_{ik}} \\ \sqrt{d_{kj}} \end{bmatrix}$ and a quasiconvex function of θ_{ikj}. Here the situation for inner-product form EDM

operator $\mathbf{D}(\Theta)$ (1119) is identical to that in §5.4.1 for list-form $\mathbf{D}(X)$; $-\mathbf{D}(\Theta)$ is not a quasiconvex function of Θ by the same reasoning, and from (1123)

$$-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(\Theta)V_{\mathcal{N}} = \Theta^{\mathrm{T}}\Theta \tag{1131}$$

is a convex quadratic function of Θ on domain $\mathbb{R}^{n\times N-1}$ achieving its minimum at $\Theta = \mathbf{0}$.

5.4.3.3 Inner-product form, discussion

We deduce that knowledge of interpoint 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 $N(N-1)/2$ in $\Theta^{\mathrm{T}}\Theta$ is unchanged[5.24] with respect to EDM D.

5.5 Invariance

When D is an EDM, there exist an infinite number of corresponding N-point lists X (79) in Euclidean space. All those lists are related by isometric transformation: rotation, reflection, and translation (*offset* or *shift*).

5.5.1 Translation

Any translation common among all the points x_ℓ in a list will be cancelled in the formation of each d_{ij}. Proof follows directly from (1045). Knowing that translation α in advance, we may remove it from the list constituting the columns of X by subtracting $\alpha\mathbf{1}^{\mathrm{T}}$. Then it stands to reason by list-form definition (1049) of an EDM, for any translation $\alpha\in\mathbb{R}^n$

$$\mathbf{D}(X-\alpha\mathbf{1}^{\mathrm{T}}) = \mathbf{D}(X) \tag{1132}$$

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

$$[\,x_2-x_1 \quad x_3-x_1 \quad \cdots \quad x_N-x_1\,] = X\sqrt{2}V_{\mathcal{N}} \in \mathbb{R}^{n\times N-1} \tag{1121}$$

and so

$$\mathbf{D}(X-x_1\mathbf{1}^{\mathrm{T}}) \;=\; \mathbf{D}(X-Xe_1\mathbf{1}^{\mathrm{T}}) \;=\; \mathbf{D}\Big(X\Big[\mathbf{0} \quad \sqrt{2}V_{\mathcal{N}}\Big]\Big) \;=\; \mathbf{D}(X) \tag{1133}$$

5.5.1.0.1 Example. *Translating geometric center to origin.*
We might choose to shift the geometric center α_c of an N-point list $\{x_\ell\}$ (arranged columnar in X) to the origin; [399] [191]

$$\alpha \;=\; \alpha_c \;\triangleq\; Xb_c \;\triangleq\; X\mathbf{1}\tfrac{1}{N} \in \mathcal{P} \subseteq \mathcal{A} \tag{1134}$$

where $\mathcal{A}$ represents the list's affine hull. If we were to associate a point-mass m_ℓ with each of the points x_ℓ in the list, then their *center of mass* (or *gravity*) would be $(\sum x_\ell\, m_\ell)\,/\sum m_\ell$. The geometric center is the same as the center of mass under the assumption of uniform mass density across points. [393] The geometric center always lies in

[5.24] The reason for amount $\mathrm{O}(N^2)$ information is because of the relative measurements. Use of a fixed reference in measurement of angles and distances would reduce required information but is antithetical. In the particular case $n=2$, for example, ordering all points x_ℓ (in a length-N list) by increasing angle of vector $x_\ell - x_1$ with respect to $x_2 - x_1$, θ_{i1j} becomes equivalent to $\sum_{k=i}^{j-1}\theta_{k,1,k+1} \le 2\pi$ and the amount of information is reduced to $2N-3$; rather, $\mathrm{O}(N)$.

the convex hull $\mathcal{P}$ of the list; *id est*, $\alpha_c \in \mathcal{P}$ because $b_c^{\mathrm{T}}\mathbf{1}=1$ and $b_c \succeq 0$.[5.25] Subtracting the geometric center from every list member,

$$X - \alpha_c \mathbf{1}^{\mathrm{T}} \;=\; X - \tfrac{1}{N} X \mathbf{1}\mathbf{1}^{\mathrm{T}} \;=\; X(I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^{\mathrm{T}}) \;=\; XV \in \mathbb{R}^{n\times N} \tag{1135}$$

where V is the geometric centering matrix (1071). So we have (*confer* (1049))

$$\mathbf{D}(X) \;=\; \mathbf{D}(XV) \;=\; \delta(V^{\mathrm{T}}X^{\mathrm{T}}XV)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\delta(V^{\mathrm{T}}X^{\mathrm{T}}XV)^{\mathrm{T}} - 2V^{\mathrm{T}}X^{\mathrm{T}}XV \in \mathbb{EDM}^N \tag{1136}$$

□

5.5.1.1 Gram-form invariance

Following from (1136) and the linear Gram-form EDM operator (1061):

$$\mathbf{D}(G) \;=\; \mathbf{D}(VGV) \;=\; \delta(VGV)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\delta(VGV)^{\mathrm{T}} - 2VGV \in \mathbb{EDM}^N \tag{1137}$$

The Gram-form consequently exhibits invariance to translation by a *doublet* $u\mathbf{1}^{\mathrm{T}} + \mathbf{1}u^{\mathrm{T}}$ (§B.2)

$$\mathbf{D}(G) = \mathbf{D}\big(G - (u\mathbf{1}^{\mathrm{T}} + \mathbf{1}u^{\mathrm{T}})\big) \tag{1138}$$

because, for any $u \in \mathbb{R}^N$, $\mathbf{D}(u\mathbf{1}^{\mathrm{T}} + \mathbf{1}u^{\mathrm{T}}) = \mathbf{0}$. The collection of all such doublets forms the nullspace (1154) to the operator; the *translation-invariant subspace* $\mathbb{S}_c^{N\perp}$ (2218) of the symmetric matrices $\mathbb{S}^N$. This means matrix G is not unique and can belong to an expanse more broad than a positive semidefinite cone; *id est*, $G \in \mathbb{S}_+^N - \mathbb{S}_c^{N\perp}$. So explains Gram matrix sufficiency in EDM definition (1061).[5.26]

5.5.2 Rotation/Reflection

Rotation of the list $X \in \mathbb{R}^{n\times N}$ about some arbitrary point $\alpha \in \mathbb{R}^n$, or reflection through some affine subset containing α, can be accomplished via $Q(X - \alpha\mathbf{1}^{\mathrm{T}})$ where Q is an orthogonal matrix (§B.5).

We rightfully expect

$$\mathbf{D}\big(Q(X - \alpha\mathbf{1}^{\mathrm{T}})\big) = \mathbf{D}(QX - \beta\mathbf{1}^{\mathrm{T}}) = \mathbf{D}(QX) = \mathbf{D}(X) \tag{1139}$$

Because list-form $\mathbf{D}(X)$ is translation invariant, we may safely ignore offset and consider only the impact of matrices that premultiply X. Interpoint distances are unaffected by rotation or reflection; we say, EDM D is *rotation/reflection invariant.* Proof follows from the fact: $Q^{\mathrm{T}} = Q^{-1} \Rightarrow X^{\mathrm{T}}Q^{\mathrm{T}}QX = X^{\mathrm{T}}X$. So (1139) follows directly from (1049).

The class of premultiplying matrices, for which interpoint distances are unaffected, is a little more broad than orthogonal matrices. Looking at EDM definition (1049), it appears that any matrix Q_{p} such that

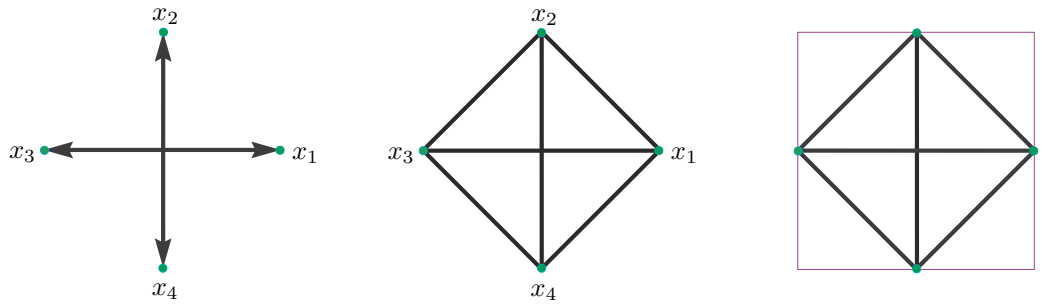
$$X^{\mathrm{T}}Q_{\mathrm{p}}^{\mathrm{T}}Q_{\mathrm{p}}\,X = X^{\mathrm{T}}X \tag{1140}$$

will have the property

$$\mathbf{D}(Q_{\mathrm{p}}X) = \mathbf{D}(X) \tag{1141}$$

An example is thin $Q_{\mathrm{p}} \in \mathbb{R}^{m\times n}$ $(m > n)$ having orthonormal columns; an orthonormal matrix.

[5.25] Any b from $\alpha = Xb$ chosen such that $b^{\mathrm{T}}\mathbf{1} = 1$, more generally, makes an auxiliary V-matrix. (§B.4.5)
[5.26] A constraint $G\mathbf{1} = \mathbf{0}$ would prevent excursion into the translation-invariant subspace (numerical unboundedness).



(a) (b) (c)

Figure 155: **(a)** Four points in quadrature in two dimensions about their geometric center. **(b)** Complete EDM graph of diamond-shaped vertices. **(c)** Quadrature rotation of Euclidean body in $\mathbb{R}^{\mathbf{2}}$ first requires shroud: the smallest Cartesian square containing it.

5.5.2.0.1 Example. *Reflection prevention and quadrature rotation.*
Consider the EDM graph in Figure **155**b representing known distance between vertices (Figure **155**a) of a tilted-square diamond in $\mathbb{R}^{\mathbf{2}}$. Suppose some geometrical optimization problem were posed where isometric transformation is allowed excepting reflection, and where rotation must be quantized so that only *quadrature* rotations are allowed; only multiples of $\pi/2$.

Counterclockwise rotation of any vector about the origin by angle θ is prescribed in two dimensions by orthogonal matrix

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{1142}$$

clockwise rotation is prescribed by negating angle, rather Q^{T}, whereas reflection of any point through a hyperplane containing the origin

$$\partial\mathcal{H} = \left\{ x\in\mathbb{R}^{\mathbf{2}} \;\middle|\; \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}^{\mathrm{T}} x = 0 \right\} \tag{1143}$$

is accomplished by multiplication with symmetric orthogonal matrix (§B.5.3)

$$R = \begin{bmatrix} \sin(\theta)^2 - \cos(\theta)^2 & -2\sin(\theta)\cos(\theta) \\ -2\sin(\theta)\cos(\theta) & \cos(\theta)^2 - \sin(\theta)^2 \end{bmatrix} \tag{1144}$$

Rotation matrix Q is characterized by identical diagonal entries and by antidiagonal entries equal but opposite in sign, whereas reflection matrix R is characterized in the reverse sense.

Assign the diamond vertices $\{x_\ell \in \mathbb{R}^{\mathbf{2}},\ \ell = 1\ldots 4\}$ to columns of a matrix

$$X = [\,x_1 \;\; x_2 \;\; x_3 \;\; x_4\,] \in \mathbb{R}^{\mathbf{2}\times\mathbf{4}} \qquad (79)$$

Our scheme to prevent reflection enforces a rotation matrix characteristic upon the coordinates of adjacent points themselves: First shift the geometric center of X to the origin; for geometric centering matrix $V \in \mathbb{S}^{\mathbf{4}}$ (§5.5.1.0.1), define

$$Y \triangleq XV \in \mathbb{R}^{\mathbf{2}\times\mathbf{4}} \tag{1145}$$

To maintain relative quadrature between points (Figure **155**a) and to prevent reflection, it is sufficient that all interpoint distances be specified and that adjacencies $Y(:,1:2)$,

$Y(:,2{:}3)$, and $Y(:,3{:}4)$ be proportional to 2×2 rotation matrices; any clockwise rotation would ascribe a reflection matrix characteristic. Counterclockwise rotation is thereby enforced by constraining equality among diagonal and antidiagonal entries as prescribed by (1142);

$$Y(:,1{:}3) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} Y(:,2{:}4) \tag{1146}$$

Quadrature quantization of rotation can be regarded as a constraint on tilt of the smallest Cartesian square containing the diamond as in Figure **155**c. Our scheme to quantize rotation requires that all square vertices be described by vectors whose entries are nonnegative when the square is translated anywhere interior to the nonnegative orthant. We capture the four square vertices as columns of a product YC where

$$C = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \tag{1147}$$

Then, assuming a unit-square shroud, the affine constraint

$$YC + \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix} \mathbf{1}^{\mathrm{T}} \geq \mathbf{0} \tag{1148}$$

quantizes rotation, as desired. □

5.5.2.1 Inner-product form invariance

Likewise, $\mathbf{D}(\Theta)$ (1119) is rotation/reflection invariant;

$$\mathbf{D}(Q_{\mathrm{p}}\Theta) = \mathbf{D}(Q\Theta) = \mathbf{D}(\Theta) \tag{1149}$$

so (1140) and (1141) similarly apply.

5.5.3 Invariance conclusion

In the making of an EDM, absolute rotation, reflection, and translation information is lost. Given an EDM, reconstruction of point position (§5.12, the list X) can be guaranteed correct only in affine dimension r and relative position. Given a noiseless complete EDM, this isometric reconstruction is unique insofar as every realization of a corresponding list X is *congruent*:

5.6 Injectivity of D & unique reconstruction

Injectivity implies uniqueness of isometric reconstruction (§5.4.2.2.10); hence, we endeavor to demonstrate it.

EDM operators list-form $\mathbf{D}(X)$ (1049), Gram-form $\mathbf{D}(G)$ (1061), and inner-product form $\mathbf{D}(\Theta)$ (1119) are many-to-one surjections (§5.5) onto the same range; the EDM cone (§6): (*confer* (1062) (1156))

$$\begin{aligned} \mathbb{EDM}^N &= \left\{ \mathbf{D}(X) : \mathbb{R}^{N-1\times N} \to \mathbb{S}_h^N \mid X \in \mathbb{R}^{N-1\times N} \right\} \\ &= \left\{ \mathbf{D}(G) : \mathbb{S}^N \to \mathbb{S}_h^N \mid G \in \mathbb{S}_+^N - \mathbb{S}_c^{N\perp} \right\} \\ &= \left\{ \mathbf{D}(\Theta) : \mathbb{R}^{N-1\times N-1} \to \mathbb{S}_h^N \mid \Theta \in \mathbb{R}^{N-1\times N-1} \right\} \end{aligned} \tag{1150}$$

where (§5.5.1.1)

$$\mathbb{S}_c^{N\perp} = \{ u\mathbf{1}^{\mathrm{T}} + \mathbf{1}u^{\mathrm{T}} \mid u \in \mathbb{R}^N \} \subseteq \mathbb{S}^N \qquad (2218)$$

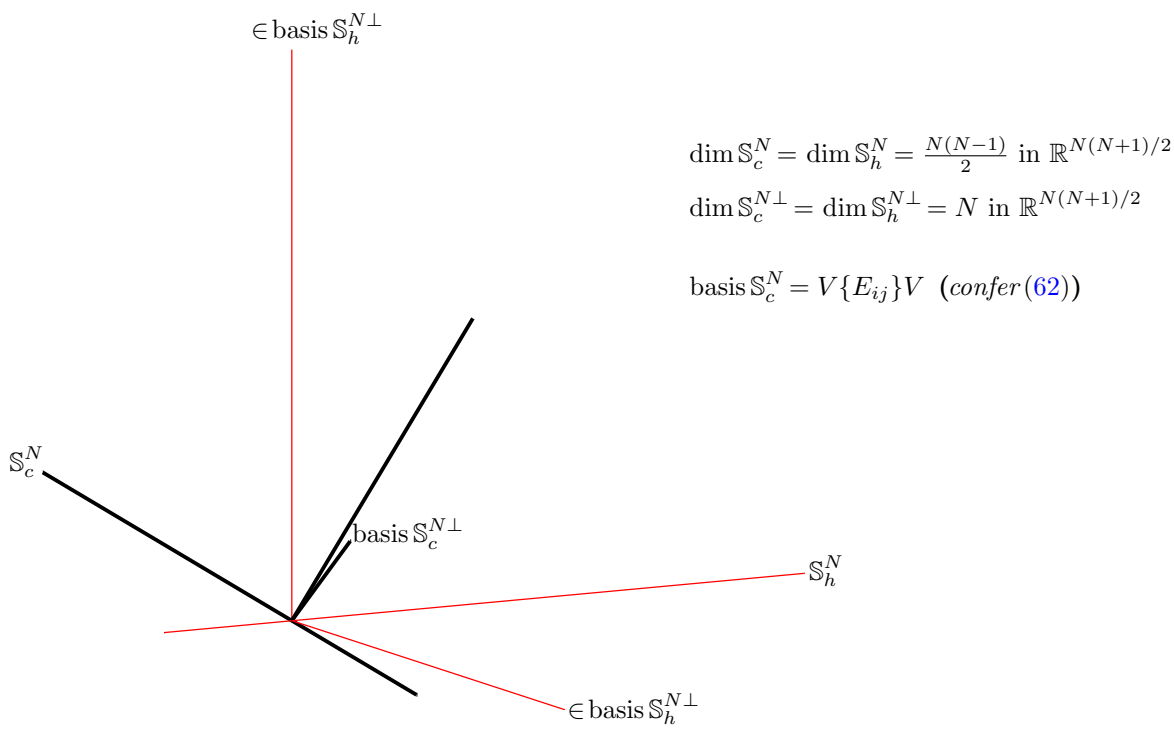


Figure 156: Orthogonal complements in $\mathbb{S}^N$ abstractly oriented in isometrically isomorphic $\mathbb{R}^{N(N+1)/2}$. Case $N=2$ accurately illustrated in $\mathbb{R}^{\mathbf{3}}$. Orthogonal projection of basis for $\mathbb{S}_h^{N\perp}$ on $\mathbb{S}_c^{N\perp}$ yields another basis for $\mathbb{S}_c^{N\perp}$. (Basis vectors for $\mathbb{S}_c^{N\perp}$ are illustrated lying in a plane orthogonal to $\mathbb{S}_c^N$ in this dimension. Basis vectors for each $\perp$ space outnumber those for its respective orthogonal complement; such is not the case in higher dimension.)

5.6.1 Gram-form bijectivity

Because linear Gram-form EDM operator

$$\mathbf{D}(G) \;=\; \delta(G)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\delta(G)^{\mathrm{T}} - 2G \qquad (1061)$$

has no nullspace [94, §A.1] on the geometric center subspace[5.27] (§E.7.2.0.2)

$$\begin{aligned}
\mathbb{S}_c^N &\triangleq \{G\in\mathbb{S}^N \mid G\mathbf{1}=\mathbf{0}\} && (2216)\\
&= \{G\in\mathbb{S}^N \mid \mathcal{N}(G)\supseteq\mathbf{1}\} \;=\; \{G\in\mathbb{S}^N \mid \mathcal{R}(G)\subseteq\mathcal{N}(\mathbf{1}^{\mathrm{T}})\}\\
&= \{VYV \mid Y\in\mathbb{S}^N\}\subset\mathbb{S}^N && (2217)\\
&\equiv \{V_{\mathcal{N}}AV_{\mathcal{N}}^{\mathrm{T}} \mid A\in\mathbb{S}^{N-1}\}
\end{aligned} \qquad (1151)$$

then $\mathbf{D}(G)$ on that subspace is injective.

