

## Chapter 6

# Cone of distance matrices

*For  $N > 3$ , the cone of EDMs is no longer a circular cone and the geometry becomes complicated...*

—Hayden, Wells, Liu, & Tarazaga, 1991 [201, §3]

In the subspace of symmetric matrices  $\mathbb{S}^N$ , we know that the convex cone of Euclidean distance matrices  $\mathbb{EDM}^N$  (the EDM cone) does not intersect the positive semidefinite cone  $\mathbb{S}_+^N$  (PSD cone) except at the origin, their only vertex; there can be no positive or negative semidefinite EDM. (1187) [251]

$$\mathbb{EDM}^N \cap \mathbb{S}_+^N = \mathbf{0} \quad (1264)$$

Even so, the two convex cones can be related. In §6.8.1 we prove the equality

$$\mathbb{EDM}^N = \mathbb{S}_h^N \cap (\mathbb{S}_c^{N\perp} - \mathbb{S}_+^N) \quad (1357)$$

a resemblance to EDM definition (976) where

$$\mathbb{S}_h^N = \left\{ A \in \mathbb{S}^N \mid \delta(A) = \mathbf{0} \right\} \quad (66)$$

is the symmetric hollow subspace (§2.2.3) and where

$$\mathbb{S}_c^{N\perp} = \left\{ u\mathbf{1}^T + \mathbf{1}u^T \mid u \in \mathbb{R}^N \right\} \quad (2115)$$

is the orthogonal complement of the geometric center subspace (§E.7.2.0.2)

$$\mathbb{S}_c^N = \left\{ Y \in \mathbb{S}^N \mid Y\mathbf{1} = \mathbf{0} \right\} \quad (2113)$$

### 6.0.1 gravity

Equality (1357) is equally important as the known isomorphisms (1095) (1096) (1107) (1108) relating the EDM cone  $\mathbb{EDM}^N$  to positive semidefinite cone  $\mathbb{S}_+^{N-1}$  (§5.6.2.1) or to an  $N(N-1)/2$ -dimensional face of  $\mathbb{S}_+^N$  (§5.6.1.1).<sup>6.1</sup> But those isomorphisms have never led to this equality relating whole cones  $\mathbb{EDM}^N$  and  $\mathbb{S}_+^N$ .

Equality (1357) is not obvious from the various EDM definitions such as (976) or (1280) because inclusion must be proved algebraically in order to establish equality;  $\mathbb{EDM}^N \supseteq \mathbb{S}_h^N \cap (\mathbb{S}_c^{N\perp} - \mathbb{S}_+^N)$ . We will instead prove (1357) using purely geometric methods.

### 6.0.2 highlight

In §6.8.1.7 we show: the Schoenberg criterion for discriminating Euclidean distance matrices

$$D \in \mathbb{EDM}^N \Leftrightarrow \begin{cases} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{S}_+^{N-1} \\ D \in \mathbb{S}_h^N \end{cases} \quad (995)$$

is a discretized membership relation (§2.13.4, dual generalized inequalities) between the EDM cone and its ordinary dual.

## 6.1 Defining EDM cone

We invoke a popular matrix criterion to illustrate correspondence between the EDM and PSD cones belonging to the ambient space of symmetric matrices:

$$D \in \mathbb{EDM}^N \Leftrightarrow \begin{cases} -V D V \in \mathbb{S}_+^N \\ D \in \mathbb{S}_h^N \end{cases} \quad (999)$$

where  $V \in \mathbb{S}^N$  is the geometric centering matrix (§B.4). The set of all EDMs of dimension  $N \times N$  forms a closed convex cone  $\mathbb{EDM}^N$  because any pair of EDMs satisfies the definition of a convex cone (175); *videlicet*, for each and every  $\zeta_1, \zeta_2 \geq 0$  (§A.3.1.0.2)

$$\begin{aligned} \zeta_1 V D_1 V + \zeta_2 V D_2 V \succeq 0 & \Leftarrow V D_1 V \succeq 0, \quad V D_2 V \succeq 0 \\ \zeta_1 D_1 + \zeta_2 D_2 \in \mathbb{S}_h^N & \Leftarrow D_1 \in \mathbb{S}_h^N, \quad D_2 \in \mathbb{S}_h^N \end{aligned} \quad (1265)$$

and convex cones are invariant to inverse linear transformation [325, p.22].

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<sup>6.1</sup>Because both positive semidefinite cones are frequently in play, dimension is explicit.