To prove injectivity of $\mathbf{D}(G)$ on $\mathbb{S}_c^N$: Any matrix $Y\in\mathbb{S}^N$ can be decomposed into orthogonal components in $\mathbb{S}^N$;

$$Y = VYV + (Y - VYV) \qquad (1152)$$

where $VYV\in\mathbb{S}_c^N$ and $Y-VYV\in\mathbb{S}_c^{N\perp}$ (2218). Because of translation invariance (§5.5.1.1) and linearity, $\mathbf{D}(Y-VYV)=\mathbf{0}$ hence $\mathcal{N}(\mathbf{D})\supseteq\mathbb{S}_c^{N\perp}$. It remains only to show

$$\mathbf{D}(VYV)=\mathbf{0} \;\Leftrightarrow\; VYV=\mathbf{0} \qquad (1153)$$

$(\Leftrightarrow\; Y=u\mathbf{1}^{\mathrm{T}}+\mathbf{1}u^{\mathrm{T}}$ for some $u\in\mathbb{R}^N)$. $\mathbf{D}(VYV)$ will vanish whenever $2VYV=\delta(VYV)\mathbf{1}^{\mathrm{T}}+\mathbf{1}\delta(VYV)^{\mathrm{T}}$. But this implies $\mathcal{R}(\mathbf{1})$ (§B.2) were a subset of $\mathcal{R}(VYV)$, which is contradictory. Thus we have

$$\mathcal{N}(\mathbf{D}) \;=\; \{Y \mid \mathbf{D}(Y)=\mathbf{0}\} \;=\; \{Y \mid VYV=\mathbf{0}\} \;=\; \mathbb{S}_c^{N\perp} \qquad (1154)$$

♦

Since $G\mathbf{1}=\mathbf{0}\Leftrightarrow X\mathbf{1}=\mathbf{0}$ (1069) simply means that list X is geometrically centered at the origin, and because the Gram-form EDM operator $\mathbf{D}$ is translation invariant with $\mathcal{N}(\mathbf{D})$ being the translation-invariant subspace $\mathbb{S}_c^{N\perp}$, then EDM definition $\mathbf{D}(G)$ (1150) on[5.28] (*confer* §6.5.1, §6.6.1, §A.7.4.0.1)

$$\mathbb{S}_c^N\cap\mathbb{S}_+^N \;=\; \{VYV\succeq 0 \mid Y\in\mathbb{S}^N\} \;\equiv\; \{V_{\mathcal{N}}AV_{\mathcal{N}}^{\mathrm{T}} \mid A\in\mathbb{S}_+^{N-1}\}\subset\mathbb{S}^N \qquad (1155)$$

must be surjective onto $\mathbb{EDM}^N$; (*confer* (1062))

$$\mathbb{EDM}^N = \left\{\mathbf{D}(G) \mid G\in\mathbb{S}_c^N\cap\mathbb{S}_+^N\right\} \qquad (1156)$$

[5.27] Equivalence $\equiv$ in (1151) follows from the fact: Given $B=VYV=V_{\mathcal{N}}AV_{\mathcal{N}}^{\mathrm{T}}\in\mathbb{S}_c^N$ with only matrix $A\in\mathbb{S}^{N-1}$ unknown, then $V_{\mathcal{N}}^{\dagger}BV_{\mathcal{N}}^{\dagger\mathrm{T}}=A$ or $V_{\mathcal{N}}^{\dagger}YV_{\mathcal{N}}^{\dagger\mathrm{T}}=A$.

[5.28] Equivalence $\equiv$ in (1155) follows from the fact: Given $B=VYV=V_{\mathcal{N}}AV_{\mathcal{N}}^{\mathrm{T}}\in\mathbb{S}_+^N$ with only matrix A unknown, then $V_{\mathcal{N}}^{\dagger}BV_{\mathcal{N}}^{\dagger\mathrm{T}}=A$ and $A\in\mathbb{S}_+^{N-1}$ must be positive semidefinite by positive semidefiniteness of B and Corollary A.3.1.0.5.

5.6.1.1 Gram-form operator D inversion

Define the linear *geometric centering operator* $\mathbf{V}$: (*confer* (1070))

$$\mathbf{V}(D) : \mathbb{S}^N \to \mathbb{S}^N \triangleq -V D V \tfrac{1}{2} \tag{1157}$$

[98, §4.3][5.29] This orthogonal projector $\mathbf{V}$ has no nullspace on

$$\mathbb{S}_h^N = \operatorname{aff} \mathbb{EDM}^N \tag{1411}$$

because the projection of $-D/2$ on $\mathbb{S}_c^N$ (2216) can be $\mathbf{0}$ if and only if $D \in \mathbb{S}_c^{N\perp}$; but $\mathbb{S}_c^{N\perp} \cap \mathbb{S}_h^N = \mathbf{0}$ (Figure **156**). Projector $\mathbf{V}$ on $\mathbb{S}_h^N$ is therefore injective hence uniquely invertible. Further, $-V\mathbb{S}_h^N V/2$ is equivalent to the geometric center subspace $\mathbb{S}_c^N$ in the ambient space of symmetric matrices; a surjection,

$$\mathbb{S}_c^N = \mathbf{V}(\mathbb{S}^N) = \mathbf{V}\Big(\mathbb{S}_h^N \oplus \mathbb{S}_h^{N\perp}\Big) = \mathbf{V}\Big(\mathbb{S}_h^N\Big) \tag{1158}$$

because (75)

$$\mathbf{V}\Big(\mathbb{S}_h^N\Big) \supseteq \mathbf{V}\Big(\mathbb{S}_h^{N\perp}\Big) = \mathbf{V}\Big(\delta^2(\mathbb{S}^N)\Big) \tag{1159}$$

Because $\mathbf{D}(G)$ on $\mathbb{S}_c^N$ is injective, and $\operatorname{aff} \mathbf{D}\Big(\mathbf{V}(\mathbb{EDM}^N)\Big) = \mathbf{D}\Big(\mathbf{V}(\operatorname{aff} \mathbb{EDM}^N)\Big)$ by property (131) of the affine hull, we find for $D \in \mathbb{S}_h^N$

$$\mathbf{D}(-V D V \tfrac{1}{2}) = \delta(-V D V \tfrac{1}{2})\mathbf{1}^{\mathrm{T}} + \mathbf{1}\,\delta(-V D V \tfrac{1}{2})^{\mathrm{T}} - 2(-V D V \tfrac{1}{2}) \tag{1160}$$

id est,

$$D = \mathbf{D}\Big(\mathbf{V}(D)\Big) \tag{1161}$$

$$-V D V = \mathbf{V}\Big(\mathbf{D}(-V D V)\Big) \tag{1162}$$

or

$$\mathbb{S}_h^N = \mathbf{D}\Big(\mathbf{V}(\mathbb{S}_h^N)\Big) \tag{1163}$$

$$-V\mathbb{S}_h^N V = \mathbf{V}\Big(\mathbf{D}(-V\mathbb{S}_h^N V)\Big) \tag{1164}$$

These operators $\mathbf{V}$ and $\mathbf{D}$ are mutual inverses.

The Gram-form $\mathbf{D}\Big(\mathbb{S}_c^N\Big)$ (1061) is equivalent to $\mathbb{S}_h^N$;

$$\mathbf{D}\Big(\mathbb{S}_c^N\Big) = \mathbf{D}\Big(\mathbf{V}(\mathbb{S}_h^N \oplus \mathbb{S}_h^{N\perp})\Big) = \mathbb{S}_h^N + \mathbf{D}\Big(\mathbf{V}(\mathbb{S}_h^{N\perp})\Big) = \mathbb{S}_h^N \tag{1165}$$

because $\mathbb{S}_h^N \supseteq \mathbf{D}\Big(\mathbf{V}(\mathbb{S}_h^{N\perp})\Big)$. In summary, for the Gram-form we have the isomorphisms [99, §2] [98, p.76, p.107] [8, §2.1][5.30] [7, §2] [9, §18.2.1] [3, §2.1]

$$\mathbb{S}_h^N = \mathbf{D}(\mathbb{S}_c^N) \tag{1166}$$

$$\mathbb{S}_c^N = \mathbf{V}(\mathbb{S}_h^N) \tag{1167}$$

and from bijectivity results in §5.6.1,

$$\mathbb{EDM}^N = \mathbf{D}(\mathbb{S}_c^N \cap \mathbb{S}_+^N) \tag{1168}$$

$$\mathbb{S}_c^N \cap \mathbb{S}_+^N = \mathbf{V}(\mathbb{EDM}^N) \tag{1169}$$

[5.29] Critchley cites Torgerson, 1958 [396, ch.11, §2], for a history and derivation of (1157).

[5.30] In [8, p.6, line 20], delete sentence: *Since G is also . . . not a singleton set.*
[8, p.10, line 11] $x_3 = 2$ (not 1).

5.6.2 Inner-product form bijectivity

The Gram-form EDM operator $\mathbf{D}(G)=\delta(G)\mathbf{1}^{\mathrm{T}}+\mathbf{1}\delta(G)^{\mathrm{T}}-2G$ (1061) is an injective map, for example, on the domain that is the subspace of symmetric matrices having all zeros in the first row and column

$$\begin{aligned}\mathbb{S}^N_{\mathbf{0}} &= \{G\in\mathbb{S}^N \mid Ge_1=\mathbf{0}\}\\ &= \left\{\begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & I\end{bmatrix} Y \begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & I\end{bmatrix} \mid Y\in\mathbb{S}^N\right\}\end{aligned} \tag{2220}$$

because it obviously has no nullspace there. Since $Ge_1=\mathbf{0}\Leftrightarrow Xe_1=\mathbf{0}$ (1063) means the first point in the list X resides at the origin, then $\mathbf{D}(G)$ on $\mathbb{S}^N_{\mathbf{0}}\cap\mathbb{S}^N_+$ must be surjective onto $\mathbb{EDM}^N$.

Substituting $\Theta^{\mathrm{T}}\Theta\leftarrow -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ (1131) into inner-product form EDM definition $\mathbf{D}(\Theta)$ (1119), it may be further decomposed:

$$\mathbf{D}(D)=\begin{bmatrix}0\\ \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)\end{bmatrix}\mathbf{1}^{\mathrm{T}}+\mathbf{1}\begin{bmatrix}0 & \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)^{\mathrm{T}}\end{bmatrix}-2\begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\end{bmatrix} \tag{1170}$$

This linear operator $\mathbf{D}$ is another flavor of inner-product form and an injective map of the EDM cone onto itself. Yet when its domain is instead the entire symmetric hollow subspace $\mathbb{S}^N_h=\operatorname{aff}\mathbb{EDM}^N$, $\mathbf{D}(D)$ becomes an injective map onto that same subspace. Proof follows directly from the fact: linear $\mathbf{D}$ has no nullspace [94, §A.1] on $\mathbb{S}^N_h=\operatorname{aff}\mathbf{D}(\mathbb{EDM}^N)=\mathbf{D}(\operatorname{aff}\mathbb{EDM}^N)$ (131).

5.6.2.1 Inversion of $\mathbf{D}\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)$

Injectivity of $\mathbf{D}(D)$ suggests inversion of (*confer* (1066))

$$\mathbf{V}_{\mathcal{N}}(D):\mathbb{S}^N\to\mathbb{S}^{N-1}\triangleq -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \tag{1171}$$

a linear surjective[5.31] mapping onto $\mathbb{S}^{N-1}$ having nullspace[5.32] $\mathbb{S}^{N\perp}_c$;

$$\mathbf{V}_{\mathcal{N}}(\mathbb{S}^N_h)=\mathbb{S}^{N-1} \tag{1172}$$

injective on domain $\mathbb{S}^N_h$ because $\mathbb{S}^{N\perp}_c\cap\mathbb{S}^N_h=\mathbf{0}$. Revising the argument of this inner-product form (1170), we get another flavor

$$\mathbf{D}\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)=\begin{bmatrix}0\\ \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)\end{bmatrix}\mathbf{1}^{\mathrm{T}}+\mathbf{1}\begin{bmatrix}0 & \delta\big(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\big)^{\mathrm{T}}\end{bmatrix}-2\begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\end{bmatrix} \tag{1173}$$

and we obtain mutual inversion of operators $\mathbf{V}_{\mathcal{N}}$ and $\mathbf{D}$, for $D\in\mathbb{S}^N_h$

$$D=\mathbf{D}\Big(\mathbf{V}_{\mathcal{N}}(D)\Big) \tag{1174}$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}=\mathbf{V}_{\mathcal{N}}\big(\mathbf{D}(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}})\big) \tag{1175}$$

[5.31] Surjectivity of $\mathbf{V}_{\mathcal{N}}(D)$ is demonstrated via the Gram-form EDM operator $\mathbf{D}(G)$: Since $\mathbb{S}^N_h=\mathbf{D}(\mathbb{S}^N_c)$ (1165), then for any $Y\in\mathbb{S}^{N-1}$, $-V_{\mathcal{N}}^{\mathrm{T}}\mathbf{D}(V_{\mathcal{N}}^{\dagger\mathrm{T}}YV_{\mathcal{N}}^{\dagger}/2)V_{\mathcal{N}}=Y$.

[5.32] $\mathcal{N}(\mathbf{V}_{\mathcal{N}})\supseteq\mathbb{S}^{N\perp}_c$ is apparent. There exists a linear mapping

$$T(\mathbf{V}_{\mathcal{N}}(D))\triangleq V_{\mathcal{N}}^{\dagger\mathrm{T}}\mathbf{V}_{\mathcal{N}}(D)V_{\mathcal{N}}^{\dagger}=-VDV\tfrac{1}{2}=\mathbf{V}(D)$$

such that

$$\mathcal{N}(T(\mathbf{V}_{\mathcal{N}}))=\mathcal{N}(\mathbf{V})\supseteq\mathcal{N}(\mathbf{V}_{\mathcal{N}})\supseteq\mathbb{S}^{N\perp}_c=\mathcal{N}(\mathbf{V})$$

where the equality $\mathbb{S}^{N\perp}_c=\mathcal{N}(\mathbf{V})$ is known (§E.7.2.0.2). ♦

or

$$\mathbb{S}_h^N = \mathbf{D}\Big(\mathbf{V}_{\mathcal{N}}(\mathbb{S}_h^N)\Big) \tag{1176}$$

$$-V_{\mathcal{N}}^{\mathrm{T}}\mathbb{S}_h^N V_{\mathcal{N}} = \mathbf{V}_{\mathcal{N}}\Big(\mathbf{D}(-V_{\mathcal{N}}^{\mathrm{T}}\mathbb{S}_h^N V_{\mathcal{N}})\Big) \tag{1177}$$

Substituting $\Theta^{\mathrm{T}}\Theta \leftarrow \Phi$ into inner-product form EDM definition (1119), any EDM may be expressed by the new flavor

$$\begin{array}{c} \mathbf{D}(\Phi) \triangleq \begin{bmatrix} 0 \\ \delta(\Phi) \end{bmatrix} \mathbf{1}^{\mathrm{T}} + \mathbf{1}\begin{bmatrix} 0 & \delta(\Phi)^{\mathrm{T}} \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \Phi \end{bmatrix} \in \mathbb{EDM}^N \\ \Leftrightarrow \\ \Phi \succeq 0 \end{array} \tag{1178}$$

where this $\mathbf{D}$ is a linear surjective operator onto $\mathbb{EDM}^N$ by definition, injective because it has no nullspace on domain $\mathbb{S}_+^{N-1}$. More broadly, $\operatorname{aff}\mathbf{D}(\mathbb{S}_+^{N-1}) = \mathbf{D}(\operatorname{aff}\mathbb{S}_+^{N-1})$ (131),

$$\begin{array}{c} \mathbb{S}_h^N = \mathbf{D}(\mathbb{S}^{N-1}) \\ \mathbb{S}^{N-1} = \mathbf{V}_{\mathcal{N}}(\mathbb{S}_h^N) \end{array} \tag{1179}$$

demonstrably isomorphisms, and by bijectivity of this inner-product form:

$$\mathbb{EDM}^N = \mathbf{D}(\mathbb{S}_+^{N-1}) \tag{1180}$$

$$\mathbb{S}_+^{N-1} = \mathbf{V}_{\mathcal{N}}(\mathbb{EDM}^N) \tag{1181}$$

5.7 Embedding in affine hull

The affine hull $\mathcal{A}$ (81) of a point list $\{x_\ell\}$ (arranged columnar in $X \in \mathbb{R}^{n\times N}$ (79)) is identical to the affine hull of that polyhedron $\mathcal{P}$ (89) formed from all convex combinations of the x_ℓ; [66, §2] [349, §17]

$$\mathcal{A} = \operatorname{aff} X = \operatorname{aff}\mathcal{P} \tag{1182}$$

Comparing hull definitions (81) and (89), it becomes obvious that the x_ℓ and their convex hull $\mathcal{P}$ are embedded in their unique affine hull $\mathcal{A}$;

$$\mathcal{A} \supseteq \mathcal{P} \supseteq \{x_\ell\} \tag{1183}$$

Recall: *affine dimension* r is a lower bound on embedding, equal to dimension of the subspace parallel to that nonempty affine set $\mathcal{A}$ in which the points are embedded. (§2.3.1) We define dimension of the convex hull $\mathcal{P}$ to be the same as dimension r of the affine hull $\mathcal{A}$ [349, §2], but r is not necessarily equal to rank of X (1202).

For the particular example illustrated in Figure **142**, $\mathcal{P}$ is the triangle in union with its relative interior while its three vertices constitute the entire list X. Affine hull $\mathcal{A}$ is the unique plane that contains the triangle, so affine dimension $r = 2$ in that example while rank of X is 3. Were there only two points in Figure **142**, then the affine hull would instead be the unique line passing through them; r would become 1 while rank would then be 2.

5.7.1 Determining affine dimension

Knowledge of affine dimension r becomes important because we lose any absolute offset common to all the generating x_ℓ in $\mathbb{R}^n$ when reconstructing convex polyhedra given only distance information. (§5.5.1) To calculate r, we first remove any offset that serves to

increase dimensionality of the subspace required to contain polyhedron $\mathcal{P}$; subtracting any $\alpha\in\mathcal{A}$ in the affine hull from every list member will work,

$$X-\alpha\mathbf{1}^{\mathrm{T}} \tag{1184}$$

translating $\mathcal{A}$ to the origin:[5.33]

$$\mathcal{A}-\alpha \;=\; \operatorname{aff}(X-\alpha\mathbf{1}^{\mathrm{T}}) \;=\; \operatorname{aff}(X)-\alpha \tag{1185}$$
$$\mathcal{P}-\alpha \;=\; \operatorname{conv}(X-\alpha\mathbf{1}^{\mathrm{T}}) \;=\; \operatorname{conv}(X)-\alpha \tag{1186}$$

Because (1182) and (1183) translate,

$$\mathbb{R}^n \;\supseteq\; \mathcal{A}-\alpha \;=\; \operatorname{aff}(X-\alpha\mathbf{1}^{\mathrm{T}}) \;=\; \operatorname{aff}(\mathcal{P}-\alpha) \;\supseteq\; \mathcal{P}-\alpha \;\supseteq\; \{x_\ell-\alpha\} \tag{1187}$$

where from the previous relations it is easily shown

$$\operatorname{aff}(\mathcal{P}-\alpha)=\operatorname{aff}(\mathcal{P})-\alpha \tag{1188}$$

Translating $\mathcal{A}$ neither changes its dimension or the dimension of the embedded polyhedron $\mathcal{P}$; (80)

$$r \;\triangleq\; \dim\mathcal{A} \;=\; \dim(\mathcal{A}-\alpha) \;\triangleq\; \dim(\mathcal{P}-\alpha) \;=\; \dim\mathcal{P} \tag{1189}$$

For any $\alpha\in\mathbb{R}^n$, (1185)-(1189) remain true. [349, p.4, p.12] Yet when $\alpha\in\mathcal{A}$, the affine set $\mathcal{A}-\alpha$ becomes a unique subspace of $\mathbb{R}^n$ in which the $\{x_\ell-\alpha\}$ and their convex hull $\mathcal{P}-\alpha$ are embedded (1187), and whose dimension is more easily calculated.

5.7.1.0.1 Example. *Translating first list-member to origin.*
Subtracting the first member $\alpha\triangleq x_1$ 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*,

$$X-x_1\mathbf{1}^{\mathrm{T}} \;=\; X-Xe_1\mathbf{1}^{\mathrm{T}} \;=\; X(I-e_1\mathbf{1}^{\mathrm{T}}) \;=\; X\begin{bmatrix}\mathbf{0} & \sqrt{2}V_{\mathcal{N}}\end{bmatrix}\in\mathbb{R}^{n\times N} \tag{1190}$$

where $V_{\mathcal{N}}$ is defined in (1055), and e_1 in (1065). Applying (1187) to (1190),

$$\mathbb{R}^n \;\supseteq\; \mathcal{R}(XV_{\mathcal{N}}) \;=\; \mathcal{A}-x_1 \;=\; \operatorname{aff}(X-x_1\mathbf{1}^{\mathrm{T}}) \;=\; \operatorname{aff}(\mathcal{P}-x_1) \;\supseteq\; \mathcal{P}-x_1 \;\ni\; \mathbf{0} \tag{1191}$$

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

$$r=\dim\mathcal{R}(XV_{\mathcal{N}}) \tag{1192}$$

□

Since shifting the geometric center to the origin (§5.5.1.0.1) translates the affine hull to the origin as well, then it must also be true

$$r \;=\; \dim\mathcal{R}(XV) \tag{1193}$$

For any matrix whose range is $\mathcal{R}(V)=\mathcal{N}(\mathbf{1}^{\mathrm{T}})$ we get the same result; *e.g*,

$$r \;=\; \dim\mathcal{R}(XV_{\mathcal{N}}^{\dagger\mathrm{T}}) \tag{1194}$$

because

$$\mathcal{R}(XV)=\{Xz \mid z\in\mathcal{N}(\mathbf{1}^{\mathrm{T}})\} \tag{1195}$$

and $\mathcal{R}(V)=\mathcal{R}(V_{\mathcal{N}})=\mathcal{R}(V_{\mathcal{N}}^{\dagger\mathrm{T}})$ (§E). These auxiliary matrices (§B.4.2) are more closely related;

$$V=V_{\mathcal{N}}V_{\mathcal{N}}^{\dagger} \qquad (1834)$$

[5.33] Manipulation of hull functions aff and conv follows from their definitions.