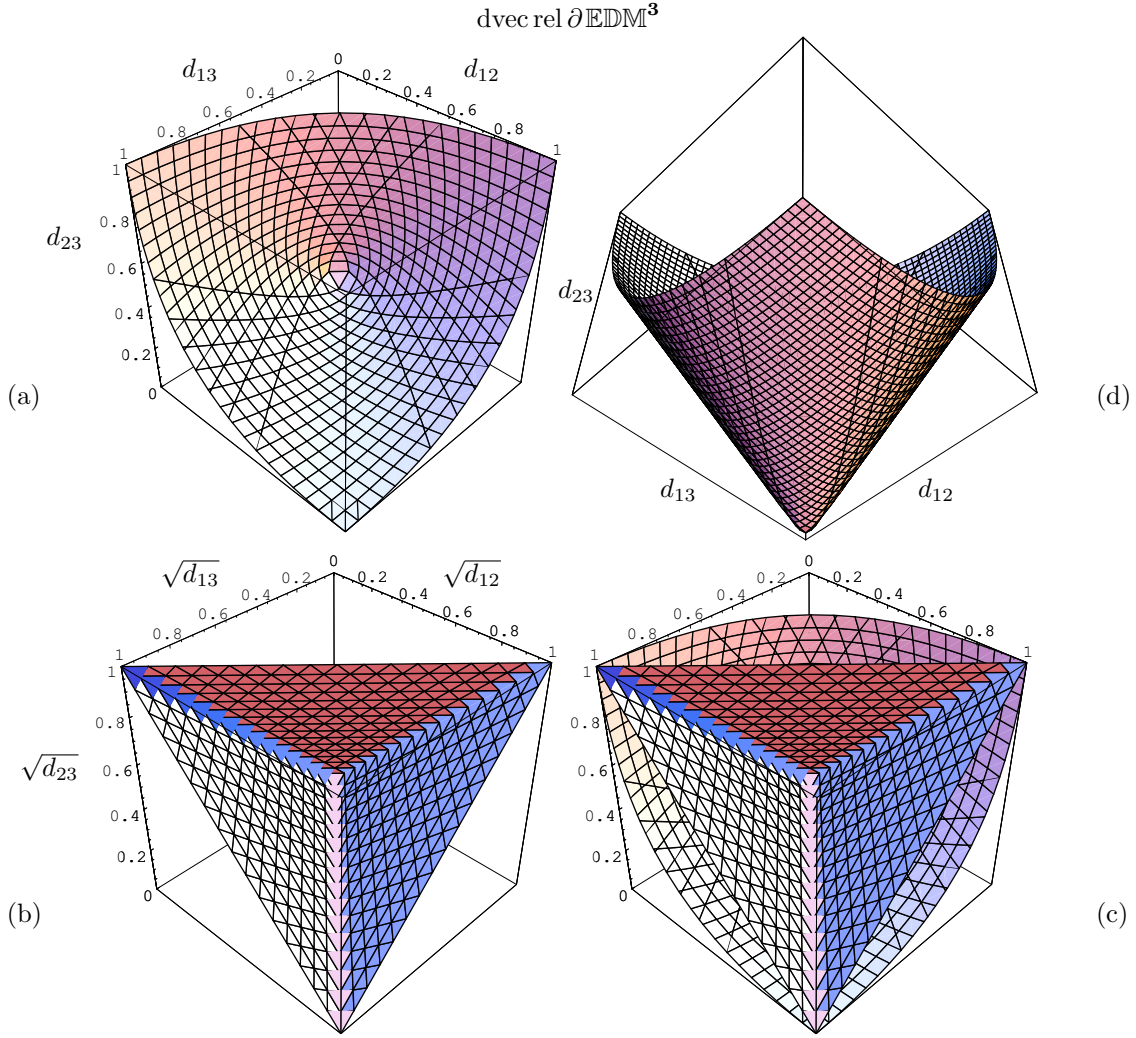


Figure 152: Relative boundary (tiled) of EDM cone  $\mathbb{EDM}^3$  drawn truncated in isometrically isomorphic subspace  $\mathbb{R}^3$ . (a) EDM cone drawn in usual distance-square coordinates  $d_{ij}$ . View is from interior toward origin. Unlike positive semidefinite cone, EDM cone is not selfdual; neither is it proper in ambient symmetric subspace (dual EDM cone for this example belongs to isomorphic  $\mathbb{R}^6$ ). (b) Drawn in its natural coordinates  $\sqrt{d_{ij}}$  (absolute distance), cone remains convex (*confer* §5.10); intersection of three halfspaces (1150) whose partial boundaries each contain origin. Cone geometry becomes nonconvex (nonpolyhedral) in higher dimension. (§6.3) (c) Two coordinate systems artificially superimposed. Coordinate transformation from  $d_{ij}$  to  $\sqrt{d_{ij}}$  appears a topological contraction. (d) Sitting on its vertex  $\mathbf{0}$ , pointed  $\mathbb{EDM}^3$  is a circular cone having axis of revolution  $\text{dvec}(-E) = \text{dvec}(\mathbf{1}\mathbf{1}^T - I)$  (1183) (73). (Rounded vertex is plot artifact.)

**6.1.0.0.1 Definition.** *Cone of Euclidean distance matrices.*

In the subspace of symmetric matrices, the set of all Euclidean distance matrices forms a unique immutable pointed closed convex cone called the *EDM cone*: for  $N > 0$

$$\begin{aligned} \mathbb{EDM}^N &\triangleq \left\{ D \in \mathbb{S}_h^N \mid -VDV \in \mathbb{S}_+^N \right\} \\ &= \bigcap_{z \in \mathcal{N}(\mathbf{1}^T)} \left\{ D \in \mathbb{S}^N \mid \langle zz^T, -D \rangle \geq 0, \delta(D) = \mathbf{0} \right\} \end{aligned} \quad (1266)$$

The EDM cone in isomorphic  $\mathbb{R}^{N(N+1)/2}$  [sic] is the intersection of an infinite number (when  $N > 2$ ) of halfspaces about the origin and a finite number of hyperplanes through the origin in vectorized variable  $D = [d_{ij}]$ . Hence  $\mathbb{EDM}^N$  is not full-dimensional with respect to  $\mathbb{S}^N$  because it is confined to the symmetric hollow subspace  $\mathbb{S}_h^N$ . The EDM cone relative interior comprises

$$\begin{aligned} \text{rel int } \mathbb{EDM}^N &= \bigcap_{z \in \mathcal{N}(\mathbf{1}^T)} \left\{ D \in \mathbb{S}^N \mid \langle zz^T, -D \rangle > 0, \delta(D) = \mathbf{0} \right\} \\ &= \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = N-1 \right\} \end{aligned} \quad (1267)$$

while its relative boundary comprises

$$\begin{aligned} \text{rel } \partial \mathbb{EDM}^N &= \left\{ D \in \mathbb{EDM}^N \mid \langle zz^T, -D \rangle = 0 \text{ for some } z \in \mathcal{N}(\mathbf{1}^T) \right\} \\ &= \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) < N-1 \right\} \end{aligned} \quad (1268)$$

△

This cone is more easily visualized in the isomorphic vector subspace  $\mathbb{R}^{N(N-1)/2}$  corresponding to  $\mathbb{S}_h^N$ :

In the case  $N=1$  point, the EDM cone is the origin in  $\mathbb{R}^0$ .

In the case  $N=2$ , the EDM cone is the nonnegative real line in  $\mathbb{R}$ ; a halfline in a subspace of the realization in Figure 156.

The EDM cone in the case  $N=3$  is a circular cone in  $\mathbb{R}^3$  illustrated in Figure 152(a)(d); rather, the set of all matrices

$$D = \begin{bmatrix} 0 & d_{12} & d_{13} \\ d_{12} & 0 & d_{23} \\ d_{13} & d_{23} & 0 \end{bmatrix} \in \mathbb{EDM}^3 \quad (1269)$$

makes a circular cone in this dimension. In this case, the first four Euclidean metric properties are necessary and sufficient tests to certify realizability of triangles; (1245). Thus triangle inequality property 4 describes three halfspaces (1150) whose intersection makes a polyhedral cone in  $\mathbb{R}^3$  of realizable  $\sqrt{d_{ij}}$  (absolute distance); an isomorphic subspace representation of the set of all EDMs  $D$  in the natural coordinates

$$\check{\sqrt{D}} \triangleq \begin{bmatrix} 0 & \sqrt{d_{12}} & \sqrt{d_{13}} \\ \sqrt{d_{12}} & 0 & \sqrt{d_{23}} \\ \sqrt{d_{13}} & \sqrt{d_{23}} & 0 \end{bmatrix} \quad (1270)$$

illustrated in Figure 152b.

## 6.2 Polyhedral bounds

The convex cone of EDMs is nonpolyhedral in  $d_{ij}$  for  $N > 2$ ; *e.g.*, Figure 152a. Still we found necessary and sufficient bounding polyhedral relations consistent with EDM cones for cardinality  $N = 1, 2, 3, 4$ :

- $N = 3$ . Transforming distance-square coordinates  $d_{ij}$  by taking their positive square root provides the polyhedral cone in Figure 152b; polyhedral because an intersection of three halfspaces in natural coordinates  $\sqrt{d_{ij}}$  is provided by triangle inequalities (1150). This polyhedral cone implicitly encompasses necessary and sufficient metric properties: nonnegativity, selfdistance, symmetry, and triangle inequality.
- $N = 4$ . Relative-angle inequality (1251) together with four Euclidean metric properties are necessary and sufficient tests for realizability of tetrahedra. (1252) Albeit relative angles  $\theta_{ikj}$  (1042) are nonlinear functions of the  $d_{ij}$ , relative-angle inequality provides a regular tetrahedron in  $\mathbb{R}^3[sic]$  (Figure 150) bounding angles  $\theta_{ikj}$  at vertex  $x_k$  consistently with EDM<sup>4</sup>.<sup>6.2</sup>

Yet were we to employ the procedure outlined in §5.14.3 for making generalized triangle inequalities, then we would find all the necessary and sufficient  $d_{ij}$ -transformations for generating bounding polyhedra consistent with EDMs of any higher dimension ( $N > 3$ ).

## 6.3 $\sqrt{\text{EDM}}$ cone is not convex

For some applications, like a molecular conformation problem (Figure 5, Figure 141) or multidimensional scaling [109] [373], absolute distance  $\sqrt{d_{ij}}$  is the preferred variable. Taking square root of the entries in all EDMs  $D$  of dimension  $N$ , we get another cone but not a convex cone when  $N > 3$  (Figure 152b): [93, §4.5.2]

$$\sqrt{\text{EDM}}^N \triangleq \{\sqrt[4]{D} \mid D \in \text{EDM}^N\} \quad (1271)$$

where  $\sqrt[4]{D}$  is defined like (1270). It is a cone simply because any cone is completely constituted by rays emanating from the origin: (§2.7) Any given ray  $\{\zeta \Gamma \in \mathbb{R}^{N(N-1)/2} \mid \zeta \geq 0\}$  remains a ray under entrywise square root:  $\{\sqrt[4]{\zeta \Gamma} \in \mathbb{R}^{N(N-1)/2} \mid \zeta \geq 0\}$ . It is already established that

$$D \in \text{EDM}^N \Rightarrow \sqrt[4]{D} \in \text{EDM}^N \quad (1182)$$

But because of how  $\sqrt{\text{EDM}}^N$  is defined, it is obvious that (*confer* §5.10)

$$D \in \text{EDM}^N \Leftrightarrow \sqrt[4]{D} \in \sqrt{\text{EDM}}^N \quad (1272)$$

Were  $\sqrt{\text{EDM}}^N$  convex, then given  $\sqrt[4]{D_1}, \sqrt[4]{D_2} \in \sqrt{\text{EDM}}^N$  we would expect their conic combination  $\sqrt[4]{D_1} + \sqrt[4]{D_2}$  to be a member of  $\sqrt{\text{EDM}}^N$ . That is easily proven false by

<sup>6.2</sup>Still, property-4 triangle inequalities (1150) corresponding to each principal  $3 \times 3$  submatrix of  $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$  demand that the corresponding  $\sqrt{d_{ij}}$  belong to a polyhedral cone like that in Figure 152b.

counterexample via (1272), for then  $(\sqrt[3]{D_1} + \sqrt[3]{D_2}) \circ (\sqrt[3]{D_1} + \sqrt[3]{D_2})$  would need to be a member of  $\mathbb{EDM}^N$ .