5.7.1.1 Affine dimension r *versus* rank

Now, suppose D is an EDM as defined by

$$\mathbf{D}(X) = \delta(X^{\mathrm{T}}X)\mathbf{1}^{\mathrm{T}} + \mathbf{1}\,\delta(X^{\mathrm{T}}X)^{\mathrm{T}} - 2X^{\mathrm{T}}X \;\in \mathbb{EDM}^N \tag{1049}$$

and we premultiply by $-V_{\mathcal{N}}^{\mathrm{T}}$ and postmultiply by $V_{\mathcal{N}}$. Then because $V_{\mathcal{N}}^{\mathrm{T}}\mathbf{1}=\mathbf{0}$ (1056), it is always true that

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^{\mathrm{T}}X^{\mathrm{T}}XV_{\mathcal{N}} \;=\; 2V_{\mathcal{N}}^{\mathrm{T}}GV_{\mathcal{N}} \in \mathbb{S}^{N-1} \tag{1196}$$

where G is a Gram matrix. Similarly pre- and postmultiplying by V (*confer* (1070))

$$-VDV \;=\; 2VX^{\mathrm{T}}XV \;=\; 2VGV \in \mathbb{S}^N \tag{1197}$$

always holds because $V\mathbf{1}=\mathbf{0}$ (1824). Likewise, multiplying inner-product form EDM definition (1119), it always holds:

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;=\; \Theta^{\mathrm{T}}\Theta \in \mathbb{S}^{N-1} \qquad (1123)$$

For any matrix A, $\operatorname{rank} A^{\mathrm{T}}A = \operatorname{rank} A = \operatorname{rank} A^{\mathrm{T}}$. (1638) [233, §0.4][5.34] So, by (1195), affine dimension

$$\begin{aligned} r \;&=\; \operatorname{rank} XV \;=\; \operatorname{rank} XV_{\mathcal{N}} \;=\; \operatorname{rank} XV_{\mathcal{N}}^{\dagger\mathrm{T}} \;=\; \operatorname{rank}\Theta \\ &=\; \operatorname{rank} VDV \;=\; \operatorname{rank} VGV \;=\; \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;=\; \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}}GV_{\mathcal{N}} \end{aligned} \tag{1198}$$

By conservation of dimension, (§A.7.3.0.1)

$$r + \dim\mathcal{N}(V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}) \;=\; N-1 \tag{1199}$$

$$r + \dim\mathcal{N}(VDV) \;=\; N \tag{1200}$$

For $D\in\mathbb{EDM}^N$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succ 0 \;\Leftrightarrow\; r = N-1 \tag{1201}$$

but $-VDV \not\succ 0$. The general fact[5.35] (*confer* (1081))

$$r \le \min\{n\,,\,N-1\} \tag{1202}$$

is evident from (1190) but can be visualized in the example illustrated in Figure **142**. 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 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.

[5.34] For $A\in\mathbb{R}^{m\times n}$, $\mathcal{N}(A^{\mathrm{T}}A) = \mathcal{N}(A)$. [374, §3.3]
[5.35] $\operatorname{rank} X \le \min\{n\,,\,N\}$

5.7.2 *Précis*

We collect expressions for affine dimension r: for list $X \in \mathbb{R}^{n\times N}$ and Gram matrix $G \in \mathbb{S}^N_+$

$$
\begin{aligned}
r \;&\triangleq\; \dim(\mathcal{P}-\alpha) \;=\; \dim\mathcal{P} \;=\; \dim\operatorname{conv} X \quad (1189)\\
&=\; \dim(\mathcal{A}-\alpha) \;=\; \dim\mathcal{A} \;=\; \dim\operatorname{aff} X\\
&=\; \operatorname{rank}(X - x_1\mathbf{1}^{\mathrm{T}}) \;=\; \operatorname{rank}(X - \tfrac{1}{N}X\mathbf{1}\mathbf{1}^{\mathrm{T}})\\
&=\; \operatorname{rank}\Theta \quad (1121)\\
&=\; \operatorname{rank} XV_{\mathcal{N}} \;=\; \operatorname{rank} XV \;=\; \operatorname{rank} XV_{\mathcal{N}}^{\dagger\mathrm{T}}\\
&=\; \operatorname{rank} X\,, \qquad Xe_1 = \mathbf{0} \quad \textbf{or} \quad X\mathbf{1} = \mathbf{0}\\
&=\; \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}}GV_{\mathcal{N}} \;=\; \operatorname{rank} VGV \;=\; \operatorname{rank} V_{\mathcal{N}}^{\dagger}GV_{\mathcal{N}}\\
&=\; \operatorname{rank} G\,, \qquad Ge_1 = \mathbf{0} \;\; (1066) \quad \textbf{or} \quad G\mathbf{1} = \mathbf{0} \;\; (1070)\\
&=\; \left.\begin{aligned}
&\operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;=\; \operatorname{rank} VDV \;=\; \operatorname{rank} V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}} \;=\; \operatorname{rank} V_{\mathcal{N}}(V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}})V_{\mathcal{N}}^{\mathrm{T}}\\
&\operatorname{rank}\Lambda \quad (1289)\\
&N-1-\dim\mathcal{N}\!\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}}\\ \mathbf{1} & -D\end{bmatrix}\right) = \operatorname{rank}\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}}\\ \mathbf{1} & -D\end{bmatrix} - 2 \quad (1210)
\end{aligned}\right\} D \in \mathbb{EDM}^N
\end{aligned}
\tag{1203}
$$

5.7.3 Eigenvalues of $-VDV$ *versus* $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$

Suppose for $D \in \mathbb{EDM}^N$ we are given eigenvectors $v_i \in \mathbb{R}^N$ of $-VDV$ and corresponding eigenvalues $\lambda \in \mathbb{R}^N$ so that

$$-VDVv_i = \lambda_i v_i\,, \quad i = 1\ldots N \tag{1204}$$

From these we can determine the eigenvectors and eigenvalues of $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$: Define

$$\nu_i \triangleq V_{\mathcal{N}}^{\dagger}v_i\,, \quad \lambda_i \neq 0 \tag{1205}$$

Then we have:

$$-VDV_{\mathcal{N}}V_{\mathcal{N}}^{\dagger}v_i = \lambda_i v_i \tag{1206}$$

$$-V_{\mathcal{N}}^{\dagger}VDV_{\mathcal{N}}\nu_i = \lambda_i V_{\mathcal{N}}^{\dagger}v_i \tag{1207}$$

$$-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}\nu_i = \lambda_i \nu_i \tag{1208}$$

the eigenvectors of $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$ are given by (1205) while its corresponding nonzero eigenvalues are identical to those of $-VDV$ although $-V_{\mathcal{N}}^{\dagger}DV_{\mathcal{N}}$ is not necessarily positive semidefinite. In contrast, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ is positive semidefinite but its nonzero eigenvalues are generally different.

5.7.3.0.1 Theorem. *EDM rank versus affine dimension r.* [191, §3] [215, §3] [190, §3] For $D \in \mathbb{EDM}^N$ (*confer* (1363))

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

$$
\begin{aligned}
\text{diameter} \;&=\; \sqrt{2}\,\left(\mathbf{1}^{\mathrm{T}}D^{\dagger}\mathbf{1}\right)^{-1/2}\\
\text{circumcenter} \;&=\; \tfrac{XD^{\dagger}\mathbf{1}}{\mathbf{1}^{\mathrm{T}}D^{\dagger}\mathbf{1}}
\end{aligned}
\tag{1209}
$$

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

3) In *Cayley-Menger form* [127, §6.2] [97, §3.3] [55, §40] (§5.11.2),

$$r \;=\; N-1-\dim\mathcal{N}\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\right) = \operatorname{rank}\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix} - 2 \tag{1210}$$

Circumhyperspheres exist for $r<\operatorname{rank}(D)-2$. [392, §7] ◇

For all practical purposes, (1202)

$$\max\{0\,,\,\operatorname{rank}(D)-2\} \;\le\; r \;\le\; \min\{n\,,\,N-1\} \tag{1211}$$

5.8 Euclidean metric *versus* matrix criteria

5.8.1 Nonnegativity property 1

When $D=[d_{ij}]$ is an EDM (1049), then it is apparent from (1196)

$$2V_{\mathcal{N}}^{\mathrm{T}}X^{\mathrm{T}}XV_{\mathcal{N}} \;=\; -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succeq 0 \tag{1212}$$

because for any matrix A, $A^{\mathrm{T}}A\succeq 0$.[5.36] We claim nonnegativity of the d_{ij} is enforced primarily by the matrix inequality (1212); *id est*,

$$\left.\begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succeq 0 \\ D\in\mathbb{S}_h^N \end{array}\right\} \Rightarrow\; d_{ij}\ge 0\,,\; i\ne j \tag{1213}$$

(The matrix inequality to enforce strict positivity differs by a stroke of the pen. (1216))

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. [185, §4.2] Given $D\in\mathbb{S}_h^N$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} =$$

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

$$= \tfrac{1}{2}(\mathbf{1}D_{1,2:N} + D_{2:N,1}\mathbf{1}^{\mathrm{T}} - D_{2:N,2:N}) \in \mathbb{S}^{N-1} \tag{1214}$$

where row, column indices $i,j\in\{1\dots N-1\}$. [355] It follows:

$$\left.\begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succeq 0 \\ D\in\mathbb{S}_h^N \end{array}\right\} \Rightarrow\; \delta(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}) = \begin{bmatrix} d_{12} \\ d_{13} \\ \vdots \\ d_{1N} \end{bmatrix} \succeq 0 \tag{1215}$$

Multiplication of $V_{\mathcal{N}}$ by any permutation matrix Ξ has null effect on its range and nullspace. In other words, any permutation of the rows or columns of $V_{\mathcal{N}}$

5.36 For $A\in\mathbb{R}^{m\times n}$, $A^{\mathrm{T}}A\succeq 0 \;\Leftrightarrow\; y^{\mathrm{T}}A^{\mathrm{T}}Ay=\|Ay\|^2\ge 0$ for all $\|y\|=1$. When A is full-rank thin-or-square, $A^{\mathrm{T}}A\succ 0$.

produces a basis for $\mathcal{N}(\mathbf{1}^{\mathrm{T}})$; *id est*, $\mathcal{R}(\Xi_{\mathrm{r}}V_{\mathcal{N}})=\mathcal{R}(V_{\mathcal{N}}\,\Xi_{\mathrm{c}})=\mathcal{R}(V_{\mathcal{N}})=\mathcal{N}(\mathbf{1}^{\mathrm{T}})$. Hence, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0 \;\Leftrightarrow\; -V_{\mathcal{N}}^{\mathrm{T}}\,\Xi_{\mathrm{r}}^{\mathrm{T}}D\Xi_{\mathrm{r}}V_{\mathcal{N}}\succeq 0 \quad (\Leftrightarrow\; -\Xi_{\mathrm{c}}^{\mathrm{T}}V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\,\Xi_{\mathrm{c}}\succeq 0)$. Various permutation matrices will sift[5.37] remaining d_{ij} similarly to (1215) thereby proving their nonnegativity. Hence $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0$ is a sufficient test for the first property (§5.2) of the Euclidean metric, nonnegativity. ♦

When affine dimension r equals 1, in particular, nonnegativity symmetry and hollowness become necessary and sufficient criteria satisfying matrix inequality (1212). (§6.5.0.0.1)

5.8.1.1 Strict positivity

Should we require the points in $\mathbb{R}^n$ to be distinct, then entries of D off the main diagonal must be strictly positive $\{d_{ij}>0\,,\; i\neq j\}$ and only those entries along the main diagonal of D are 0. By similar argument, the strict matrix inequality is a sufficient test for strict positivity of Euclidean distance-square;

$$\left.\begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succ 0 \\ D\in\mathbb{S}_h^N \end{array}\right\}\Rightarrow\; d_{ij}>0\,,\quad i\neq j \tag{1216}$$

5.8.2 Triangle inequality property 4

In light of Kreyszig's observation [259, §1.1 prob.15] that properties 2 through 4 of the Euclidean metric (§5.2) together imply nonnegativity property 1,

$$2\sqrt{d_{jk}}=\sqrt{d_{jk}}+\sqrt{d_{kj}}\;\geq\;\sqrt{d_{jj}}=0\,,\quad j\neq k \tag{1217}$$

nonnegativity criterion (1213) suggests that matrix inequality $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0$ might somehow take on the role of triangle inequality; *id est*,

$$\left.\begin{array}{r} \delta(D)=\mathbf{0} \\ D^{\mathrm{T}}=D \\ -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0 \end{array}\right\}\Rightarrow\sqrt{d_{ij}}\;\leq\;\sqrt{d_{ik}}+\sqrt{d_{kj}}\;,\quad i\neq j\neq k \tag{1218}$$

We now show that is indeed the case: Let T be the *leading principal submatrix* in $\mathbb{S}^{\mathbf{2}}$ of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ (upper left 2×2 submatrix from (1214));

$$T\triangleq\begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) \\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} \end{bmatrix} \tag{1219}$$

Submatrix T must be positive (semi)definite whenever $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ is. (§A.3.1.0.4, §5.8.3) Now we have,

$$\begin{array}{l} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0\;\Rightarrow\;T\succeq 0\;\Leftrightarrow\;\lambda_1\geq\lambda_2\geq 0 \\ -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succ 0\;\Rightarrow\;T\succ 0\;\Leftrightarrow\;\lambda_1\geq\lambda_2>0 \end{array} \tag{1220}$$

where λ_1 and λ_2 are the eigenvalues of T, real due only to symmetry of T:

$$\begin{array}{l} \lambda_1=\frac{1}{2}\left(d_{12}+d_{13}+\sqrt{d_{23}^2-2(d_{12}+d_{13})d_{23}+2(d_{12}^2+d_{13}^2)}\right)\in\mathbb{R} \\ \lambda_2=\frac{1}{2}\left(d_{12}+d_{13}-\sqrt{d_{23}^2-2(d_{12}+d_{13})d_{23}+2(d_{12}^2+d_{13}^2)}\right)\in\mathbb{R} \end{array} \tag{1221}$$

Nonnegativity of eigenvalue λ_1 is guaranteed by only nonnegativity of the d_{ij} which in turn is guaranteed by matrix inequality (1213). Inequality between the eigenvalues in (1220) follows from only realness of the d_{ij}. Since λ_1 always equals or exceeds λ_2,

[5.37] Rule of thumb: If $\Xi_{\mathrm{r}}(i\,,1)=1$, then $\delta(-V_{\mathcal{N}}^{\mathrm{T}}\Xi_{\mathrm{r}}^{\mathrm{T}}D\Xi_{\mathrm{r}}V_{\mathcal{N}})\in\mathbb{R}^{N-1}$ is some permutation of the ith row or column of D excepting the 0 entry from the main diagonal.

conditions for positive (semi)definiteness of submatrix T can be completely determined by examining λ_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*,

$$\begin{aligned} T \succeq 0 \quad \Leftrightarrow \quad \det T = \lambda_1 \lambda_2 \geq 0\,, \quad d_{12}\,, d_{13} \geq 0 \qquad & \text{(c)} \\ \Leftrightarrow \\ \lambda_2 \geq 0 \qquad & \text{(b)} \\ \Leftrightarrow \\ |\sqrt{d_{12}} - \sqrt{d_{23}}\,| \;\leq\; \sqrt{d_{13}} \;\leq\; \sqrt{d_{12}} + \sqrt{d_{23}} \qquad & \text{(a)} \end{aligned} \tag{1222}$$

Triangle inequality (1222a) (*confer* (1117) (1234)), in terms of three rooted entries from D, is equivalent to metric property 4

$$\begin{aligned} \sqrt{d_{13}} &\leq \sqrt{d_{12}} + \sqrt{d_{23}} \\ \sqrt{d_{23}} &\leq \sqrt{d_{12}} + \sqrt{d_{13}} \\ \sqrt{d_{12}} &\leq \sqrt{d_{13}} + \sqrt{d_{23}} \end{aligned} \tag{1223}$$

for the corresponding points x_1, x_2, x_3 from some length-N list.[5.38]

5.8.2.1 Comment

Given D whose dimension N equals or exceeds 3, there are $N!/(3!(N-3)!)$ distinct triangle inequalities in total like (1117) 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, (1222a) that came from T (1219). Yet we claim if $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0$ then all triangle inequalities will be satisfied simultaneously;

$$|\sqrt{d_{ik}} - \sqrt{d_{kj}}\,| \;\leq\; \sqrt{d_{ij}} \;\leq\; \sqrt{d_{ik}} + \sqrt{d_{kj}}\,, \quad i<k<j \tag{1224}$$

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

5.8.2.1.1 Shore. The columns of $\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}}$ hold a basis for $\mathcal{N}(\mathbf{1}^{\mathrm{T}})$ when Ξ_{r} and Ξ_{c} are permutation matrices. In other words, any permutation of the rows or columns of $V_{\mathcal{N}}$ leaves its range and nullspace unchanged; *id est*, $\mathcal{R}(\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}}) = \mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^{\mathrm{T}})$ (1056). Hence, two distinct matrix inequalities can be equivalent tests of the positive semidefiniteness of D on $\mathcal{R}(V_{\mathcal{N}})$; *id est*, $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0 \;\Leftrightarrow\; -(\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}})^{\mathrm{T}} D (\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}}) \succeq 0$. By properly choosing permutation matrices,[5.39] the leading principal submatrix $T_{\Xi} \in \mathbb{S}^{\mathbf{2}}$ of $-(\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}})^{\mathrm{T}} D (\Xi_{\mathrm{r}} V_{\mathcal{N}} \Xi_{\mathrm{c}})$ may be loaded with the entries of D needed to test any particular triangle inequality (similarly to (1214)-(1222)). Because all the triangle inequalities can be individually tested using a test equivalent to the lone matrix inequality $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0$, it logically follows that the lone matrix inequality tests all those triangle inequalities simultaneously. We conclude that $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0$ is a sufficient test for the fourth property of the Euclidean metric, triangle inequality. ♠

[5.38] Accounting for symmetry property 3, the fourth metric property demands three inequalities be satisfied per one of type (1222a). The first of those inequalities in (1223) is self evident from (1222a), while the two remaining follow from the left side of (1222a) and the fact (for scalars) $|a| \leq b \Leftrightarrow a \leq b$ and $-a \leq b$.

[5.39] 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 $\Xi_{\mathrm{r}}(i,1) = \Xi_{\mathrm{r}}(k,2) = \Xi_{\mathrm{r}}(j,3) = 1$ and $\Xi_{\mathrm{c}} = I$.

5.8.2.2 Strict triangle inequality

Without exception, all the inequalities in (1222) and (1223) can be made strict while their corresponding implications remain true. The then strict inequality (1222a) or (1223) may be interpreted as a *strict triangle inequality* under which collinear arrangement of points is not allowed. [255, §24/6, p.322] Hence by similar reasoning, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succ 0$ is a sufficient test of all the strict triangle inequalities; *id est*,

$$\left.\begin{array}{r}\delta(D)=\mathbf{0}\\ D^{\mathrm{T}}=D\\ -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succ 0\end{array}\right\}\Rightarrow \sqrt{d_{ij}}\;<\;\sqrt{d_{ik}}+\sqrt{d_{kj}}\;,\quad i\neq j\neq k \tag{1225}$$

5.8.3 $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ nesting

From (1219) observe that $T=-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow 3}$. In fact, for $D\in\mathbb{EDM}^N$, the leading principal submatrices of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ form a nested sequence (by inclusion) whose members are individually positive semidefinite [185] [233] [374] and have the same form as T; *videlicet*,[5.40]

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow 1} \;=\; [\,\emptyset\,] \tag{o}$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow 2} \;=\; [d_{12}]\in\mathbb{S}_+ \tag{a}$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow 3} \;=\; \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23})\\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13}\end{bmatrix} \;=\; T\in\mathbb{S}_+^{\mathbf{2}} \tag{b}$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow 4} \;=\; \begin{bmatrix} d_{12} & \frac{1}{2}(d_{12}+d_{13}-d_{23}) & \frac{1}{2}(d_{12}+d_{14}-d_{24})\\ \frac{1}{2}(d_{12}+d_{13}-d_{23}) & d_{13} & \frac{1}{2}(d_{13}+d_{14}-d_{34})\\ \frac{1}{2}(d_{12}+d_{14}-d_{24}) & \frac{1}{2}(d_{13}+d_{14}-d_{34}) & d_{14}\end{bmatrix} \tag{c}$$

$$\vdots$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow i} \;=\; \begin{bmatrix} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow i-1} & \nu(i)\\ \nu(i)^{\mathrm{T}} & d_{1i}\end{bmatrix}\in\mathbb{S}_+^{i-1} \tag{d}$$

$$\vdots$$

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;=\; \begin{bmatrix} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}|_{N\leftarrow N-1} & \nu(N)\\ \nu(N)^{\mathrm{T}} & d_{1N}\end{bmatrix}\in\mathbb{S}_+^{N-1} \tag{e}$$

(1226)

where

$$\nu(i)\triangleq\frac{1}{2}\begin{bmatrix} d_{12}+d_{1i}-d_{2i}\\ d_{13}+d_{1i}-d_{3i}\\ \vdots\\ d_{1,i-1}+d_{1i}-d_{i-1,i}\end{bmatrix}\in\mathbb{R}^{i-2},\quad i>2 \tag{1227}$$

Hence, the leading principal submatrices of EDM D must also be EDMs.[5.41]

[5.40] $-VDV|_{N\leftarrow 1}=0\in\mathbb{S}_+^0$ (§B.4.1)

[5.41] In fact, each and every principal submatrix of an EDM D is another EDM. [269, §4.1]

Bordered symmetric matrices in the form (1226d) are known to have *intertwined* [374, §6.4] (or *interlaced* [233, §4.3] [370, §IV.4.1]) eigenvalues; (*confer* §5.11.1) that means, for the particular submatrices (1226a) and (1226b),

$$\lambda_2 \leq d_{12} \leq \lambda_1 \tag{1228}$$

where d_{12} is the eigenvalue of submatrix (1226a) and λ_1, λ_2 are the eigenvalues of T (1226b) (1219). Intertwining in (1228) predicts that should d_{12} become 0, then λ_2 must go to 0.[5.42] Eigenvalues are similarly intertwined for submatrices (1226b) and (1226c);

$$\gamma_3 \leq \lambda_2 \leq \gamma_2 \leq \lambda_1 \leq \gamma_1 \tag{1229}$$

where $\gamma_1, \gamma_2, \gamma_3$ are the eigenvalues of submatrix (1226c). Intertwining likewise predicts that should λ_2 become 0 (a possibility revealed in §5.8.3.1), then γ_3 must go to 0. Combining results so far for $N = 2, 3, 4$: (1228) (1229)

$$\gamma_3 \leq \lambda_2 \leq d_{12} \leq \lambda_1 \leq \gamma_1 \tag{1230}$$

The preceding logic extends by induction through the remaining members of the sequence (1226).