Notwithstanding,

$$\sqrt{\mathbb{EDM}^N} \subseteq \mathbb{EDM}^N \quad (1273)$$

by (1182) (Figure 152), and we learn how to transform a nonconvex *proximity problem* in the natural coordinates  $\sqrt{d_{ij}}$  to a convex optimization in §7.2.1.

## 6.4 EDM definition in $\mathbf{11}^T$

Any EDM  $D$  corresponding to affine dimension  $r$  has representation

$$\mathbf{D}(V_{\mathcal{X}}) \triangleq \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \mathbf{1}^T + \mathbf{1} \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)^T - 2V_{\mathcal{X}} V_{\mathcal{X}}^T \in \mathbb{EDM}^N \quad (1274)$$

where  $\mathcal{R}(V_{\mathcal{X}} \in \mathbb{R}^{N \times r}) \subseteq \mathcal{N}(\mathbf{1}^T) = \mathbf{1}^\perp$

$$V_{\mathcal{X}}^T V_{\mathcal{X}} = \delta^2(V_{\mathcal{X}}^T V_{\mathcal{X}}) \quad \text{and} \quad V_{\mathcal{X}} \text{ is full-rank with orthogonal columns.} \quad (1275)$$

Equation (1274) is simply the standard EDM definition (976) with a centered list  $X$  as in (1063); Gram matrix  $X^T X$  has been replaced with the subcompact singular value decomposition (§A.6.2)<sup>6.3</sup>

$$V_{\mathcal{X}} V_{\mathcal{X}}^T \equiv V^T X^T X V \in \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1276)$$

This means: inner product  $V_{\mathcal{X}}^T V_{\mathcal{X}}$  is an  $r \times r$  diagonal matrix  $\Sigma$  of nonzero singular values.

Vector  $\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)$  may be decomposed into complementary parts by projecting it on orthogonal subspaces  $\mathbf{1}^\perp$  and  $\mathcal{R}(\mathbf{1})$ : namely,

$$P_{\mathbf{1}^\perp}(\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)) = V \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \quad (1277)$$

$$P_{\mathbf{1}}(\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)) = \frac{1}{N} \mathbf{1} \mathbf{1}^T \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \quad (1278)$$

Of course

$$\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) = V \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) + \frac{1}{N} \mathbf{1} \mathbf{1}^T \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \quad (1279)$$

by (998). Substituting this into EDM definition (1274), we get the Hayden, Wells, Liu, & Tarazaga EDM formula [201, §2]

$$\mathbf{D}(V_{\mathcal{X}}, y) \triangleq y \mathbf{1}^T + \mathbf{1} y^T + \frac{\lambda}{N} \mathbf{1} \mathbf{1}^T - 2V_{\mathcal{X}} V_{\mathcal{X}}^T \in \mathbb{EDM}^N \quad (1280)$$

where

$$\lambda \triangleq 2\|V_{\mathcal{X}}\|_F^2 = \mathbf{1}^T \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \mathbf{1} \quad \text{and} \quad y \triangleq \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) - \frac{\lambda}{2N} \mathbf{1} = V \delta(V_{\mathcal{X}} V_{\mathcal{X}}^T) \quad (1281)$$

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<sup>6.3</sup>Subcompact SVD:  $V_{\mathcal{X}} V_{\mathcal{X}}^T \triangleq Q \sqrt{\Sigma} \sqrt{\Sigma}^T \equiv V^T X^T X V$ . So  $V_{\mathcal{X}}^T$  is not necessarily  $XV$  (§5.5.1.0.1), although affine dimension  $r = \text{rank}(V_{\mathcal{X}}^T) = \text{rank}(XV)$ . (1120)

and  $y=\mathbf{0}$  if and only if  $\mathbf{1}$  is an eigenvector of EDM  $D$ . Scalar  $\lambda$  becomes an eigenvalue when corresponding eigenvector  $\mathbf{1}$  exists.<sup>6.4</sup>

Then the particular dyad sum from (1280)

$$y\mathbf{1}^T + \mathbf{1}y^T + \frac{\lambda}{N}\mathbf{1}\mathbf{1}^T \in \mathbb{S}_c^{N\perp} \quad (1282)$$

must belong to the orthogonal complement of the geometric center subspace (p.632), whereas  $V_{\mathcal{X}}V_{\mathcal{X}}^T \in \mathbb{S}_c^N \cap \mathbb{S}_+^N$  (1276) belongs to the positive semidefinite cone in the geometric center subspace.

**Proof.** We validate eigenvector  $\mathbf{1}$  and eigenvalue  $\lambda$ .

( $\Rightarrow$ ) Suppose  $\mathbf{1}$  is an eigenvector of EDM  $D$ . Then because

$$V_{\mathcal{X}}^T \mathbf{1} = \mathbf{0} \quad (1283)$$

it follows

$$\begin{aligned} D\mathbf{1} &= \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\mathbf{1}\mathbf{1}^T + \mathbf{1}\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)^T\mathbf{1} = N\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) + \|V_{\mathcal{X}}\|_{\text{F}}^2\mathbf{1} \\ &\Rightarrow \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \propto \mathbf{1} \end{aligned} \quad (1284)$$

For some  $\kappa \in \mathbb{R}_+$

$$\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)^T\mathbf{1} = N\kappa = \text{tr}(V_{\mathcal{X}}^TV_{\mathcal{X}}) = \|V_{\mathcal{X}}\|_{\text{F}}^2 \Rightarrow \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) = \frac{1}{N}\|V_{\mathcal{X}}\|_{\text{F}}^2\mathbf{1} \quad (1285)$$

so  $y=\mathbf{0}$ .