5.8.3.1 Tightening the triangle inequality

Now we apply Schur complement from §A.4 to tighten the triangle inequality from (1218) in case: cardinality $N = 4$. We find that the gains by doing so are modest. From (1226) we identify:

$$\begin{bmatrix} A & B \\ B^{\mathrm{T}} & C \end{bmatrix} \triangleq -V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}|_{N\leftarrow 4} \tag{1231}$$

$$A \triangleq T = -V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}|_{N\leftarrow 3} \tag{1232}$$

both positive semidefinite by assumption, where $B = \nu(4)$ (1227), and $C = d_{14}$. Using nonstrict $CC^{\dagger}$-form (1679), $C \succeq 0$ by assumption (§5.8.1) and $CC^{\dagger} = I$. So by the *positive semidefinite ordering of eigenvalues theorem* (§A.3.1.0.1),

$$-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}|_{N\leftarrow 4} \succeq 0 \;\Leftrightarrow\; T \succeq d_{14}^{-1}\nu(4)\nu(4)^{\mathrm{T}} \;\Rightarrow\; \begin{cases} \lambda_1 \geq d_{14}^{-1}\|\nu(4)\|^2 \\ \lambda_2 \geq 0 \end{cases} \tag{1233}$$

where $\{d_{14}^{-1}\|\nu(4)\|^2, 0\}$ are the eigenvalues of $d_{14}^{-1}\nu(4)\nu(4)^{\mathrm{T}}$ while λ_1, λ_2 are the eigenvalues of T.

5.8.3.1.1 Example. *Small completion problem,* II.
Applying the inequality for λ_1 in (1233) to the *small completion problem* on page 345 Figure **143**, the lower bound on $\sqrt{d_{14}}$ (1.236 in (1042)) is tightened to 1.289. The correct value of $\sqrt{d_{14}}$ to three significant figures is 1.414. □

[5.42] If d_{12} were 0, eigenvalue λ_2 becomes 0 (1221) because d_{13} must then be equal to d_{23}; *id est*, $d_{12} = 0 \;\Leftrightarrow\; x_1 = x_2$. (§5.4)

5.8.4 Affine dimension reduction in two dimensions

(*confer* §5.14.4) The leading principal 2×2 submatrix T of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ has largest eigenvalue λ_1 (1221) which is a convex function of D.[5.43] λ_1 can never be 0 unless $d_{12}=d_{13}=d_{23}=0$. Eigenvalue λ_1 can never be negative while the d_{ij} are nonnegative. The remaining eigenvalue λ_2 (1221) is a concave function of D that becomes 0 only at the upper and lower bounds of triangle inequality (1222a) and its equivalent forms: (*confer* (1224))

$$\begin{array}{rcccl} |\sqrt{d_{12}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{13}} & \leq & \sqrt{d_{12}}+\sqrt{d_{23}} \qquad \text{(a)} \\ & & \Leftrightarrow & & \\ |\sqrt{d_{12}}-\sqrt{d_{13}}\,| & \leq & \sqrt{d_{23}} & \leq & \sqrt{d_{12}}+\sqrt{d_{13}} \qquad \text{(b)} \\ & & \Leftrightarrow & & \\ |\sqrt{d_{13}}-\sqrt{d_{23}}\,| & \leq & \sqrt{d_{12}} & \leq & \sqrt{d_{13}}+\sqrt{d_{23}} \qquad \text{(c)} \end{array} \tag{1234}$$

In between those bounds, λ_2 is strictly positive; otherwise, it would be negative but prevented by the condition $T\succeq 0$.

When λ_2 becomes 0, it means triangle $\triangle_{123}$ has collapsed to a line segment; a potential reduction in affine dimension r. The same logic is valid for any particular principal 2×2 submatrix of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$, hence applicable to other triangles.

5.9 Bridge: Convex polyhedra to EDMs

The criteria for the existence of an EDM include, by definition (1049) (1119), the properties imposed upon its entries d_{ij} by the Euclidean metric. From §5.8.1 and §5.8.2, we know there is a relationship of matrix criteria to those properties. Here is a snapshot of what we are sure: for $i\,,j\,,k\in\{1\dots N\}$ (*confer* §5.2)

$$\begin{array}{l} \sqrt{d_{ij}}\geq 0\,,\quad i\neq j \\ \sqrt{d_{ij}}=0\,,\quad i=j \\ \sqrt{d_{ij}}=\sqrt{d_{ji}} \\ \sqrt{d_{ij}}\;\leq\;\sqrt{d_{ik}}+\sqrt{d_{kj}}\;,\quad i\neq j\neq k \end{array} \quad\Leftarrow\quad \begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0 \\ \delta(D)=\mathbf{0} \\ D^{\mathrm{T}}=D \end{array} \tag{1235}$$

all implied by $D\in\mathbb{EDM}^N$. In words, these four Euclidean metric properties are necessary conditions for D to be a distance matrix. At the moment, we have no converse. As of concern in §5.3, we have yet to establish metric requirements beyond the four Euclidean metric properties that would allow D to be certified an EDM or might facilitate polyhedron or list reconstruction from an incomplete EDM. We deal with this problem in §5.14. Our present goal is to establish *ab initio* the necessary and sufficient matrix criteria that will subsume all the Euclidean metric properties and any further requirements[5.44] for all $N>1$ (§5.8.3); *id est*,

$$\left.\begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0 \\ D\in\mathbb{S}_h^N \end{array}\right\}\;\Leftrightarrow\;\; D\in\mathbb{EDM}^N \tag{1068}$$

[5.43] The largest eigenvalue of any symmetric matrix is always a convex function of its entries, while the smallest eigenvalue is always concave. [66, exmp.3.10] In our particular case, say $\underline{d}\triangleq\begin{bmatrix}d_{12}\\ d_{13}\\ d_{23}\end{bmatrix}\in\mathbb{R}^{\mathbf{3}}$. Then the Hessian (1956) $\nabla^2\lambda_1(\underline{d})\succeq 0$ certifies convexity whereas $\nabla^2\lambda_2(\underline{d})\preceq 0$ certifies concavity. Each Hessian has rank 1. The respective gradients $\nabla\lambda_1(\underline{d})$ and $\nabla\lambda_2(\underline{d})$ are nowhere $\mathbf{0}$ and can be uniquely defined.

[5.44] Schoenberg [355, (1)] first extolled matrix product $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ (1214) (predicated on symmetry and selfdistance) in 1935, specifically incorporating $V_{\mathcal{N}}$, albeit algebraically. He showed: nonnegativity $-y^{\mathrm{T}}V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\,y\geq 0\,,\;\forall\,y\in\mathbb{R}^{N-1}$, is necessary and sufficient for D to be an EDM. Gower [190, §3] remarks how surprising it is that such a fundamental property of Euclidean geometry was obtained so late.

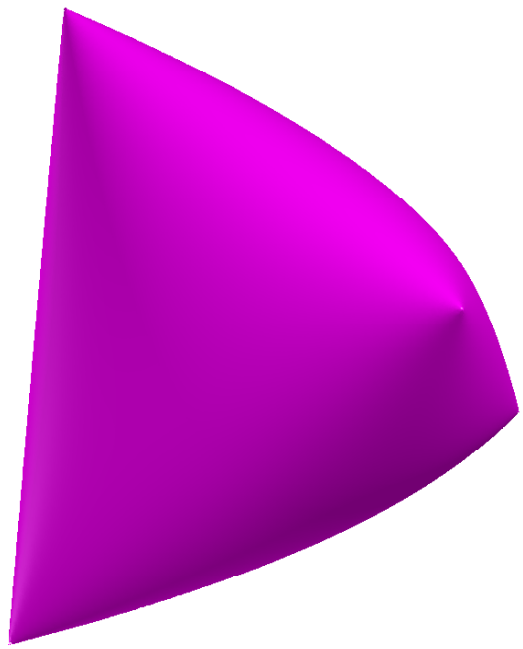


Figure 157: Elliptope $\mathcal{E}^{\mathbf{3}}$ in isometrically isomorphic $\mathbb{R}^{\mathbf{6}}$ (projected on $\mathbb{R}^{\mathbf{3}}$) is a convex body that appears to possess some kind of symmetry in this dimension; it resembles a malformed pillow in the shape of a bulging tetrahedron. Elliptope relative boundary is not *smooth* and comprises all set members (1237) having at least one 0 eigenvalue. [272, §2.1] This elliptope has an infinity of vertices, but there are only four vertices corresponding to a rank-1 matrix. Those yy^{T}, evident in the illustration, have binary vector $y \in \mathbb{R}^{\mathbf{3}}$ with entries in $\{\pm 1\}$.

or for EDM definition (1128),

$$\left.\begin{array}{r} \Omega \succeq 0 \\ \sqrt{\delta(d)} \succeq 0 \end{array}\right\} \;\Leftrightarrow\; D = \mathbf{D}(\Omega\,, d) \in \mathbb{EDM}^N \tag{1236}$$

5.9.1 Geometric arguments

5.9.1.0.1 Definition. *Elliptope*: [272] [269, §2.3] [127, §31.5]
a unique bounded immutable convex Euclidean body in $\mathbb{S}^n$; intersection of positive semidefinite cone $\mathbb{S}^n_+$ with that set of n hyperplanes defined by unity main diagonal;

$$\mathcal{E}^n \triangleq \mathbb{S}^n_+ \cap \{\Phi \in \mathbb{S}^n \mid \delta(\Phi) = \mathbf{1}\} \tag{1237}$$

`a.k.a` the set of all *correlation matrices* of dimension

$$\dim \mathcal{E}^n = n(n-1)/2 \;\text{ in }\; \mathbb{R}^{n(n+1)/2} \tag{1238}$$

An elliptope $\mathcal{E}^n$ is not a polyhedron, in general, but has some polyhedral faces and an infinity of vertices.[5.45] Of those, 2^{n-1} vertices (some extreme points of the elliptope) are

[5.45] Laurent defines vertex distinctly from the sense herein (§2.6.1.0.1); she defines *vertex* as a point with full-dimensional (nonempty interior) normal cone (§E.10.3.2.1). Her definition excludes point C in Figure **35**, for example.

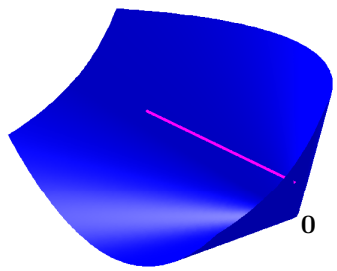


Figure 158: Elliptope $\mathcal{E}^{\mathbf{2}}$ in isometrically isomorphic $\mathbb{R}^{\mathbf{3}}$ is a line segment illustrated interior to positive semidefinite cone $\mathbb{S}^{\mathbf{2}}_{+}$ (Figure **46**). Two vertices on boundary are rank-1 binary.

extreme directions yy^{T} of the positive semidefinite cone where entries of vector $y \in \mathbb{R}^n$ belong to $\{\pm 1\}$ and exercise every combination. Each of the remaining vertices has rank, greater than 1, belonging to the set $\{k > 0 \mid k(k+1)/2 \leq n\}$. Each and every face of an elliptope is exposed. $\triangle$

In fact, any positive semidefinite matrix whose entries belong to $\{\pm 1\}$ is a rank-1 correlation matrix; and *vice versa*:[5.46]

5.9.1.0.2 Theorem. *Elliptope vertices rank-1.* (*confer* §2.3.1.0.1) [144, §2.1.1]
For $Y \in \mathbb{S}^n$, $y \in \mathbb{R}^n$, and all $i, j \in \{1 \dots n\}$

$$Y \succeq 0\,, \quad Y_{ij} \in \{\pm 1\} \qquad \Leftrightarrow \qquad Y = yy^{\mathrm{T}}, \quad y_i \in \{\pm 1\} \tag{1239}$$

$\diamond$

The elliptope for dimension $n = 2$ is a line segment in isometrically isomorphic $\mathbb{R}^{n(n+1)/2}$ (Figure **158**). Obviously, $\mathrm{cone}(\mathcal{E}^n) \neq \mathbb{S}^n_{+}$. The elliptope for dimension $n = 3$ is realized in Figure **157**.

5.9.1.0.3 Lemma. *Hypersphere.* (*confer* bullet p.352) [19, §4]
Matrix $\Psi = [\Psi_{ij}] \in \mathbb{S}^N$ belongs to the elliptope in $\mathbb{S}^N$ iff there exist N points p on the boundary of a hypersphere in $\mathbb{R}^{\mathrm{rank}\,\Psi}$ having radius 1 such that

$$\|p_i - p_j\|^2 = 2(1 - \Psi_{ij})\,, \quad i, j = 1 \dots N \tag{1240}$$

$\diamond$

There is a similar theorem for Euclidean distance matrices:

We derive matrix criteria for D to be an EDM, validating (1068) using simple geometry; distance to the polyhedron formed by the convex hull of a list of points (79) in Euclidean space $\mathbb{R}^n$.

[5.46] As there are few equivalent conditions for rank constraints, this device is rather important for relaxing integer, combinatorial, or Boolean problems.

5.9.1.0.4 EDM assertion.

D is a Euclidean distance matrix if and only if $D \in \mathbb{S}_h^N$ and distances-square from the origin

$$\{\|p(y)\|^2 = -y^{\mathrm{T}} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}\, y \mid y \in \mathcal{S} - \beta\} \tag{1241}$$

correspond to points p in some bounded convex polyhedron

$$\mathcal{P} - \alpha \;=\; \{p(y) \mid y \in \mathcal{S} - \beta\} \tag{1242}$$

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 domain of linear surjection $p(y)$ is the unit simplex $\mathcal{S} \subset \mathbb{R}_+^{N-1}$ shifted such that its vertex at the origin is translated to $-\beta$ in $\mathbb{R}^{N-1}$. When $\beta = 0$, then $\alpha = x_1$. ◇

In terms of $V_{\mathcal{N}}$, the unit simplex (300) in $\mathbb{R}^{N-1}$ has an equivalent representation:

$$\mathcal{S} \;=\; \{s \in \mathbb{R}^{N-1} \mid \sqrt{2} V_{\mathcal{N}}\, s \succeq -e_1\} \tag{1243}$$

where e_1 is as in (1065). 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 map from vertices of the unit simplex to members of the list generating $\mathcal{P}$;

$$\begin{array}{rcccc} p & : & \mathbb{R}^{N-1} & \rightarrow & \mathbb{R}^n \\ p\left(\left\{\begin{array}{c} -\beta \\ e_1 - \beta \\ e_2 - \beta \\ \vdots \\ e_{N-1} - \beta \end{array}\right\}\right) & = & & & \left\{\begin{array}{c} x_1 - \alpha \\ x_2 - \alpha \\ x_3 - \alpha \\ \vdots \\ x_N - \alpha \end{array}\right\} \end{array} \tag{1244}$$

5.9.1.0.5 Proof. *EDM assertion.*

(⇒) We demonstrate that if D is an EDM, then each distance-square $\|p(y)\|^2$ described by (1241) corresponds to a point p in some embedded polyhedron $\mathcal{P} - \alpha$. Assume D is indeed an EDM; *id est*, D can be made from some list X of N unknown points in Euclidean space $\mathbb{R}^n$; $D = \mathbf{D}(X)$ for $X \in \mathbb{R}^{n \times N}$ as in (1049). Since D is translation invariant (§5.5.1), we may shift the affine hull $\mathcal{A}$ of those unknown points to the origin as in (1184). Then take any point p in their convex hull (89);

$$\mathcal{P} - \alpha \;=\; \{p = (X - X b\, \mathbf{1}^{\mathrm{T}}) a \mid a^{\mathrm{T}} \mathbf{1} = 1,\; a \succeq 0\} \tag{1245}$$

where $\alpha = X b \in \mathcal{A} \;\Leftrightarrow\; b^{\mathrm{T}} \mathbf{1} = 1$. Solutions to $a^{\mathrm{T}} \mathbf{1} = 1$ are:[5.47]

$$a \in \left\{ e_1 + \sqrt{2} V_{\mathcal{N}}\, s \mid s \in \mathbb{R}^{N-1} \right\} \tag{1246}$$

where e_1 is as in (1065). Similarly, $b = e_1 + \sqrt{2} V_{\mathcal{N}}\, \beta$.

$$\begin{array}{rcl} \mathcal{P} - \alpha & = & \{p = X(I - (e_1 + \sqrt{2} V_{\mathcal{N}} \beta) \mathbf{1}^{\mathrm{T}})(e_1 + \sqrt{2} V_{\mathcal{N}}\, s) \mid \sqrt{2} V_{\mathcal{N}}\, s \succeq -e_1\} \\ & = & \{p = X \sqrt{2} V_{\mathcal{N}} (s - \beta) \mid \sqrt{2} V_{\mathcal{N}}\, s \succeq -e_1\} \end{array} \tag{1247}$$

that describes the domain of $p(s)$ as the unit simplex

$$\mathcal{S} = \{s \mid \sqrt{2} V_{\mathcal{N}}\, s \succeq -e_1\} \subset \mathbb{R}_+^{N-1} \qquad (1243)$$

[5.47] Since $\mathcal{R}(V_{\mathcal{N}}) = \mathcal{N}(\mathbf{1}^{\mathrm{T}})$ and $\mathcal{N}(\mathbf{1}^{\mathrm{T}}) \perp \mathcal{R}(\mathbf{1})$, 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, $a = e_1$.

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

$$\mathcal{P}-\alpha \;=\; \{p = X\sqrt{2}V_{\mathcal{N}}\,y \mid y\in\mathcal{S}-\beta\} \tag{1248}$$

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 $\mathcal{P}-\alpha$ (1187) and the origin (when $\alpha\in\mathcal{A}$), and because $\mathcal{A}$ has dimension r by definition (1189). Now, any distance-square from the origin to the polyhedron $\mathcal{P}-\alpha$ can be formulated

$$\{p^{\mathrm{T}}p \;=\; \|p\|^2 \;=\; 2y^{\mathrm{T}}V_{\mathcal{N}}^{\mathrm{T}}X^{\mathrm{T}}XV_{\mathcal{N}}\,y \mid y\in\mathcal{S}-\beta\} \tag{1249}$$

Applying (1196) to (1249) we get (1241).
(⇐) To validate the *EDM assertion* in the reverse direction, we prove: If each distance-square $\|p(y)\|^2$ (1241) 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

$$p(\mathcal{S}-\beta) = \mathcal{P}-\alpha \tag{1250}$$

because $\mathcal{A}-\alpha = \operatorname{aff}(\mathcal{P}-\alpha)\supseteq\mathcal{P}-\alpha$ (1187). So, outside domain $\mathcal{S}-\beta$ of linear surjection $p(y)$, simplex complement $\backslash\mathcal{S}-\beta\subset\mathbb{R}^{N-1}$ must contain domain of the distance-square $\|p(y)\|^2 = p(y)^{\mathrm{T}}p(y)$ to remaining points in 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 $\mathcal{A}-\alpha$, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ must be positive semidefinite and is assumed symmetric;[5.48]

$$-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \;\triangleq\; \Theta_{\mathrm{p}}^{\mathrm{T}}\Theta_{\mathrm{p}} \tag{1251}$$

where[5.49] $\Theta_{\mathrm{p}}\in\mathbb{R}^{m\times N-1}$ for some $m\geq r$. Because $p(\mathcal{S}-\beta)$ is a convex polyhedron, it is necessarily a set of linear combinations of points from some length-N list because every convex polyhedron having N or fewer vertices can be generated that way (§2.12.2). Equivalent to (1241) are

$$\{p^{\mathrm{T}}p \mid p\in\mathcal{P}-\alpha\} \;=\; \{p^{\mathrm{T}}p = y^{\mathrm{T}}\Theta_{\mathrm{p}}^{\mathrm{T}}\Theta_{\mathrm{p}}\,y \mid y\in\mathcal{S}-\beta\} \tag{1252}$$

Because $p\in\mathcal{P}-\alpha$ may be found by factoring (1252), the list Θ_{p} is found by factoring (1251). A unique EDM can be made from that list using inner-product form definition $\mathbf{D}(\Theta)|_{\Theta=\Theta_{\mathrm{p}}}$ (1119). That EDM will be identical to D if $\delta(D)=\mathbf{0}$, by injectivity of $\mathbf{D}$ (1170). ♦

5.9.2 Necessity and sufficiency

From (1212) we learned that matrix inequality $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0$ is a necessary test for D to be an EDM. In §5.9.1, the connection between convex polyhedra and EDMs was pronounced by the *EDM assertion*; the matrix inequality together with $D\in\mathbb{S}_h^N$ became a sufficient test when the *EDM assertion* demanded that every bounded convex polyhedron have a corresponding EDM. For all $N>1$ (§5.8.3), the matrix criteria for the existence of an EDM in (1068), (1236), and (1044) are therefore necessary and sufficient and subsume all the Euclidean metric properties and further requirements.