( $\Leftarrow$ ) Now suppose  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) = \frac{\lambda}{2N}\mathbf{1}\mathbf{1}^T$ ; *id est*,  $y=\mathbf{0}$ . Then

$$D = \frac{\lambda}{N}\mathbf{1}\mathbf{1}^T - 2V_{\mathcal{X}}V_{\mathcal{X}}^T \in \mathbb{EDM}^N \quad (1286)$$

$\mathbf{1}$  is an eigenvector with corresponding eigenvalue  $\lambda$ . ♦

### 6.4.1 Range of EDM $D$

From §B.1.1 pertaining to linear independence of dyad sums: If the transpose halves of all the dyads in the sum (1274)<sup>6.5</sup> make a linearly independent set, then the nontranspose halves constitute a basis for the range of EDM  $D$ . Saying this mathematically: For  $D \in \mathbb{EDM}^N$

$$\begin{aligned} \mathcal{R}(D) &= \mathcal{R}([\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \quad \mathbf{1} \quad V_{\mathcal{X}}]) \Leftarrow \text{rank}([\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \quad \mathbf{1} \quad V_{\mathcal{X}}]) = 2 + r \\ \mathcal{R}(D) &= \mathcal{R}([\mathbf{1} \quad V_{\mathcal{X}}]) \Leftarrow \text{otherwise} \end{aligned} \quad (1287)$$

<sup>6.4</sup> *e.g.*, when  $X=I$  in EDM definition (976).

<sup>6.5</sup> Identifying columns  $V_{\mathcal{X}} \triangleq [v_1 \cdots v_r]$ , then  $V_{\mathcal{X}}V_{\mathcal{X}}^T = \sum_i v_i v_i^T$  is also a sum of dyads.

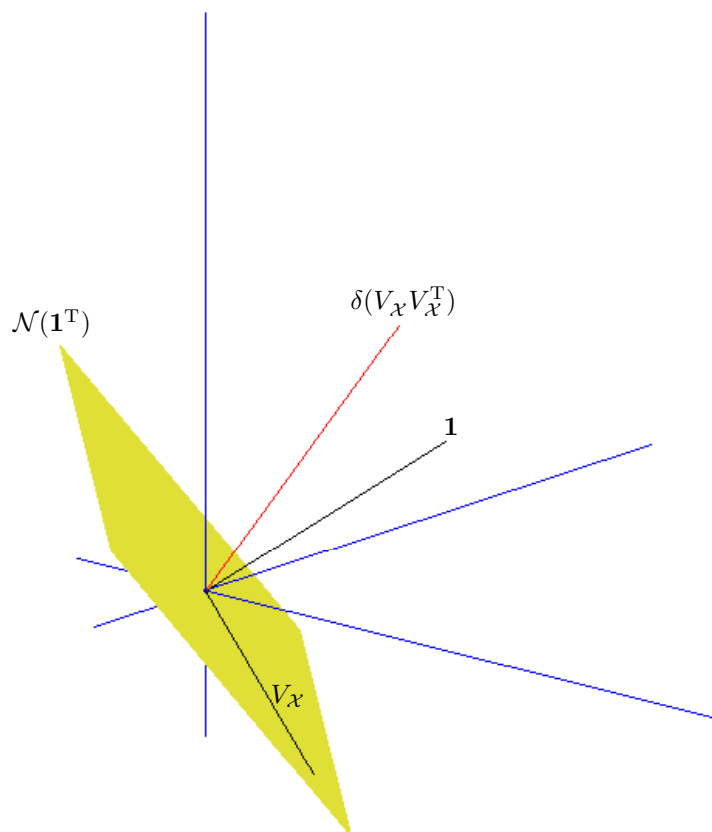


Figure 153: Example of  $V_{\mathcal{X}}$  selection to make an EDM corresponding to cardinality  $N=3$  and affine dimension  $r=1$ ;  $V_{\mathcal{X}}$  is a vector in nullspace  $\mathcal{N}(\mathbf{1}^T) \subset \mathbb{R}^3$ . Nullspace of  $\mathbf{1}^T$  is hyperplane in  $\mathbb{R}^3$  (drawn truncated) having normal  $\mathbf{1}$ . Vector  $\delta(V_{\mathcal{X}} V_{\mathcal{X}}^T)$  may or may not be in plane spanned by  $\{\mathbf{1}, V_{\mathcal{X}}\}$ , but belongs to nonnegative orthant which is strictly supported by  $\mathcal{N}(\mathbf{1}^T)$ .



**6.4.1.0.1 Proof.** We need that condition under which the rank equality is satisfied: We know  $\mathcal{R}(V_{\mathcal{X}}) \perp \mathbf{1}$ , but what is the relative geometric orientation of  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$ ?  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \succeq 0$  because  $V_{\mathcal{X}}V_{\mathcal{X}}^T \succeq 0$ , and  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \propto \mathbf{1}$  remains possible (1284); this means  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) \notin \mathcal{N}(\mathbf{1}^T)$  simply because it has no negative entries. (Figure 153) If the projection of  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$  on  $\mathcal{N}(\mathbf{1}^T)$  does not belong to  $\mathcal{R}(V_{\mathcal{X}})$ , then that is a necessary and sufficient condition for linear independence (l.i.) of  $\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)$  with respect to  $\mathcal{R}([\mathbf{1} \ V_{\mathcal{X}}])$ ; *id est*,

$$\begin{aligned} V\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) &\neq V_{\mathcal{X}}a \quad \text{for any } a \in \mathbb{R}^r \\ (I - \frac{1}{N}\mathbf{11}^T)\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) &\neq V_{\mathcal{X}}a \\ \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) - \frac{1}{N}\|V_{\mathcal{X}}\|_{\text{F}}^2\mathbf{1} &\neq V_{\mathcal{X}}a \\ \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T) - \frac{\lambda}{2N}\mathbf{1} = y &\neq V_{\mathcal{X}}a \Leftrightarrow \{\mathbf{1}, \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T), V_{\mathcal{X}}\} \text{ is l.i.} \end{aligned} \quad (1288)$$