Now we apply the necessary and sufficient EDM criteria (1068) to an earlier problem:

[5.48] The antisymmetric part $(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} - (-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}})^{\mathrm{T}})/2$ 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 $(A+A^{\mathrm{T}})/2$ survives the test $y^{\mathrm{T}}Ay\geq 0$. [233, §7.1]
[5.49] $A^{\mathrm{T}}=A\succeq 0 \;\Leftrightarrow\; A=R^{\mathrm{T}}R$ for some real matrix R. [374, §6.3]

5.9.2.0.1 Example. *Small completion problem,* III. (*confer* §5.8.3.1.1)
Continuing Example 5.3.0.0.2 pertaining to Figure **143** where $N=4$, distance-square d_{14} is ascertainable from the matrix inequality $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0$. Because all distances in (1041) are known except $\sqrt{d_{14}}$, we may simply calculate the smallest eigenvalue of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ over a range of d_{14} as in Figure **159**. We observe a unique value of d_{14} satisfying (1068) where the abscissa axis is tangent to the hypograph of the smallest eigenvalue. Since the smallest eigenvalue of a symmetric matrix is known to be a concave function (§5.8.4), we calculate its second partial derivative with respect to d_{14} evaluated at 2 and find $-1/3$. We conclude there are no other satisfying values of d_{14}. Further, that value of d_{14} does not meet an upper or lower bound of a triangle inequality like (1224), so neither does it cause collapse of any triangle. Because the smallest eigenvalue is 0, affine dimension r of any point list corresponding to D cannot exceed $N-2$. (§5.7.1.1) □

5.10 EDM-entry composition

Laurent [269, §2.3] applies results from Schoenberg, 1938 [356], to show certain nonlinear compositions of individual EDM entries yield EDMs; in particular,

$$\begin{aligned} D\in\mathbb{EDM}^N \;&\Leftrightarrow\; [1-e^{-\alpha\, d_{ij}}]\in\mathbb{EDM}^N \quad \forall\,\alpha>0 \qquad \text{(a)}\\ &\Leftrightarrow\; [e^{-\alpha\, d_{ij}}]\in\mathcal{E}^N \qquad\qquad \forall\,\alpha>0 \qquad \text{(b)}\end{aligned} \tag{1253}$$

where $D=[d_{ij}]$ and $\mathcal{E}^N$ is the elliptope (1237).

5.10.0.0.1 Proof. (Monique Laurent, 2003) [356] (*confer* [259])

Lemma 2.1. from *A Tour d'Horizon ... on Completion Problems.* [269]
For $D=[d_{ij}\,,\; i,j=1\dots N]\in\mathbb{S}_h^N$ and $\mathcal{E}^N$ the elliptope in $\mathbb{S}^N$ (§5.9.1.0.1), the following assertions are equivalent:

(i) $D\in\mathbb{EDM}^N$

(ii) $e^{-\alpha D}\triangleq[e^{-\alpha d_{ij}}]\in\mathcal{E}^N$ for all $\alpha>0$

(iii) $\mathbf{1}\mathbf{1}^{\mathrm{T}}-e^{-\alpha D}\triangleq[1-e^{-\alpha d_{ij}}]\in\mathbb{EDM}^N$ for all $\alpha>0$ ◇

1) Equivalence of Lemma 2.1 (i) (ii) is stated in Schoenberg's Theorem 1 [356, p.527].

2) (ii) ⇒ (iii) can be seen from the statement in the beginning of section 3, saying that a distance space embeds in L_2 iff some associated matrix is PSD. We reformulate it:

Let $d=(d_{ij})_{i,j=0,1\dots N}$ be a distance space on $N+1$ points (*i.e,* symmetric hollow matrix of order $N+1$) and let $p=(p_{ij})_{i,j=1\dots N}$ be the symmetric matrix of order N related by:

(A) $2p_{ij}=d_{0i}+d_{0j}-d_{ij}$ for $i,j=1\dots N$

or equivalently

(B) $d_{0i}=p_{ii}\;,\quad d_{ij}=p_{ii}+p_{jj}-2p_{ij}$ for $i,j=1\dots N$

Then d embeds in L_2 iff p is a positive semidefinite matrix iff d is of negative type (second half page 525/top of page 526 in [356]).

For the implication from (ii) to (iii), set: $p=e^{-\alpha d}$ and define d' from p using (B) above. Then d' is a distance space on $N+1$ points that embeds in L_2. Thus its subspace of N points also embeds in L_2 and is precisely $1-e^{-\alpha d}$.

Note that (iii) ⇒ (ii) cannot be read immediately from this argument since (iii) involves the subdistance of d' on N points (and not the full d' on $N+1$ points).

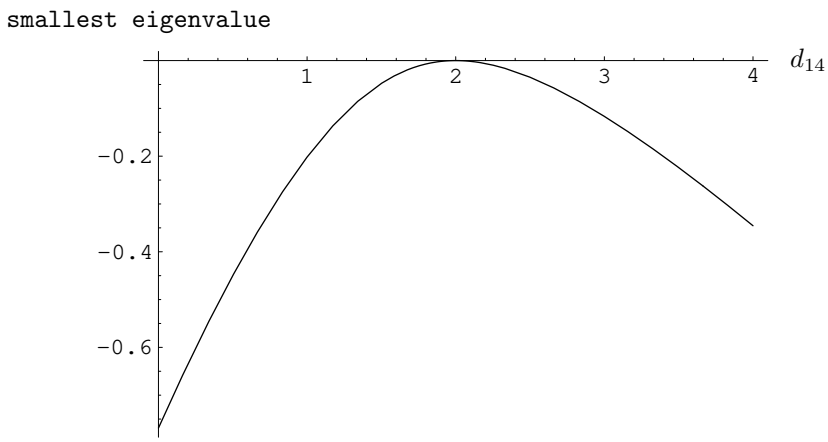


Figure 159: Smallest eigenvalue of $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ makes it a PSD matrix for only one value of d_{14}: 2.

(a)

(b)

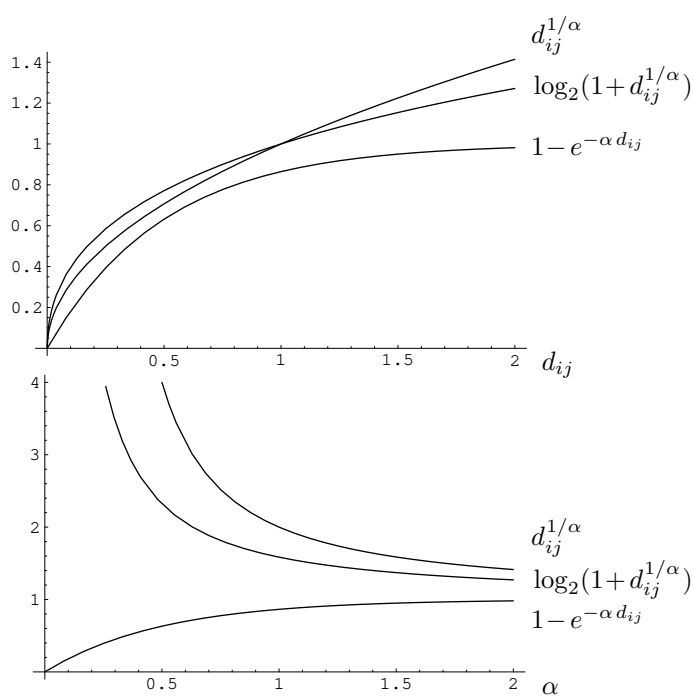


Figure 160: Some entrywise EDM compositions: **(a)** $\alpha = 2$. Concave nondecreasing in d_{ij}. **(b)** Trajectory convergence in α for $d_{ij} = 2$.

3) Show (iii) $\Rightarrow$ (i) by using the series expansion of the function $1-e^{-\alpha d}$: the constant term cancels, α factors out; there remains a summation of d plus a multiple of α. Letting α go to 0 gives the result.

This is not explicitly written in Schoenberg, but he also uses such an argument; expansion of the exponential function then $\alpha \to 0$ (first proof on [356, p.526]). ♦

Schoenberg's results [356, §6 thm.5] (*confer* [259, p.108-109]) also suggest certain finite positive roots of EDM entries produce EDMs; specifically,

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; [d_{ij}^{1/\alpha}] \in \mathbb{EDM}^N \quad \forall\, \alpha > 1 \tag{1254}$$

The special case $\alpha = 2$ is of interest because it corresponds to absolute distance; *e.g*,

$$D \in \mathbb{EDM}^N \Rightarrow \sqrt[\circ]{D} \in \mathbb{EDM}^N \tag{1255}$$

Assuming that points constituting a corresponding list X are distinct (1216), then it follows: for $D \in \mathbb{S}_h^N$

$$\lim_{\alpha\to\infty} [d_{ij}^{1/\alpha}] \;=\; \lim_{\alpha\to\infty} [1 - e^{-\alpha\, d_{ij}}] \;=\; -E \;\triangleq\; \mathbf{1}\mathbf{1}^{\mathrm{T}} - I \tag{1256}$$

Negative elementary matrix $-E$ (§B.3) is: relatively interior to the EDM cone (§6.5), on its axis, and terminal to respective trajectories (1253a) and (1254) as functions of α. Both trajectories are confined to the EDM cone; in engineering terms, the EDM cone is an *invariant set* [352] to either trajectory. Further, if D is not an EDM but for some particular α_{p} it becomes an EDM, then for all greater values of α it remains an EDM.

5.10.0.0.2 Exercise. *Concave nondecreasing EDM-entry composition.*
Given EDM $D = [d_{ij}]$, empirical evidence suggests that the composition $[\log_2(1 + d_{ij}^{1/\alpha})]$ is also an EDM for each fixed $\alpha \geq 1$ [*sic*]. Its concavity in d_{ij} is illustrated in Figure **160** together with functions from (1253a) and (1254). Prove whether it holds more generally: Any concave nondecreasing composition of individual EDM entries d_{ij} on $\mathbb{R}_+$ produces another EDM. ▼

5.10.0.0.3 Exercise. *Taxicab distance matrix as EDM.*
Determine whether taxicab distance matrices $(\mathbf{D}_1(X)$ in Example 3.10.0.0.2$)$ are all numerically equivalent to EDMs. Explain why or why not. ▼

5.10.1 EDM by elliptope

(*confer* (1075)) For some $\kappa \in \mathbb{R}_+$ and $C \in \mathbb{S}_+^N$ in elliptope $\mathcal{E}^N$ (§5.9.1.0.1), Alfakih asserts: any given EDM D is expressible [10] [127, §31.5]

$$D = \kappa(\mathbf{1}\mathbf{1}^{\mathrm{T}} - C) \in \mathbb{EDM}^N \tag{1257}$$

This expression exhibits nonlinear combination of variables κ and C. We therefore propose a different expression requiring redefinition of the elliptope (1237) by scalar parametrization;

$$\mathcal{E}_t^n \triangleq \mathbb{S}_+^n \cap \{\Phi \in \mathbb{S}^n \mid \delta(\Phi) = t\,\mathbf{1}\} \tag{1258}$$

where, of course, $\mathcal{E}^n = \mathcal{E}_1^n$. Then any given EDM D is expressible

$$D = t\mathbf{1}\mathbf{1}^{\mathrm{T}} - \mathfrak{E} \in \mathbb{EDM}^N \tag{1259}$$

which is linear in variables $t \in \mathbb{R}_+$ and $\mathfrak{E} \in \mathcal{E}_t^N$.

5.11 EDM indefiniteness

By known result (§A.7.2) regarding a 0-valued entry on the main diagonal of a symmetric positive semidefinite matrix, there can be no positive or negative semidefinite EDM except the $\mathbf{0}$ matrix because $\mathbb{EDM}^N \subseteq \mathbb{S}_h^N$ (1048) and

$$\mathbb{S}_h^N \cap \mathbb{S}_+^N = \mathbf{0} \tag{1260}$$

the origin. So when $D \in \mathbb{EDM}^N$, there can be no factorization $D = A^{\mathrm{T}}A$ or $-D = A^{\mathrm{T}}A$. [374, §6.3] Hence eigenvalues of an EDM are neither all nonnegative or all nonpositive; an EDM is indefinite and possibly invertible.

5.11.1 EDM eigenvalues, congruence transformation

For any symmetric $-D$, we can characterize its eigenvalues by congruence transformation: [374, §6.3]

$$-W^{\mathrm{T}}DW \;=\; -\begin{bmatrix} V_{\mathcal{N}}^{\mathrm{T}} \\ \mathbf{1}^{\mathrm{T}} \end{bmatrix} D \begin{bmatrix} V_{\mathcal{N}} & \mathbf{1} \end{bmatrix} \;=\; -\begin{bmatrix} V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} & V_{\mathcal{N}}^{\mathrm{T}}D\mathbf{1} \\ \mathbf{1}^{\mathrm{T}}DV_{\mathcal{N}} & \mathbf{1}^{\mathrm{T}}D\mathbf{1} \end{bmatrix} \in \mathbb{S}^N \tag{1261}$$

Because

$$W \triangleq \begin{bmatrix} V_{\mathcal{N}} & \mathbf{1} \end{bmatrix} \in \mathbb{R}^{N\times N} \tag{1262}$$

is full-rank, then (1684)

$$\operatorname{inertia}(-D) = \operatorname{inertia}\big(-W^{\mathrm{T}}DW\big) \tag{1263}$$

the congruence (1261) has the same number of positive, zero, and negative eigenvalues as $-D$. Further, if we denote by $\{\gamma_i\,,\; i=1\dots N-1\}$ the eigenvalues of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ and denote eigenvalues of the congruence $-W^{\mathrm{T}}DW$ by $\{\zeta_i\,,\; i=1\dots N\}$ and if we arrange each respective set of eigenvalues in nonincreasing order, then by theory of *interlacing eigenvalues for bordered symmetric matrices* [233, §4.3] [374, §6.4] [370, §IV.4.1]

$$\zeta_N \le \gamma_{N-1} \le \zeta_{N-1} \le \gamma_{N-2} \le \cdots \le \gamma_2 \le \zeta_2 \le \gamma_1 \le \zeta_1 \tag{1264}$$

When $D \in \mathbb{EDM}^N$, then $\gamma_i \ge 0\;\forall\, i$ (1620) because $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \succeq 0$ as we know. That means the congruence must have $N-1$ nonnegative eigenvalues; $\zeta_i \ge 0$, $i=1\dots N-1$. The remaining eigenvalue ζ_N cannot be nonnegative because then $-D$ would be positive semidefinite, an impossibility; so $\zeta_N < 0$. By congruence, nontrivial $-D$ must therefore have exactly one negative eigenvalue;[5.50] [127, §2.4.5]

$$D \in \mathbb{EDM}^N \Rightarrow \begin{cases} \lambda(-D)_i \;\ge\; 0\,, \quad i=1\dots N-1 \\ \left(\sum\limits_{i=1}^{N} \lambda(-D)_i = 0\right) \\ D \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N\times N} \end{cases} \tag{1265}$$

where the $\lambda(-D)_i$ are nonincreasingly ordered eigenvalues of $-D$ whose sum must be 0 only because $\operatorname{tr} D = 0$ [374, §5.1]. The eigenvalue summation condition, therefore, can be considered redundant. Even so, all these conditions are insufficient to determine whether some given $H \in \mathbb{S}_h^N$ is an EDM; as shown by counterexample.[5.51]

[5.50] All entries of the corresponding eigenvector must have the same sign, with respect to each other, [98, p.116] because that eigenvector is the *Perron vector* corresponding to *spectral radius*; [233, §8.3.1] the predominant characteristic of square nonnegative matrices. Unlike positive semidefinite matrices, nonnegative matrices are guaranteed only to have at least one nonnegative eigenvalue.

[5.51] When $N=3$, for example, the symmetric hollow matrix

$$H = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 5 \\ 1 & 5 & 0 \end{bmatrix} \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N\times N}$$

5.11.1.0.1 Exercise. *Spectral inequality.*
Prove whether it holds: for $D=[d_{ij}]\in\mathbb{EDM}^N$

$$\lambda(-D)_1 \geq d_{ij} \geq \lambda(-D)_{N-1} \qquad \forall\, i\neq j \tag{1266}$$

▼

5.11.1.0.2 Definition. *Spectral cone $\mathcal{K}_\lambda$.*
A convex cone containing all *eigenspectra* corresponding to some given set of matrices is called a *spectral cone.* △

5.11.1.0.3 Definition. *Eigenspectrum.* [259, p.365] [370, p.26] (*confer* §A.5.0.1)
The eigenvalues of a matrix, including duplicates, are referred to as its *eigenspectrum.* △

Any positive semidefinite matrix, for example, possesses a vector (or nonincreasing list) of nonnegative eigenvalues corresponding to an eigenspectrum contained in a spectral cone $\mathcal{K}_\lambda$ that is a nonnegative orthant (or monotone nonnegative cone).

5.11.2 Spectral cones $\mathcal{K}_\lambda$ for distance matrices

Denoting the eigenvalues of Cayley-Menger matrix $\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\in\mathbb{S}^{N+1}$ by

$$\lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\right)\in\mathbb{R}^{N+1} \tag{1267}$$

we have the Cayley-Menger form (§5.7.3.0.1) of necessary and sufficient conditions for $D\in\mathbb{EDM}^N$ from the literature: [215, §3][5.52] [81, §3] [127, §6.2] (*confer* (1068) (1044))

$$D\in\mathbb{EDM}^N \Leftrightarrow \left\{\begin{array}{l} \lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\right)_i \geq 0\,, \quad i=1\ldots N \\ D\in\mathbb{S}_h^N \end{array}\right\} \Leftrightarrow \left\{\begin{array}{c} -V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0 \\ D\in\mathbb{S}_h^N \end{array}\right. \tag{1268}$$

These conditions say the Cayley-Menger form has one and only one negative eigenvalue. When D is an EDM, eigenvalues $\lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\right)$ belong to that particular orthant in $\mathbb{R}^{N+1}$ having the $N+1^{\mathrm{th}}$ coordinate as sole negative coordinate:[5.53]

$$\begin{bmatrix} \mathbb{R}_+^N \\ \mathbb{R}_- \end{bmatrix} = \operatorname{cone}\{e_1\,,\ e_2\,,\ \cdots\ e_N\,,\ -e_{N+1}\} \tag{1269}$$

5.11.2.1 Cayley-Menger *versus* Schoenberg

Connection to the Schoenberg criterion (1068) is made when the Cayley-Menger form is further partitioned:

$$\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} \mathbf{1}^{\mathrm{T}} \\ -D_{1,\,2:N} \end{bmatrix} \\ [\,\mathbf{1} \quad -D_{2:N,\,1}\,] & -D_{2:N,\,2:N} \end{bmatrix} \tag{1270}$$

is not an EDM, although $\lambda(-H)=[5\ \ 0.3723\ \ -5.3723]^{\mathrm{T}}$ conforms to (1265).

[5.52] Recall: for $D\in\mathbb{S}_h^N$, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0$ subsumes nonnegativity property 1 (§5.8.1).

[5.53] Empirically, all except one entry of the corresponding eigenvector have the same sign with respect to each other.

Matrix $D \in \mathbb{S}_h^N$ is an EDM if and only if the Schur complement of $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ (§A.4) in this partition is positive semidefinite; [19, §1] [249, §3] *id est*, (*confer* (1214))

$$\begin{gathered} D \in \mathbb{EDM}^N \\ \Leftrightarrow \\ -D_{2:N,\,2:N} - [\,\mathbf{1} \quad -D_{2:N,\,1}\,] \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{1}^{\mathrm{T}} \\ -D_{1,\,2:N} \end{bmatrix} = -2V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0 \\ \textbf{and} \\ D \in \mathbb{S}_h^N \end{gathered} \tag{1271}$$

Positive semidefiniteness of that Schur complement insures nonnegativity ($D \in \mathbb{R}_+^{N\times N}$, §5.8.1), whereas *complementary inertia* (1686) insures existence of that lone negative eigenvalue of the Cayley-Menger form.

Now we apply results from chapter 2 with regard to polyhedral cones and their duals.

5.11.2.2 Ordered eigenspectra

Conditions (1268) specify eigenvalue membership to $\mathcal{K}_\lambda$ the smallest pointed polyhedral *spectral cone* for $\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix}$:

$$\begin{aligned} \mathcal{K}_\lambda &\triangleq \{\zeta \in \mathbb{R}^{N+1} \mid \zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_N \geq 0 \geq \zeta_{N+1}\,,\ \mathbf{1}^{\mathrm{T}}\zeta = 0\} \\ &= \mathcal{K}_{\mathcal{M}} \cap \begin{bmatrix} \mathbb{R}_+^N \\ \mathbb{R}_- \end{bmatrix} \cap \partial\mathcal{H} \\ &= \lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix}\right) \end{aligned} \tag{1272}$$

where

$$\partial\mathcal{H} \triangleq \{\zeta \in \mathbb{R}^{N+1} \mid \mathbf{1}^{\mathrm{T}}\zeta = 0\} \tag{1273}$$

is a hyperplane through the origin, and $\mathcal{K}_{\mathcal{M}}$ is the monotone cone (§2.13.10.4.3, implying ordered eigenspectra) which is full-dimensional but is not pointed;

$$\mathcal{K}_{\mathcal{M}} = \{\zeta \in \mathbb{R}^{N+1} \mid \zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_{N+1}\} \qquad (445)$$

$$\mathcal{K}_{\mathcal{M}}^* = \{[\,e_1 - e_2 \quad e_2 - e_3 \quad \cdots \quad e_N - e_{N+1}\,]\,a \mid a \succeq 0\} \subset \mathbb{R}^{N+1} \qquad (446)$$

So because of the hyperplane,

$$\dim \operatorname{aff} \mathcal{K}_\lambda \;=\; \dim \partial\mathcal{H} \;=\; N \tag{1274}$$

indicating that spectral cone $\mathcal{K}_\lambda$ is not full-dimensional. Defining

$$A \triangleq \begin{bmatrix} e_1^{\mathrm{T}} - e_2^{\mathrm{T}} \\ e_2^{\mathrm{T}} - e_3^{\mathrm{T}} \\ \vdots \\ e_N^{\mathrm{T}} - e_{N+1}^{\mathrm{T}} \end{bmatrix} \in \mathbb{R}^{N\times N+1}, \qquad B \triangleq \begin{bmatrix} e_1^{\mathrm{T}} \\ e_2^{\mathrm{T}} \\ \vdots \\ e_N^{\mathrm{T}} \\ -e_{N+1}^{\mathrm{T}} \end{bmatrix} \in \mathbb{R}^{N+1\times N+1} \tag{1275}$$

we have the halfspace-description:

$$\mathcal{K}_\lambda \;=\; \{\zeta \in \mathbb{R}^{N+1} \mid A\zeta \succeq 0\,,\ B\zeta \succeq 0\,,\ \mathbf{1}^{\mathrm{T}}\zeta = 0\} \tag{1276}$$

From this and (453) we get a vertex-description for a pointed spectral cone that is not full-dimensional:

$$\mathcal{K}_\lambda = \left\{ V_\mathcal{N} \left(\begin{bmatrix} \hat{A} \\ \hat{B} \end{bmatrix} V_\mathcal{N} \right)^\dagger b \mid b \succeq 0 \right\} \tag{1277}$$

where $V_\mathcal{N} \in \mathbb{R}^{N+1\times N}$, and where [*sic*]

$$\hat{B} = e_N^\mathrm{T} \in \mathbb{R}^{1\times N+1} \tag{1278}$$

and

$$\hat{A} = \begin{bmatrix} e_1^\mathrm{T} - e_2^\mathrm{T} \\ e_2^\mathrm{T} - e_3^\mathrm{T} \\ \vdots \\ e_{N-1}^\mathrm{T} - e_N^\mathrm{T} \end{bmatrix} \in \mathbb{R}^{N-1\times N+1} \tag{1279}$$

hold those rows of A and B corresponding to conically independent rows (§2.10) in $\begin{bmatrix} A \\ B \end{bmatrix} V_\mathcal{N}$.

Conditions (1268) can be equivalently restated in terms of a spectral cone for Euclidean distance matrices:

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \begin{cases} \lambda\left(\begin{bmatrix} 0 & \mathbf{1}^\mathrm{T} \\ \mathbf{1} & -D \end{bmatrix} \right) \in \mathcal{K}_\mathcal{M} \cap \begin{bmatrix} \mathbb{R}_+^N \\ \mathbb{R}_- \end{bmatrix} \cap \partial\mathcal{H} \\ D \in \mathbb{S}_h^N \end{cases} \tag{1280}$$

Vertex-description of the dual spectral cone is, (323)

$$\begin{aligned} \mathcal{K}_\lambda^* &= \overline{\mathcal{K}_\mathcal{M}^* + \begin{bmatrix} \mathbb{R}_+^N \\ \mathbb{R}_- \end{bmatrix}^* + \partial\mathcal{H}^*} \subseteq \mathbb{R}^{N+1} \\ &= \left\{ \begin{bmatrix} A^\mathrm{T} & B^\mathrm{T} & \mathbf{1} & -\mathbf{1} \end{bmatrix} b \mid b \succeq 0 \right\} = \left\{ \begin{bmatrix} \hat{A}^\mathrm{T} & \hat{B}^\mathrm{T} & \mathbf{1} & -\mathbf{1} \end{bmatrix} a \mid a \succeq 0 \right\} \end{aligned} \tag{1281}$$

From (1277) and (454) we get a halfspace-description:

$$\mathcal{K}_\lambda^* = \{ y \in \mathbb{R}^{N+1} \mid (V_\mathcal{N}^\mathrm{T} [\, \hat{A}^\mathrm{T} \;\; \hat{B}^\mathrm{T} \,])^\dagger V_\mathcal{N}^\mathrm{T} y \succeq 0 \} \tag{1282}$$

This polyhedral dual spectral cone $\mathcal{K}_\lambda^*$ is closed, convex, full-dimensional because $\mathcal{K}_\lambda$ is pointed, but is not pointed because $\mathcal{K}_\lambda$ is not full-dimensional.

5.11.2.3 Unordered eigenspectra

Spectral cones are not unique; eigenspectra ordering can be rendered benign within a cone by presorting a vector of eigenvalues into nonincreasing order.[5.54] Then things simplify: Conditions (1268) now specify eigenvalue membership to the spectral cone

$$\begin{aligned} \lambda\left(\begin{bmatrix} 0 & \mathbf{1}^\mathrm{T} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix} \right) &= \begin{bmatrix} \mathbb{R}_+^N \\ \mathbb{R}_- \end{bmatrix} \cap \partial\mathcal{H} \\ &= \{ \zeta \in \mathbb{R}^{N+1} \mid B\zeta \succeq 0 \,,\; \mathbf{1}^\mathrm{T}\zeta = 0 \} \end{aligned} \tag{1283}$$

[5.54] Eigenspectra ordering (represented by a cone having monotone description such as (1272)) becomes benign in (1495), for example, where projection of a given presorted vector on the nonnegative orthant in a subspace is equivalent to its projection on the monotone nonnegative cone in that same subspace; equivalence is a consequence of presorting.

where B is defined in (1275), and $\partial\mathcal{H}$ in (1273). From (453) we get a vertex-description for a pointed spectral cone not full-dimensional:

$$\begin{aligned}\lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix}\right) &= \left\{V_{\mathcal{N}}(\tilde{B}V_{\mathcal{N}})^{\dagger}\, b \mid b \succeq 0\right\} \\ &= \left\{\begin{bmatrix} I \\ -\mathbf{1}^{\mathrm{T}} \end{bmatrix} b \mid b \succeq 0\right\}\end{aligned} \tag{1284}$$

where $V_{\mathcal{N}} \in \mathbb{R}^{N+1\times N}$ and

$$\tilde{B} \triangleq \begin{bmatrix} e_1^{\mathrm{T}} \\ e_2^{\mathrm{T}} \\ \vdots \\ e_N^{\mathrm{T}} \end{bmatrix} \in \mathbb{R}^{N\times N+1} \tag{1285}$$

holds only those rows of B corresponding to conically independent rows in $BV_{\mathcal{N}}$.

For presorted eigenvalues, (1268) can be equivalently restated

$$D \in \mathbb{EDM}^N \;\Leftrightarrow\; \begin{cases} \lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D \end{bmatrix}\right) \in \begin{bmatrix} \mathbb{R}^N_+ \\ \mathbb{R}_- \end{bmatrix} \cap \partial\mathcal{H} \\ D \in \mathbb{S}^N_h \end{cases} \tag{1286}$$

Vertex-description of the dual spectral cone is, (323)

$$\begin{aligned}\lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix}\right)^* &= \begin{bmatrix} \mathbb{R}^N_+ \\ \mathbb{R}_- \end{bmatrix} + \partial\mathcal{H}^* \subseteq \mathbb{R}^{N+1} \\ &= \left\{\begin{bmatrix} B^{\mathrm{T}} & \mathbf{1} & -\mathbf{1}\end{bmatrix} b \mid b \succeq 0\right\} = \left\{\begin{bmatrix} \tilde{B}^{\mathrm{T}} & \mathbf{1} & -\mathbf{1}\end{bmatrix} a \mid a \succeq 0\right\}\end{aligned} \tag{1287}$$

From (454) we get a halfspace-description:

$$\begin{aligned}\lambda\left(\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbb{EDM}^N \end{bmatrix}\right)^* &= \{y \in \mathbb{R}^{N+1} \mid (V_{\mathcal{N}}^{\mathrm{T}}\tilde{B}^{\mathrm{T}})^{\dagger}\, V_{\mathcal{N}}^{\mathrm{T}} y \succeq 0\} \\ &= \{y \in \mathbb{R}^{N+1} \mid [\,I \;\; -\mathbf{1}\,]\, y \succeq 0\}\end{aligned} \tag{1288}$$

This polyhedral dual spectral cone is closed, convex, full-dimensional but not pointed.[5.55]

5.11.2.4 Dual cone *versus* dual spectral cone

An open question regards the relationship of convex cones and their duals to the corresponding spectral cones and their duals. A positive semidefinite cone, for example, is selfdual. Both the nonnegative orthant and the monotone nonnegative cone are spectral cones for it. When we consider the nonnegative orthant, then that spectral cone for the selfdual positive semidefinite cone is also selfdual.

5.12 List reconstruction

The term *metric multidimensional scaling*[5.56] [292] [119] [400] [117] [296] [98] refers to any reconstruction of a list $X \in \mathbb{R}^{n\times N}$ in Euclidean space from interpoint distance information, possibly incomplete (§6.7), ordinal (§5.13.2), or specified perhaps only by

[5.55] Notice that any nonincreasingly ordered eigenspectrum belongs to this dual spectral cone.

[5.56] Scaling [396] *means making a scale,* i.e, *a numerical representation of qualitative data. If the scale is multidimensional, it's* multidimensional scaling. —Jan de Leeuw
In one dimension, N coordinates in X define the scale; *e.g*, §7.2.2.7.1.

bounding-constraints (§5.4.2.2.12) [398]. Techniques for reconstruction are essentially methods for optimally embedding an unknown list of points, corresponding to given Euclidean distance data, in an affine subset of desired or minimum dimension. The oldest known precursor is called *principal component analysis* [193] which analyzes the correlation matrix (§5.9.1.0.1); [57, §22] `a.k.a,` *Karhunen-Loéve transform* in digital signal processing literature.

A goal of multidimensional scaling is to find a low-dimensional representation of list X so that distances between its elements best preserve a given set of pairwise dissimilarities. *Dissimilarity* is some measure or perception of unlikeness. *Similarity* between vectors (in Euclidean space) is measured by inner product, [334, §2] whereas dissimilarity is measured by distance-square.[5.57] When dissimilarity data comprises measurable distances, then reconstruction is termed *metric* multidimensional scaling.

Isometric reconstruction (§5.5.3) of point list X is best performed by eigenvalue decomposition of a Gram matrix; for then, numerical errors of factorization are easily spotted in the eigenvalues: Now we consider how rotation/reflection and translation invariance factor into a reconstruction.

5.12.1 x_1 at the origin. $V_{\mathcal{N}}$

At the stage of reconstruction, we have $D \in \mathbb{EDM}^N$ and wish to find a generating list (§2.3.2) for polyhedron $\mathcal{P} - \alpha$ by factoring Gram matrix $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ (1066) as in (1251). One way to factor $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ is via diagonalization of symmetric matrices; [374, §5.6] [233] (§A.5.1, §A.3)

$$-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \triangleq Q \Lambda Q^{\mathrm{T}} \tag{1289}$$

$$Q \Lambda Q^{\mathrm{T}} \succeq 0 \;\Leftrightarrow\; \Lambda \succeq 0 \tag{1290}$$

where $Q \in \mathbb{R}^{N-1 \times N-1}$ is an orthogonal matrix containing eigenvectors while $\Lambda \in \mathbb{S}^{N-1}$ is a diagonal matrix containing corresponding nonnegative eigenvalues ordered by nonincreasing value. From the diagonalization, identify the list using (1196);

$$-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \;=\; 2 V_{\mathcal{N}}^{\mathrm{T}} X^{\mathrm{T}} X V_{\mathcal{N}} \;\triangleq\; Q \sqrt{\Lambda}\, Q_{\mathrm{p}}^{\mathrm{T}} Q_{\mathrm{p}} \sqrt{\Lambda}\, Q^{\mathrm{T}} \tag{1291}$$

where $\sqrt{\Lambda}\, Q_{\mathrm{p}}^{\mathrm{T}} Q_{\mathrm{p}} \sqrt{\Lambda} \triangleq \Lambda = \sqrt{\Lambda}\sqrt{\Lambda}$ and where $Q_{\mathrm{p}} \in \mathbb{R}^{n \times N-1}$ is unknown as is its dimension n. Rotation/reflection is accounted for by Q_{p} yet only its first r columns are necessarily orthonormal.[5.58] Assuming membership to the unit simplex $y \in \mathcal{S}$ (1248), then point $p = X\sqrt{2} V_{\mathcal{N}}\, y = Q_{\mathrm{p}} \sqrt{\Lambda}\, Q^{\mathrm{T}} y$ in $\mathbb{R}^n$ belongs to the translated polyhedron

$$\mathcal{P} - x_1 \tag{1292}$$

whose generating list constitutes the columns of (1190)

$$\begin{aligned} \begin{bmatrix} \mathbf{0} & X\sqrt{2} V_{\mathcal{N}} \end{bmatrix} &= \begin{bmatrix} \mathbf{0} & Q_{\mathrm{p}} \sqrt{\Lambda}\, Q^{\mathrm{T}} \end{bmatrix} \in \mathbb{R}^{n \times N} \\ &= \begin{bmatrix} \mathbf{0} & x_2 - x_1 & x_3 - x_1 & \cdots & x_N - x_1 \end{bmatrix} \end{aligned} \tag{1293}$$

The scaled auxiliary matrix $V_{\mathcal{N}}$ represents that translation. A simple choice for Q_{p} has n set to $N-1$; *id est*, $Q_{\mathrm{p}} = I$. Ideally, each member of the generating list has at most r nonzero entries; r being, affine dimension

$$\operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \;=\; \operatorname{rank} Q_{\mathrm{p}} \sqrt{\Lambda}\, Q^{\mathrm{T}} \;=\; \operatorname{rank} \Lambda \;=\; r \tag{1294}$$

[5.57] This sense reversal is analogous to autocorrelation *versus* total power of lagged differences in digital signal processing. [106, p.9]

[5.58] Recall r signifies affine dimension. Q_{p} is not necessarily an orthogonal matrix. Q_{p} is constrained such that only its first r columns are necessarily orthonormal because there are only r nonzero eigenvalues in Λ when $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ has rank r (§5.7.1.1). Remaining columns of Q_{p} are arbitrary.

Each member then has at least $N-1-r$ zeros in its higher-dimensional coordinates because $r \leq N-1$. (1202) To truncate those zeros, choose n equal to affine dimension which is the smallest n possible because $XV_{\mathcal{N}}$ has rank $r \leq n$ (1198).[5.59] In that case, the simplest choice for Q_{p} is $[\,I \;\; \mathbf{0}\,]$ having dimension $r \times N-1$.

We may wish to verify the list (1293) found from the diagonalization of $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$. Because of rotation/reflection and translation invariance (§5.5), EDM D can be uniquely made from that list by calculating: (1049)

$$\mathbf{D}(X) \;=\; \mathbf{D}(X[\,\mathbf{0} \;\; \sqrt{2}V_{\mathcal{N}}\,]) \;=\; \mathbf{D}(Q_{\mathrm{p}}[\,\mathbf{0} \;\; \sqrt{\Lambda}\,Q^{\mathrm{T}}\,]) \;=\; \mathbf{D}([\,\mathbf{0} \;\; \sqrt{\Lambda}\,Q^{\mathrm{T}}\,]) \tag{1295}$$

This suggests a way to find EDM D given $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$ (*confer* (1174))

$$D = \begin{bmatrix} 0 \\ \delta\big(-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}\big) \end{bmatrix} \mathbf{1}^{\mathrm{T}} + \mathbf{1}\begin{bmatrix} 0 & \delta\big(-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}\big)^{\mathrm{T}} \end{bmatrix} - 2\begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & -V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \end{bmatrix} \tag{1170}$$

5.12.2 0 geometric center. V

Alternatively we may perform reconstruction using auxiliary matrix V (§B.4.1) and Gram matrix $-VDV\frac{1}{2}$ (1070) instead; to find a generating list for polyhedron

$$\mathcal{P} - \alpha_c \tag{1296}$$

whose geometric center α_c has been translated to the origin. Redimensioning diagonalization factors $Q\,,\Lambda \in \mathbb{R}^{N\times N}$ and unknown $Q_{\mathrm{p}} \in \mathbb{R}^{n\times N}$, (1197)

$$-VDV \;=\; 2VX^{\mathrm{T}}XV \;\triangleq\; Q\Lambda Q^{\mathrm{T}} \;\triangleq\; Q\sqrt{\Lambda}\,Q_{\mathrm{p}}^{\mathrm{T}}Q_{\mathrm{p}}\sqrt{\Lambda}\,Q^{\mathrm{T}} \tag{1297}$$

where the geometrically centered generating list constitutes (*confer* (1293))

$$\begin{aligned} XV \;&=\; \tfrac{1}{\sqrt{2}}\,Q_{\mathrm{p}}\sqrt{\Lambda}\,Q^{\mathrm{T}} \in \mathbb{R}^{n\times N} \\ &=\; [\,x_1 - \tfrac{1}{N}X\mathbf{1} \quad x_2 - \tfrac{1}{N}X\mathbf{1} \quad x_3 - \tfrac{1}{N}X\mathbf{1} \quad \cdots \quad x_N - \tfrac{1}{N}X\mathbf{1}\,] \end{aligned} \tag{1298}$$

where $\alpha_c = \frac{1}{N}X\mathbf{1}$. (§5.5.1.0.1) Recall, Q_{p} accounts for list rotation/reflection. The simplest choice for Q_{p} is $[\,I \;\; \mathbf{0}\,] \in \mathbb{R}^{r\times N}$ with affine dimension r.

Now EDM D can be uniquely made from the list found: (1049)

$$\mathbf{D}(X) \;=\; \mathbf{D}(XV) \;=\; \mathbf{D}(\tfrac{1}{\sqrt{2}}\,Q_{\mathrm{p}}\sqrt{\Lambda}\,Q^{\mathrm{T}}) \;=\; \mathbf{D}(\sqrt{\Lambda}\,Q^{\mathrm{T}})\tfrac{1}{2} \tag{1299}$$

This EDM is, of course, identical to (1295). Similarly to (1170), from $-VDV$ we can find EDM D (*confer* (1161))

$$D = \delta(-VDV\tfrac{1}{2})\mathbf{1}^{\mathrm{T}} + \mathbf{1}\,\delta(-VDV\tfrac{1}{2})^{\mathrm{T}} - 2(-VDV\tfrac{1}{2}) \tag{1160}$$

[5.59] If we write $Q^{\mathrm{T}} = \begin{bmatrix} q_1^{\mathrm{T}} \\ \vdots \\ q_{N-1}^{\mathrm{T}} \end{bmatrix}$ as rowwise eigenvectors, $\Lambda = \begin{bmatrix} \lambda_1 & & & & & \mathbf{0} \\ & \ddots & & & & \\ & & \lambda_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ \mathbf{0} & & & & & 0 \end{bmatrix}$ in terms of eigenvalues, and $Q_{\mathrm{p}} = [\,q_{\mathrm{p}1} \cdots q_{\mathrm{p}N-1}\,]$ as column vectors, then $Q_{\mathrm{p}}\sqrt{\Lambda}\,Q^{\mathrm{T}} = \sum_{i=1}^{r}\sqrt{\lambda_i}\,q_{\mathrm{p}i}\,q_i^{\mathrm{T}}$ is a sum of r linearly independent rank-1 matrices (§B.1.1). Hence the summation has rank r.