When this condition is violated (when (1281)  $y = V_{\mathcal{X}}a_p$  for some particular  $a \in \mathbb{R}^r$ ), on the other hand, then from (1280) we have

$$\begin{aligned} \mathcal{R}(D = y\mathbf{1}^T + \mathbf{1}y^T + \frac{\lambda}{N}\mathbf{11}^T - 2V_{\mathcal{X}}V_{\mathcal{X}}^T) &= \mathcal{R}((V_{\mathcal{X}}a_p + \frac{\lambda}{N}\mathbf{1})\mathbf{1}^T + (\mathbf{1}a_p^T - 2V_{\mathcal{X}})V_{\mathcal{X}}^T) \\ &= \mathcal{R}([V_{\mathcal{X}}a_p + \frac{\lambda}{N}\mathbf{1} \quad \mathbf{1}a_p^T - 2V_{\mathcal{X}}]) \\ &= \mathcal{R}([\mathbf{1} \ V_{\mathcal{X}}]) \end{aligned} \quad (1289)$$

An example of such a violation is (1286) where, in particular,  $a_p = \mathbf{0}$ .  $\blacklozenge$

Then a statement parallel to (1287) is, for  $D \in \mathbb{EDM}^N$  (Theorem 5.7.3.0.1)

$$\begin{aligned} \text{rank}(D) = r + 2 &\Leftrightarrow y \notin \mathcal{R}(V_{\mathcal{X}}) \quad (\Leftrightarrow \mathbf{1}^T D^\dagger \mathbf{1} = 0) \\ \text{rank}(D) = r + 1 &\Leftrightarrow y \in \mathcal{R}(V_{\mathcal{X}}) \quad (\Leftrightarrow \mathbf{1}^T D^\dagger \mathbf{1} \neq 0) \end{aligned} \quad (1290)$$

## 6.4.2 Boundary constituents of EDM cone

Expression (1274) has utility in forming the set of all EDMs corresponding to affine dimension  $r$ :

$$\begin{aligned} &\left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = r \right\} \\ &= \left\{ D(V_{\mathcal{X}}) \mid V_{\mathcal{X}} \in \mathbb{R}^{N \times r}, \text{rank } V_{\mathcal{X}} = r, V_{\mathcal{X}}^T V_{\mathcal{X}} = \delta^2(V_{\mathcal{X}}^T V_{\mathcal{X}}), \mathcal{R}(V_{\mathcal{X}}) \subseteq \mathcal{N}(\mathbf{1}^T) \right\} \end{aligned} \quad (1291)$$

whereas  $\{D \in \mathbb{EDM}^N \mid \text{rank}(VDV) \leq r\}$  is the closure of this same set;

$$\left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) \leq r \right\} = \overline{\left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = r \right\}} \quad (1292)$$

For example,

$$\begin{aligned} \text{rel } \partial \mathbb{EDM}^N &= \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) < N - 1 \right\} \\ &= \bigcup_{r=0}^{N-2} \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = r \right\} \end{aligned} \quad (1293)$$