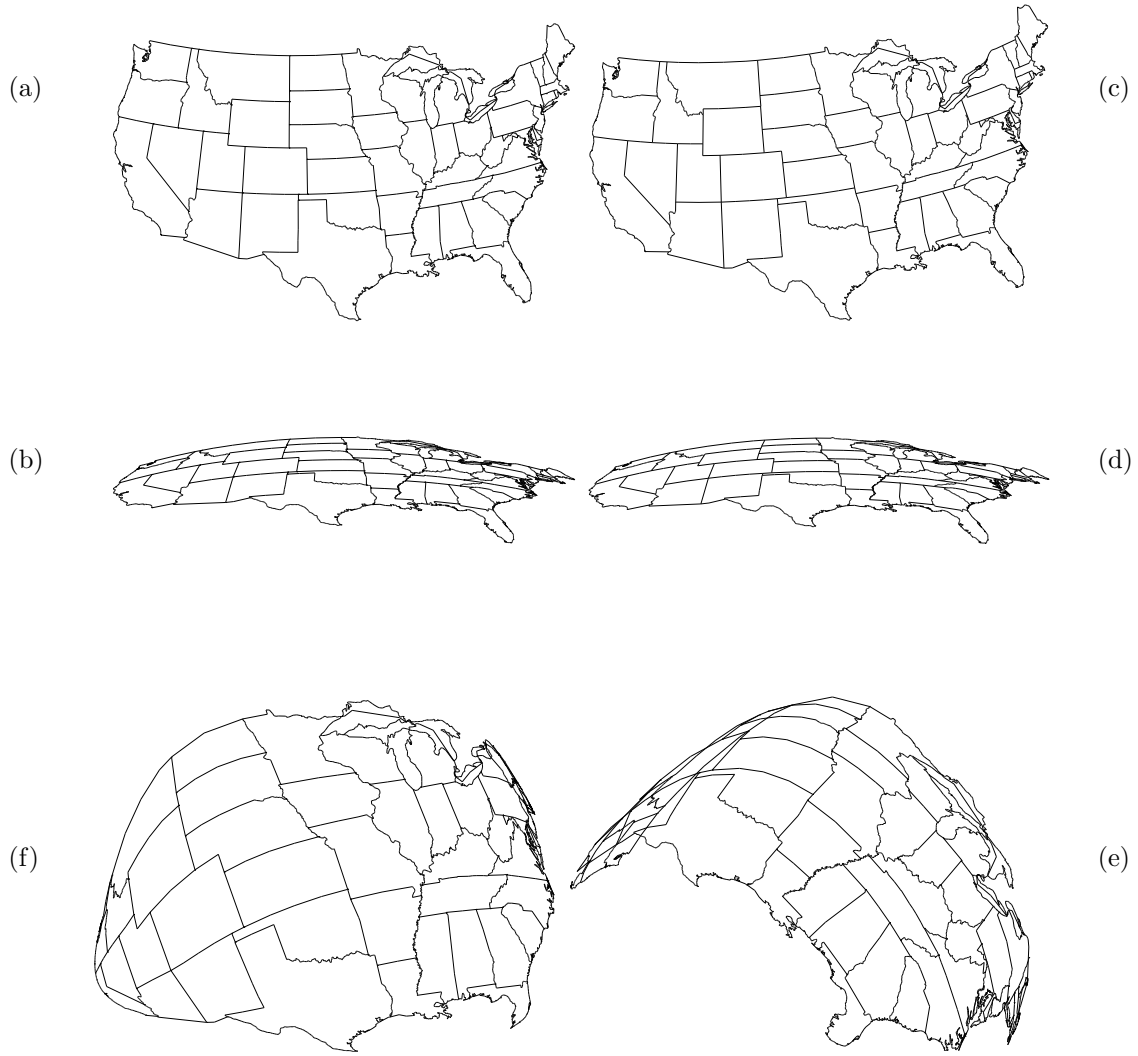


Figure 161: (*confer* Figure 8) Nonconvex map of United States of America showing some state boundaries and the Great Lakes. All plots made by connecting 5020 points. Any difference in scale in (a) through (d) is artifact of plotting routine.
(a) Shows original map made from decimated (latitude, longitude) data.
(b) Original map data rotated (freehand) to highlight curvature of Earth.
(c) Map isometrically reconstructed from an EDM (from distance only).
(d) Same reconstructed map illustrating curvature.
(e)(f) Two views of one isotonic reconstruction (from comparative distance); problem (1309) with no sort constraint $\Pi\,\underline{d}$ (and no hidden line removal).

5.13 Reconstruction examples

5.13.1 Isometric reconstruction

5.13.1.0.1 Example. *Cartography.*
The most fundamental application of EDMs is to reconstruct relative point position given only interpoint distance information. Drawing a map of the United States is a good illustration of isometric reconstruction (§5.4.2.2.10) from complete distance data. We obtained latitude and longitude information for the coast, border, states, and Great Lakes from the *usalo atlas data file* within MATLAB Mapping Toolbox; conversion to Cartesian coordinates (x, y, z) via:

$$\begin{aligned} \phi &\triangleq \pi/2 - \text{latitude} \\ \theta &\triangleq \text{longitude} \\ x &= \sin(\phi)\cos(\theta) \\ y &= \sin(\phi)\sin(\theta) \\ z &= \cos(\phi) \end{aligned} \tag{1300}$$

We used 64% of the available map data to calculate EDM D from $N = 5020$ points. The original (decimated) data and its isometric reconstruction via (1291) are shown in Figure **161**a-d. [430, MATLAB code] The eigenvalues computed for (1289) are

$$\lambda(-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}) = [199.8 \;\; 152.3 \;\; 2.465 \;\; 0 \;\; 0 \;\; 0 \;\cdots\;]^{\mathrm{T}} \tag{1301}$$

The 0 eigenvalues have absolute numerical error on the order of `2E-13`; meaning, the EDM data indicates three dimensions ($r = 3$) are required for reconstruction to nearly machine precision. □

5.13.2 Isotonic reconstruction

Sometimes only comparative information about distance is known (Earth is closer to the Moon than it is to the Sun). Suppose, for example, EDM D for three points is unknown:

$$D = [d_{ij}] = \begin{bmatrix} 0 & d_{12} & d_{13} \\ d_{12} & 0 & d_{23} \\ d_{13} & d_{23} & 0 \end{bmatrix} \in \mathbb{S}_h^{\mathbf{3}} \tag{1038}$$

but comparative distance data is available:

$$d_{13} \geq d_{23} \geq d_{12} \tag{1302}$$

With vectorization $\underline{d} = [d_{12} \; d_{13} \; d_{23}]^{\mathrm{T}} \in \mathbb{R}^{\mathbf{3}}$, we express the comparative data as the nonincreasing sorting

$$\Pi\,\underline{d} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} d_{12} \\ d_{13} \\ d_{23} \end{bmatrix} = \begin{bmatrix} d_{13} \\ d_{23} \\ d_{12} \end{bmatrix} \in \mathcal{K}_{\mathcal{M}+} \tag{1303}$$

where Π is a given permutation matrix expressing known sorting action on the entries of unknown EDM D, and $\mathcal{K}_{\mathcal{M}+}$ is the monotone nonnegative cone (§2.13.10.4.2)

$$\mathcal{K}_{\mathcal{M}+} = \{z \mid z_1 \geq z_2 \geq \cdots \geq z_{N(N-1)/2} \geq 0\} \subseteq \mathbb{R}_+^{N(N-1)/2} \tag{438}$$

where $N(N-1)/2 = 3$ for the present example. From sorted vectorization (1303) we create the *sort-index matrix*

$$O = \begin{bmatrix} 0 & 1^2 & 3^2 \\ 1^2 & 0 & 2^2 \\ 3^2 & 2^2 & 0 \end{bmatrix} \in \mathbb{S}_h^{\mathbf{3}} \cap \mathbb{R}_+^{\mathbf{3}\times\mathbf{3}} \tag{1304}$$

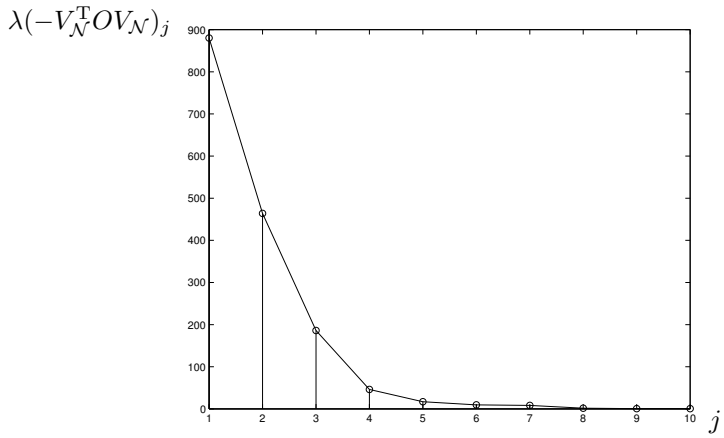


Figure 162: Largest ten eigenvalues, of $-V_{\mathcal{N}}^{\mathrm{T}}OV_{\mathcal{N}}$ for USA map, sorted by decreasing value.

generally defined

$$O_{ij} \triangleq k^2 \mid d_{ij} = (\Xi\,\Pi\,\underline{d})_k \;, \qquad j \neq i \tag{1305}$$

where Ξ is a permutation matrix (1920) completely reversing order of vector entries.

Replacing EDM data with indices-square of a nonincreasing sorting like this is, of course, a heuristic we invented and may be regarded as a nonlinear introduction of much noise into the Euclidean distance matrix. For large data sets, this heuristic makes an otherwise intense problem computationally tractable; we see an example in relaxed problem (1310).

Any process of reconstruction that leaves comparative distance information intact is called *ordinal multidimensional scaling* or *isotonic reconstruction.* Beyond rotation, reflection, and translation error, (§5.5) list reconstruction by isotonic reconstruction is subject to error in absolute scale (*dilation*) and distance ratio. Yet Borg & Groenen argue: [57, §2.2] reconstruction from complete comparative distance information for a large number of points is as highly constrained as reconstruction from an EDM; the larger the number, the smaller the optimal solution set; whereas,

$$\text{isotonic solution set} \supseteq \text{isometric solution set} \tag{1306}$$

5.13.2.1 Isotonic cartography

To test Borg & Groenen's conjecture, suppose we make a complete sort-index matrix $O \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N\times N}$ for the map of USA and then substitute O in place of EDM D in the reconstruction process of §5.12. Whereas EDM D returned only three significant eigenvalues (1301), the sort-index matrix O is generally not an EDM (certainly not an EDM with corresponding affine dimension 3) so returns many more. The eigenvalues, calculated with absolute numerical error approximately `5E-7`, are plotted in Figure **162**:

$$\lambda(-V_{\mathcal{N}}^{\mathrm{T}}OV_{\mathcal{N}}) = [\texttt{880.1 463.9 186.1 46.20 17.12 9.625 8.257 1.701 0.7128 0.6460} \cdots\,]^{\mathrm{T}} \tag{1307}$$

The extra eigenvalues indicate that affine dimension corresponding to an EDM near O is likely to exceed 3. To realize the map, we must simultaneously reduce that dimensionality and find an EDM D closest to O in some sense[5.60] while maintaining

[5.60] a problem explored more in §7.

the known comparative distance relationship. For example: given permutation matrix Π expressing the known sorting action like (1303) on entries

$$\underline{d} \triangleq \frac{1}{\sqrt{2}} \operatorname{dvec} D = \begin{bmatrix} d_{12} \\ d_{13} \\ d_{23} \\ d_{14} \\ d_{24} \\ d_{34} \\ \vdots \\ d_{N-1,N} \end{bmatrix} \in \mathbb{R}^{N(N-1)/2} \tag{1308}$$

of unknown $D \in \mathbb{S}_h^N$, we can make sort-index matrix O input to the optimization problem

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^{\mathrm{T}}(D-O)V_{\mathcal{N}}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \leq 3 \\ & \Pi\,\underline{d} \in \mathcal{K}_{\mathcal{M}+} \\ & D \in \mathbb{EDM}^N \end{array} \tag{1309}$$

that finds the EDM D (corresponding to affine dimension not exceeding 3 in isomorphic $\operatorname{dvec}\mathbb{EDM}^N \cap \Pi^{\mathrm{T}}\mathcal{K}_{\mathcal{M}+}$) closest to O in the sense of Schoenberg (1068).

Analytical solution to this problem, ignoring the sort constraint $\Pi\,\underline{d} \in \mathcal{K}_{\mathcal{M}+}$, is known [400]: we get the convex optimization [*sic*] (§7.1)

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^{\mathrm{T}}(D-O)V_{\mathcal{N}}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \leq 3 \\ & D \in \mathbb{EDM}^N \end{array} \tag{1310}$$

Only the three largest nonnegative eigenvalues in (1307) need be retained to make list (1293); the rest are discarded. The reconstruction from EDM D found in this manner is plotted in Figure **161**e-f. (In the MATLAB code on *Wikimization* [423], matrix O is normalized by $(N(N-1)/2)^2$.) From these plots it becomes obvious that inclusion of the sort constraint is necessary for isotonic reconstruction.

That sort constraint demands: any optimal solution $D^\star$ must possess the known comparative distance relationship that produces the original ordinal distance data O (1305). Ignoring the sort constraint, apparently, violates it. Yet even more remarkable is how much the map, reconstructed using only ordinal data, still resembles the original map of USA after suffering the many violations produced by solving relaxed problem (1310). This suggests the simple reconstruction techniques of §5.12 are robust to a significant amount of noise.

5.13.2.2 Isotonic solution with sort constraint

Because problems involving rank are generally difficult, we will partition (1309) into two problems we know how to solve and then alternate their solution until convergence:

$$\begin{array}{lll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^{\mathrm{T}}(D-O)V_{\mathcal{N}}\|_{\mathrm{F}} & \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \leq 3 & \text{(a) (1310)} \\ & D \in \mathbb{EDM}^N & \\ & & \\ \underset{\sigma}{\text{minimize}} & \|\sigma - \Pi\,\underline{d}\| & \\ \text{subject to} & \sigma \in \mathcal{K}_{\mathcal{M}+} & \text{(b)} \end{array} \tag{1311}$$

where sort-index matrix O (a given constant in (a)) becomes an implicit vector variable $\underline{o}_i$ solving the ith instance of (1311b)

$$\frac{1}{\sqrt{2}}\operatorname{dvec} O_i \;=\; \underline{o}_i \;\triangleq\; \Pi^{\mathrm{T}}\sigma^{\star} \in \mathbb{R}^{N(N-1)/2}\,, \qquad i\in\{1,2,3\ldots\} \tag{1312}$$

As mentioned in discussion of relaxed problem (1310), a closed-form solution to problem (1311a) exists. Only the first iteration of (1311a) sees the original sort-index matrix O whose entries are nonnegative whole numbers; *id est*, $O_0 = O \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N\times N}$ (1305). Subsequent iterations i take the previous solution of (1311b) as input

$$O_i = \operatorname{dvec}^{-1}(\sqrt{2}\,\underline{o}_i) \in \mathbb{S}^N \tag{1313}$$

real successors, estimating distance-square not order, to the sort-index matrix O.

New convex problem (1311b) finds the unique minimum-distance projection of $\Pi\,\underline{d}$ on the monotone nonnegative cone $\mathcal{K}_{\mathcal{M}+}$. By defining

$$Y^{\dagger\mathrm{T}} = [e_1 - e_2 \quad e_2 - e_3 \quad e_3 - e_4 \quad \cdots \quad e_m] \in \mathbb{R}^{m\times m} \tag{439}$$

where $m \triangleq N(N-1)/2$, we may rewrite (1311b) as an equivalent quadratic program; a convex problem in terms of the halfspace-description of $\mathcal{K}_{\mathcal{M}+}$:

$$\begin{array}{ll} \underset{\sigma}{\text{minimize}} & (\sigma - \Pi\,\underline{d})^{\mathrm{T}}(\sigma - \Pi\,\underline{d}) \\ \text{subject to} & Y^{\dagger}\sigma \;\succeq\; 0 \end{array} \tag{1314}$$

This quadratic program can be converted to a semidefinite program via Schur-form (§3.5.3); we get the equivalent problem

$$\begin{array}{ll} \underset{t\in\mathbb{R}\,,\,\sigma}{\text{minimize}} & t \\ \text{subject to} & \begin{bmatrix} t\,I & \sigma - \Pi\,\underline{d} \\ (\sigma - \Pi\,\underline{d})^{\mathrm{T}} & 1 \end{bmatrix} \succeq 0 \\ & Y^{\dagger}\sigma \;\succeq\; 0 \end{array} \tag{1315}$$

5.13.2.3 Convergence

In §E.10 we discuss convergence of alternating projection on intersecting convex sets in a Euclidean vector space; convergence to a point in their intersection. Here the situation is different for two reasons:

Firstly, sets of positive semidefinite matrices having an upper bound on rank are generally not convex. Yet in §7.1.4.0.1 we prove that (1311a) is equivalent to a projection of nonincreasingly ordered eigenvalues on a subset of the nonnegative orthant:

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \|-V_{\mathcal{N}}^{\mathrm{T}}(D-O)V_{\mathcal{N}}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank} V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \le 3 \\ & D \in \mathbb{EDM}^N \end{array} \quad\equiv\quad \begin{array}{ll} \underset{\Upsilon}{\text{minimize}} & \|\Upsilon - \Lambda\|_{\mathrm{F}} \\ \text{subject to} & \delta(\Upsilon) \in \begin{bmatrix} \mathbb{R}_+^{\mathbf{3}} \\ \mathbf{0} \end{bmatrix} \end{array} \tag{1316}$$

where $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}} \triangleq U\Upsilon U^{\mathrm{T}} \in \mathbb{S}^{N-1}$ and $-V_{\mathcal{N}}^{\mathrm{T}}OV_{\mathcal{N}} \triangleq Q\Lambda Q^{\mathrm{T}} \in \mathbb{S}^{N-1}$ are ordered diagonalizations (§A.5). It so happens: optimal orthogonal $U^{\star}$ always equals Q given. Linear operator $T(A) = U^{\star\mathrm{T}}AU^{\star}$, acting on square matrix A, is an isometry because Frobenius' norm is orthogonally invariant (51). This isometric isomorphism T thus maps a nonconvex problem to a convex one that preserves distance.

Secondly, the second half (1311b) of the *alternation* takes place in a different vector space; $\mathbb{S}_h^N$ (*versus* $\mathbb{S}^{N-1}$). From §5.6 we know these two vector spaces are related by an isomorphism, $\mathbb{S}^{N-1} = \mathbf{V}_{\mathcal{N}}(\mathbb{S}_h^N)$ (1179), but not by an isometry.

We have, therefore, no guarantee from theory of alternating projection that alternation (1311) converges to a point, in the set of all EDMs corresponding to affine dimension not in excess of 3, belonging to $\operatorname{dvec}\mathbb{EDM}^N \cap \Pi^{\mathrm{T}}\mathcal{K}_{\mathcal{M}+}$.

5.13.2.4 Interlude

Map reconstruction from comparative distance data, isotonic reconstruction, would also prove invaluable to stellar cartography where absolute interstellar distance is difficult to acquire. But we have not yet implemented the second half (1314) of alternation (1311) for USA map data because memory-demands exceed capability of our computer.

5.13.2.4.1 Exercise. *Convergence of isotonic solution by alternation.*
Empirically demonstrate convergence, discussed in §5.13.2.3, on a smaller data set. ▼

It would be remiss not to mention another method of solution to this isotonic reconstruction problem: Once again we assume only comparative distance data like (1302) is available. Given known set of indices $\mathcal{I}$

$$\begin{array}{ll} \underset{D}{\text{minimize}} & \operatorname{rank} V D V \\ \text{subject to} & d_{ij} \le d_{kl} \le d_{mn} \qquad \forall (i,j,k,l,m,n) \in \mathcal{I} \\ & D \in \mathbb{EDM}^N \end{array} \tag{1317}$$

this problem minimizes affine dimension while finding an EDM whose entries satisfy known comparative relationships. Suitable rank heuristics are discussed in §4.5.1 and §7.2.2 that will transform this to a convex optimization problem.

Using contemporary computers, even with a rank heuristic in place of the objective function, this problem formulation is more difficult to compute than the relaxed counterpart problem (1310). That is because there exist efficient algorithms to compute a selected few eigenvalues and eigenvectors from a very large matrix. Regardless, it is important to recognize: the optimal solution set for this problem (1317) is practically always different from the optimal solution set for its counterpart, problem (1309).