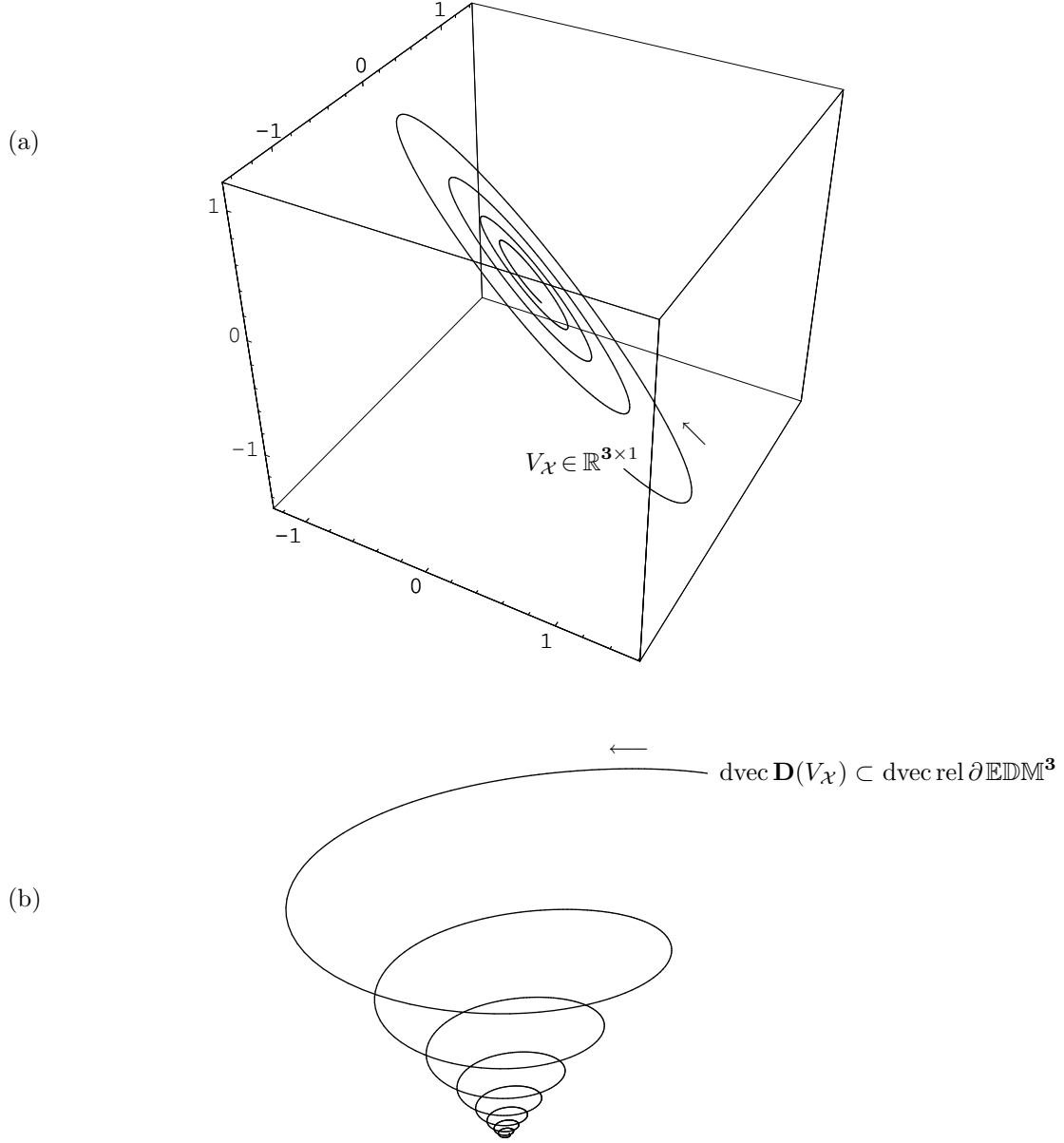


Figure 154: **(a)** Vector  $V_X$  from Figure 153 spirals in  $\mathcal{N}(\mathbf{1}^T) \subset \mathbb{R}^3$  decaying toward origin. (Spiral is two-dimensional in vector space  $\mathbb{R}^3$ .) **(b)** Corresponding trajectory  $\mathbf{D}(V_X)$  on EDM cone relative boundary creates a vortex also decaying toward origin. There are two complete orbits on EDM cone boundary about axis of revolution for every single revolution of  $V_X$  about origin. (Vortex is three-dimensional in isometrically isomorphic  $\mathbb{R}^3$ .)

None of these are necessarily convex sets, although

$$\begin{aligned}\mathbb{EDM}^N &= \bigcup_{r=0}^{N-1} \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = r \right\} \\ &= \overline{\left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = N-1 \right\}} \\ \text{rel int } \mathbb{EDM}^N &= \left\{ D \in \mathbb{EDM}^N \mid \text{rank}(VDV) = N-1 \right\}\end{aligned}\tag{1294}$$

are pointed convex cones.

When cardinality  $N = 3$  and affine dimension  $r = 2$ , for example, the relative interior  $\text{rel int } \mathbb{EDM}^3$  is realized via (1291). (§6.5)

When  $N = 3$  and  $r = 1$ , the relative boundary of the EDM cone  $\text{dvec rel } \partial \mathbb{EDM}^3$  is realized in isomorphic  $\mathbb{R}^3$  as in Figure 152d. This figure could be constructed via (1292) by spiraling vector  $V_{\mathcal{X}}$  tightly about the origin in  $\mathcal{N}(\mathbf{1}^T)$ ; as can be imagined with aid of Figure 153. Vectors close to the origin in  $\mathcal{N}(\mathbf{1}^T)$  are correspondingly close to the origin in  $\mathbb{EDM}^N$ . As vector  $V_{\mathcal{X}}$  orbits the origin in  $\mathcal{N}(\mathbf{1}^T)$ , the corresponding EDM orbits the axis of revolution while remaining on the boundary of the circular cone  $\text{dvec rel } \partial \mathbb{EDM}^3$ . (Figure 154)

### 6.4.3 Faces of EDM cone

Like the positive semidefinite cone, EDM cone faces are EDM cones.

#### 6.4.3.0.1 Exercise. Isomorphic faces.

Prove that in high cardinality  $N$ , any set of EDMs made via (1291) or (1292) with particular affine dimension  $r$  is isomorphic with any set admitting the same affine dimension but made in lower cardinality. ▼

#### 6.4.3.1 smallest face that contains an EDM

Now suppose we are given a particular EDM  $\mathbf{D}(V_{\mathcal{X}_p}) \in \mathbb{EDM}^N$  corresponding to affine dimension  $r$  and parametrized by  $V_{\mathcal{X}_p}$  in (1274). The EDM cone's smallest face that contains  $\mathbf{D}(V_{\mathcal{X}_p})$  is

$$\begin{aligned}\mathcal{F}\left(\mathbb{EDM}^N \ni \mathbf{D}(V_{\mathcal{X}_p})\right) &= \overline{\left\{ \mathbf{D}(V_{\mathcal{X}}) \mid V_{\mathcal{X}} \in \mathbb{R}^{N \times r}, \text{rank } V_{\mathcal{X}} = r, V_{\mathcal{X}}^T V_{\mathcal{X}} = \delta^2(V_{\mathcal{X}}^T V_{\mathcal{X}}), \mathcal{R}(V_{\mathcal{X}}) \subseteq \mathcal{R}(V_{\mathcal{X}_p}) \right\}} \\ &\simeq \mathbb{EDM}^{r+1}\end{aligned}\tag{1295}$$

which is isomorphic<sup>6.6</sup> with convex cone  $\mathbb{EDM}^{r+1}$ , hence of dimension

$$\dim \mathcal{F}\left(\mathbb{EDM}^N \ni \mathbf{D}(V_{\mathcal{X}_p})\right) = (r+1)r/2\tag{1296}$$

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<sup>6.6</sup>The fact that the smallest face is isomorphic with another EDM cone (perhaps smaller than  $\mathbb{EDM}^N$ ) is implicit in [201, §2].

in isomorphic  $\mathbb{R}^{N(N-1)/2}$ . Not all dimensions are represented; *e.g.*, the EDM cone has no two-dimensional faces.