5.14 Fifth property of Euclidean metric

We continue now with the question raised in §5.3 regarding necessity for at least one requirement more than the four properties of the Euclidean metric (§5.2) to certify realizability of a bounded convex polyhedron or to reconstruct a generating list for it from incomplete distance information. There we saw that the four Euclidean metric properties are necessary for $D \in \mathbb{EDM}^N$ in the case $N=3$, but become insufficient when cardinality N exceeds 3 (regardless of affine dimension).

5.14.1 Recapitulate

In the particular case $N=3$, $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0$ (1220) and $D \in \mathbb{S}_h^{\mathbf{3}}$ are necessary and sufficient conditions for D to be an EDM. By (1222), triangle inequality is then the only Euclidean condition bounding the necessarily nonnegative d_{ij}; and those bounds are tight. That means the first four properties of the Euclidean metric are necessary and sufficient conditions for D to be an EDM in the case $N=3$; for $i,j \in \{1,2,3\}$

$$\begin{array}{l} \sqrt{d_{ij}} \ge 0\,, \quad i \ne j \\ \sqrt{d_{ij}} = 0\,, \quad i = j \\ \sqrt{d_{ij}} = \sqrt{d_{ji}} \\ \sqrt{d_{ij}} \le \sqrt{d_{ik}} + \sqrt{d_{kj}}\,, \quad i \ne j \ne k \end{array} \quad \Leftrightarrow \quad \begin{array}{r} -V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_h^{\mathbf{3}} \end{array} \quad \Leftrightarrow \quad D \in \mathbb{EDM}^{\mathbf{3}} \tag{1318}$$

Yet those four properties become insufficient when $N > 3$.

5.14.2 Derivation of the Fifth

Correspondence between the triangle inequality and the EDM was developed in §5.8.2 where a triangle inequality (1222a) was revealed within the leading principal 2×2 submatrix of $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ when positive semidefinite. Our choice of the leading principal submatrix was arbitrary; actually, a unique triangle inequality like (1117) corresponds to any one of the $(N-1)!/(2!(N-1-2)!)$ principal 2×2 submatrices.[5.61] Assuming $D\in\mathbb{S}_h^{\mathbf{4}}$ and $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\in\mathbb{S}^{\mathbf{3}}$, then by the *positive (semi)definite principal submatrices theorem* (§A.3.1.0.4) it is sufficient to prove: all d_{ij} are nonnegative, all triangle inequalities are satisfied, and $\det(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}})$ is nonnegative. When $N=4$, in other words, that nonnegative determinant becomes the fifth and last Euclidean metric requirement for $D\in\mathbb{EDM}^N$. We now endeavor to ascribe geometric meaning to it.

5.14.2.1 Nonnegative determinant

By (1123) when $D\in\mathbb{EDM}^{\mathbf{4}}$, $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ is equal to inner product (1118),

$$\Theta^{\mathrm{T}}\Theta=\begin{bmatrix} d_{12} & \sqrt{d_{12}d_{13}}\cos\theta_{213} & \sqrt{d_{12}d_{14}}\cos\theta_{214}\\ \sqrt{d_{12}d_{13}}\cos\theta_{213} & d_{13} & \sqrt{d_{13}d_{14}}\cos\theta_{314}\\ \sqrt{d_{12}d_{14}}\cos\theta_{214} & \sqrt{d_{13}d_{14}}\cos\theta_{314} & d_{14}\end{bmatrix} \tag{1319}$$

Because Euclidean space is an inner-product space, the more concise inner-product form of the determinant is admitted;

$$\det(\Theta^{\mathrm{T}}\Theta)=-d_{12}d_{13}d_{14}\big(\cos(\theta_{213})^2+\cos(\theta_{214})^2+\cos(\theta_{314})^2-2\cos\theta_{213}\cos\theta_{214}\cos\theta_{314}-1\big) \tag{1320}$$

The determinant is nonnegative if and only if

$$\begin{gathered}\cos\theta_{214}\cos\theta_{314}-\sqrt{\sin(\theta_{214})^2\sin(\theta_{314})^2}\;\le\;\cos\theta_{213}\;\le\;\cos\theta_{214}\cos\theta_{314}+\sqrt{\sin(\theta_{214})^2\sin(\theta_{314})^2}\\ \Leftrightarrow\\ \cos\theta_{213}\cos\theta_{314}-\sqrt{\sin(\theta_{213})^2\sin(\theta_{314})^2}\;\le\;\cos\theta_{214}\;\le\;\cos\theta_{213}\cos\theta_{314}+\sqrt{\sin(\theta_{213})^2\sin(\theta_{314})^2}\\ \Leftrightarrow\\ \cos\theta_{213}\cos\theta_{214}-\sqrt{\sin(\theta_{213})^2\sin(\theta_{214})^2}\;\le\;\cos\theta_{314}\;\le\;\cos\theta_{213}\cos\theta_{214}+\sqrt{\sin(\theta_{213})^2\sin(\theta_{214})^2}\end{gathered} \tag{1321}$$

which simplifies, for $0\le\theta_{i1\ell},\theta_{\ell 1j},\theta_{i1j}\le\pi$ and all $i\neq j\neq\ell\in\{2,3,4\}$, to

$$\cos(\theta_{i1\ell}+\theta_{\ell 1j})\;\le\;\cos\theta_{i1j}\;\le\;\cos(\theta_{i1\ell}-\theta_{\ell 1j}) \tag{1322}$$

Analogously to triangle inequality (1234), the determinant is 0 upon equality on either side of (1322) which is tight. Inequality (1322) can be equivalently written linearly as a triangle inequality between relative angles [463, §1.4];

$$\begin{gathered}|\theta_{i1\ell}-\theta_{\ell 1j}|\;\le\;\theta_{i1j}\;\le\;\theta_{i1\ell}+\theta_{\ell 1j}\\ \theta_{i1\ell}+\theta_{\ell 1j}+\theta_{i1j}\;\le\;2\pi\\ 0\le\theta_{i1\ell},\theta_{\ell 1j},\theta_{i1j}\le\pi\end{gathered} \tag{1323}$$

Generalizing this:

[5.61] There are fewer principal 2×2 submatrices in $-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}$ 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* §5.8.2.1)

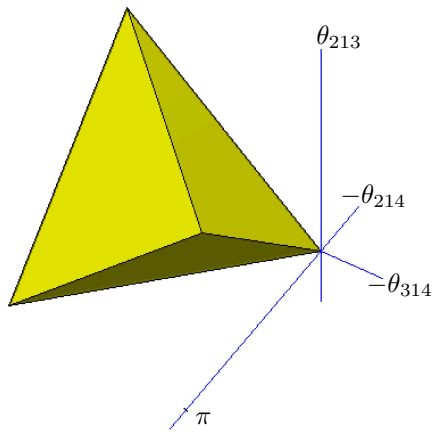


Figure 163: The *relative-angle inequality tetrahedron* (1324) bounding $\mathbb{EDM}^{\mathbf{4}}$ is regular; drawn in entirety. Each angle θ (1115) must belong to this solid to be realizable.

5.14.2.1.1 Fifth property of Euclidean metric - restatement.

Relative-angle inequality. [54] [55, p.17, p.107] [269, §3.1] (*confer* §5.3.1.0.1) Augmenting the four fundamental Euclidean metric properties in $\mathbb{R}^n$, for all $i,j,\ell \neq k \in \{1\dots N\}$, $i<j<\ell$, and for $N \geq 4$ distinct points $\{x_k\}$, the inequalities

$$\begin{aligned} |\theta_{ik\ell} - \theta_{\ell kj}| \;\leq\; \theta_{ikj} \;\leq\; \theta_{ik\ell} + \theta_{\ell kj} & \qquad \text{(a)} \\ \theta_{ik\ell} + \theta_{\ell kj} + \theta_{ikj} \;\leq\; 2\pi & \qquad \text{(b)} \\ 0 \leq \theta_{ik\ell}\,, \theta_{\ell kj}\,, \theta_{ikj} \leq \pi & \qquad \text{(c)} \end{aligned} \tag{1324}$$

must be satisfied at each point x_k regardless of affine dimension, where $\theta_{ikj} = \theta_{jki}$ is the angle between vectors at vertex x_k as defined in (1115) and illustrated in Figure **144**.

◇

Because point labelling is arbitrary, this fifth Euclidean metric requirement must apply to each of the N points as though each were in turn labelled x_1; hence the new index k in (1324). Just as the triangle inequality is the ultimate test for realizability of only three points, the relative-angle inequality is the ultimate test for only four. For four distinct points, the triangle inequality remains a necessary although penultimate test; (§5.4.3)

$$\begin{array}{l} \text{Four Euclidean metric properties (§5.2).} \\ \text{Angle } \theta \text{ inequality (1043) or (1324).} \end{array} \;\Leftrightarrow\; \begin{array}{c} -V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_h^{\mathbf{4}} \end{array} \;\Leftrightarrow\; D = \mathbf{D}(\Theta) \in \mathbb{EDM}^{\mathbf{4}} \tag{1325}$$

The relative-angle inequality, for this case, is illustrated in Figure **163**.

5.14.2.2 Beyond the fifth metric property

When cardinality N exceeds 4, the first four properties of the Euclidean metric and the relative-angle inequality together become insufficient conditions for realizability. In other words, the four Euclidean metric properties and relative-angle inequality remain necessary but become a sufficient test only for positive semidefiniteness of all the principal 3×3 submatrices [*sic*] in $-V_{\mathcal{N}}^{\mathrm{T}} D V_{\mathcal{N}}$. Relative-angle inequality can be considered the ultimate

test only for realizability at each vertex x_k of each and every purported tetrahedron constituting a hyperdimensional body.

When $N=5$ in particular, relative-angle inequality becomes the penultimate Euclidean metric requirement while nonnegativity of then unwieldy $\det(\Theta^{\mathrm{T}}\Theta)$ corresponds (by the *positive* (*semi*)*definite principal submatrices theorem* in §A.3.1.0.4) to the sixth and last Euclidean metric requirement. Together these six tests become necessary and sufficient, and so on.

Yet for all values of N, only assuming nonnegative d_{ij}, relative-angle matrix inequality in (1236) is necessary and sufficient to certify realizability; (§5.4.3.1)

$$\begin{array}{l}\text{Euclidean metric property 1 (§5.2).}\\ \text{Angle matrix inequality } \Omega\succeq 0 \text{ (1124).}\end{array} \;\Leftrightarrow\; \begin{array}{c}-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}}\succeq 0\\ D\in\mathbb{S}_h^N\end{array} \;\Leftrightarrow\; D=\mathbf{D}(\Omega\,,d)\in\mathbb{EDM}^N \tag{1326}$$

Like matrix criteria (1044), (1068), and (1236), the relative-angle matrix inequality and nonnegativity property subsume all the Euclidean metric properties and further requirements.

5.14.3 Path not followed

As a means to test for realizability of four or more points, an intuitively appealing way to augment the four Euclidean metric properties is to recognize generalizations of the triangle inequality: In the case of cardinality $N=4$ the three-dimensional analogue to triangle & distance is tetrahedron & facet-area, whereas in case $N=5$ the four-dimensional analogue is polychoron & facet-volume, *ad infinitum.* For N points, $N+1$ metric properties are required.

5.14.3.1 $N = 4$

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-square: $\mathrm{c}_1\,,\mathrm{c}_2\,,\mathrm{c}_3\,,\mathrm{c}_4$. Then analogous to metric property 4, we may write a tight[5.62] area inequality for the facets

$$\sqrt{\mathrm{c}_i}\;\leq\;\sqrt{\mathrm{c}_j}+\sqrt{\mathrm{c}_k}+\sqrt{\mathrm{c}_\ell}\;,\quad i\neq j\neq k\neq\ell\in\{1,2,3,4\} \tag{1327}$$

which is a generalized "triangle" inequality [259, §1.1] that follows from

$$\sqrt{\mathrm{c}_i}=\sqrt{\mathrm{c}_j}\cos\varphi_{ij}+\sqrt{\mathrm{c}_k}\cos\varphi_{ik}+\sqrt{\mathrm{c}_\ell}\cos\varphi_{i\ell} \tag{1328}$$

[276] [444, *Law of Cosines*] where φ_{ij} is the dihedral angle at the common edge between triangular facets i and j.

If D is the EDM corresponding to the whole tetrahedron, then area-square of the ith triangular facet has a convenient formula in terms of $D_i\in\mathbb{EDM}^{N-1}$ the EDM corresponding to that particular facet: From the *Cayley-Menger determinant*[5.63] for simplices, [444] [151] [190, §4] [97, §3.3] the ith facet

[5.62] The upper bound is met when all angles in (1328) are simultaneously 0; that occurs, for example, if one point is relatively interior to the convex hull of the three remaining.

[5.63] whose foremost characteristic is: the determinant vanishes if and only if affine dimension does not equal penultimate cardinality; *id est*, $\det\begin{bmatrix}0 & \mathbf{1}^{\mathrm{T}}\\ \mathbf{1} & -D\end{bmatrix}=0\Leftrightarrow r<N-1$ where D is any EDM (§5.7.3.0.1). Otherwise, the determinant is negative.

area-square for $i\in\{1\dots N\}$ is (§A.4.1)

$$\mathrm{c}_i = \frac{-1}{2^{N-2}(N-2)!^2}\det\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -D_i \end{bmatrix} \tag{1329}$$

$$= \frac{(-1)^N}{2^{N-2}(N-2)!^2}\det D_i\left(\mathbf{1}^{\mathrm{T}}D_i^{-1}\mathbf{1}\right) \tag{1330}$$

$$= \frac{(-1)^N}{2^{N-2}(N-2)!^2}\,\mathbf{1}^{\mathrm{T}}\mathrm{cof}(D_i)^{\mathrm{T}}\mathbf{1} \tag{1331}$$

where D_i is the ith principal $N-1\times N-1$ submatrix[5.64] of $D\in\mathbb{EDM}^N$, and $\mathrm{cof}(D_i)$ is the $N-1\times N-1$ matrix of *cofactors* [374, §4] corresponding to D_i. The number of principal 3×3 submatrices in D is, of course, equal to the number of triangular facets in the tetrahedron; four $\left(N!/(3!(N-3)!)\right)$ when $N=4$.

5.14.3.1.1 Exercise. *Sufficiency conditions for an EDM of four points.* Triangle inequality (property 4) and area inequality (1327) are conditions necessary for D to be an EDM. Prove their sufficiency in conjunction with the remaining three Euclidean metric properties. ▼

5.14.3.2 $N = 5$

Moving to the next level, we might encounter a Euclidean body called *polychoron*: a bounded polyhedron in four dimensions.[5.65] Our polychoron has five $\left(N!/(4!(N-4)!)\right)$ facets, each of them a general tetrahedron whose volume-square c_i is calculated using the same formula; (1329) where D is the EDM corresponding to the polychoron, and D_i is the EDM corresponding to the ith facet (the principal 4×4 submatrix of $D\in\mathbb{EDM}^N$ corresponding to the ith tetrahedron). The analogue to triangle & distance is now polychoron & facet-volume. We could then write another generalized "triangle" inequality like (1327) but in terms of facet volume; [449, §IV]

$$\sqrt{\mathrm{c}_i} \le \sqrt{\mathrm{c}_j} + \sqrt{\mathrm{c}_k} + \sqrt{\mathrm{c}_\ell} + \sqrt{\mathrm{c}_m}\,, \quad i\neq j\neq k\neq \ell\neq m\in\{1\dots 5\} \tag{1332}$$

5.14.3.2.1 Exercise. *Sufficiency for an EDM of five points.* For $N=5$, triangle (distance) inequality (§5.2), area inequality (1327), and volume inequality (1332) are conditions necessary for D to be an EDM. Prove their sufficiency. ▼

5.14.3.3 Volume of simplices

There is no known formula for the volume of a bounded general convex polyhedron expressed either by halfspace or vertex-description. [461, §2.1] [320, p.173] [266] [202] [203] Volume is a concept germane to $\mathbb{R}^{\mathbf{3}}$; in higher dimensions it is called *content*. Applying the *EDM assertion* (§5.9.1.0.4) and a result from [66, p.407], a general nonempty simplex (§2.12.3) in $\mathbb{R}^{N-1}$ corresponding to an EDM $D\in\mathbb{S}_h^N$ has content

$$\sqrt{\mathrm{c}} = \mathrm{content}(\mathcal{S})\sqrt{\det(-V_{\mathcal{N}}^{\mathrm{T}}DV_{\mathcal{N}})} \tag{1333}$$

[5.64] Every principal submatrix of an EDM remains an EDM. [269, §4.1]

[5.65] The simplest polychoron is called a *pentatope* [444]; a regular simplex hence convex. (A *pentahedron* is a three-dimensional body having five vertices.)

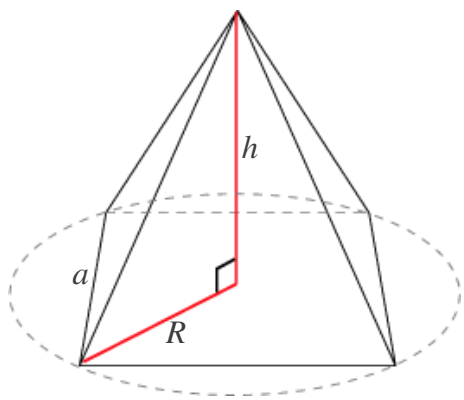


Figure 164: Length of one-dimensional face a equals height $h=a=1$ of this convex nonsimplicial pyramid in $\mathbb{R}^{\mathbf{3}}$ with square base inscribed in a circle of radius R centered at the origin. [444, *Pyramid*]

where content-square of the unit simplex $\mathcal{S}\subset\mathbb{R}^{N-1}$ is proportional to its Cayley-Menger determinant;

$$\operatorname{content}(\mathcal{S})^2 = \frac{-1}{2^{N-1}(N-1)!^2}\det\begin{bmatrix} 0 & \mathbf{1}^{\mathrm{T}} \\ \mathbf{1} & -\mathbf{D}([\,\mathbf{0}\;\; e_1\;\; e_2\;\; \cdots\;\; e_{N-1}\,]) \end{bmatrix} \tag{1334}$$

where $e_i\in\mathbb{R}^{N-1}$ and the EDM operator used is $\mathbf{D}(X)$ (1049).

5.14.3.3.1 Example. *Pyramid.*
A formula for volume of a pyramid is known:[5.66] it is $\frac{1}{3}$ the product of its base area with its height. [255] The pyramid in Figure **164** has volume $\frac{1}{3}$. To find its volume using EDMs, we must first decompose the pyramid into simplicial parts. Slicing it in half along the plane containing the line segments corresponding to radius R and height h we find the vertices of one simplex,

$$X = \begin{bmatrix} 1/2 & 1/2 & -1/2 & 0 \\ 1/2 & -1/2 & -1/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{n\times N} \tag{1335}$$

where $N=n+1$ for any nonempty simplex in $\mathbb{R}^n$. The volume of this simplex is half that of the entire pyramid; *id est*, $\sqrt{\mathrm{c}}=\frac{1}{6}$ found by evaluating (1333).
□

With that, we conclude digression of path.

5.14.4 Affine dimension reduction in three dimensions

(*confer* §5.8.4) The determinant of any $M\times M$ matrix is equal to the product of its M eigenvalues. [374, §5.1] When $N=4$ and $\det(\Theta^{\mathrm{T}}\Theta)$ is 0, that means one or more eigenvalues of $\Theta^{\mathrm{T}}\Theta\in\mathbb{R}^{\mathbf{3}\times\mathbf{3}}$ are 0. The determinant will go to 0 whenever equality is attained on either side of (1043), (1324a), or (1324b), meaning that a tetrahedron has

[5.66] Pyramid volume is independent of the paramount vertex position as long as its height remains constant.

collapsed to a lower affine dimension; *id est*, $r = \operatorname{rank}\Theta^{\mathrm{T}}\Theta = \operatorname{rank}\Theta$ is reduced below $N-1$ exactly by the number of 0 eigenvalues (§5.7.1.1).

In solving completion problems of any size N where one or more entries of an EDM are unknown, therefore, dimension r of the affine hull required to contain the unknown points is potentially reduced by selecting distances to attain equality in (1043) or (1324a) or (1324b).

5.14.4.1 *Exemplum redux*

We now apply the *fifth Euclidean metric property* to an earlier problem:

5.14.4.1.1 Example. *Small completion problem,* IV. (*confer* §5.9.2.0.1)
Returning again to Example 5.3.0.0.2 that pertains to Figure **143** where $N=4$, distance-square d_{14} is ascertainable from the fifth Euclidean metric property. Because all distances in (1041) are known except $\sqrt{d_{14}}$, then $\cos\theta_{123}=0$ and $\theta_{324}=0$ result from identity (1115). Applying (1043),

$$\begin{aligned} \cos(\theta_{123}+\theta_{324}) \;&\leq\; \cos\theta_{124} \;\leq\; \cos(\theta_{123}-\theta_{324}) \\ 0 \;&\leq\; \cos\theta_{124} \;\leq\; 0 \end{aligned} \tag{1336}$$

It follows again from (1115) that d_{14} can only be 2. As explained in this subsection, affine dimension r cannot exceed $N-2$ because equality is attained in (1336). □