When cardinality  $N=4$  and affine dimension  $r=2$  so that  $\mathcal{R}(V_{\mathcal{X}_p})$  is any two-dimensional subspace of three-dimensional  $\mathcal{N}(\mathbf{1}^T)$  in  $\mathbb{R}^4$ , for example, then the corresponding face of  $\mathbb{EDM}^4$  is isometrically isomorphic with: (1292)

$$\mathbb{EDM}^3 = \{D \in \mathbb{EDM}^3 \mid \text{rank}(VDV) \leq 2\} \simeq \mathcal{F}(\mathbb{EDM}^4 \ni \mathbf{D}(V_{\mathcal{X}_p})) \quad (1297)$$

Each two-dimensional subspace of  $\mathcal{N}(\mathbf{1}^T)$  corresponds to another three-dimensional face.

Because each and every principal submatrix of an EDM in  $\mathbb{EDM}^N$  (§5.14.3) is another EDM [251, §4.1], for example, then each principal submatrix belongs to a particular face of  $\mathbb{EDM}^N$ .

#### 6.4.3.2 extreme directions of EDM cone

In particular, extreme directions (§2.8.1) of  $\mathbb{EDM}^N$  correspond to affine dimension  $r=1$  and are simply represented: for any particular cardinality  $N \geq 2$  (§2.8.2) and each and every nonzero vector  $z$  in  $\mathcal{N}(\mathbf{1}^T)$

$$\begin{aligned} \Gamma &\triangleq (z \circ z)\mathbf{1}^T + \mathbf{1}(z \circ z)^T - 2zz^T \in \mathbb{EDM}^N \\ &= \delta(zz^T)\mathbf{1}^T + \mathbf{1}\delta(zz^T)^T - 2zz^T \end{aligned} \quad (1298)$$

is an extreme direction corresponding to a one-dimensional face of the EDM cone  $\mathbb{EDM}^N$  that is a ray in isomorphic subspace  $\mathbb{R}^{N(N-1)/2}$ .

Proving this would exercise the fundamental definition (186) of extreme direction. Here is a sketch: Any EDM may be represented

$$\mathbf{D}(V_{\mathcal{X}}) = \delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)\mathbf{1}^T + \mathbf{1}\delta(V_{\mathcal{X}}V_{\mathcal{X}}^T)^T - 2V_{\mathcal{X}}V_{\mathcal{X}}^T \in \mathbb{EDM}^N \quad (1274)$$

where matrix  $V_{\mathcal{X}}$  (1275) has orthogonal columns. For the same reason (1556) that  $zz^T$  is an extreme direction of the positive semidefinite cone (§2.9.2.7) for any particular nonzero vector  $z$ , there is no conic combination of distinct EDMs (each conically independent of  $\Gamma$  (§2.10)) equal to  $\Gamma$ . ■

##### 6.4.3.2.1 Example. Biorthogonal expansion of an EDM. (confer §2.13.7.1.1)

When matrix  $D$  belongs to the EDM cone, nonnegative coordinates for biorthogonal expansion are the eigenvalues  $\lambda \in \mathbb{R}^N$  of  $-VDV_{\frac{1}{2}}$ : For any  $D \in \mathbb{S}_h^N$  it holds

$$D = \delta(-VDV_{\frac{1}{2}})\mathbf{1}^T + \mathbf{1}\delta(-VDV_{\frac{1}{2}})^T - 2(-VDV_{\frac{1}{2}}) \quad (1087)$$

By diagonalization  $-VDV_{\frac{1}{2}} \triangleq Q\Lambda Q^T \in \mathbb{S}_c^N$  (§A.5.1) we may write

$$\begin{aligned} D &= \delta\left(\sum_{i=1}^N \lambda_i q_i q_i^T\right)\mathbf{1}^T + \mathbf{1}\delta\left(\sum_{i=1}^N \lambda_i q_i q_i^T\right)^T - 2\sum_{i=1}^N \lambda_i q_i q_i^T \\ &= \sum_{i=1}^N \lambda_i (\delta(q_i q_i^T)\mathbf{1}^T + \mathbf{1}\delta(q_i q_i^T)^T - 2q_i q_i^T) \end{aligned} \quad (1299)$$

where  $q_i$  is the  $i^{\text{th}}$  eigenvector of  $-VDV_{\frac{1}{2}}$  arranged columnar in orthogonal matrix

$$Q = [q_1 \ q_2 \ \cdots \ q_N] \in \mathbb{R}^{N \times N} \quad (399)$$

and where  $\{\delta(q_i q_i^T) \mathbf{1}^T + \mathbf{1} \delta(q_i q_i^T)^T - 2q_i q_i^T, \ i=1 \dots N\}$  are extreme directions of some pointed polyhedral cone  $\mathcal{K} \subset \mathbb{S}_h^N$  and extreme directions of  $\mathbb{EDM}^N$ . Invertibility of (1299)

$$\begin{aligned} -VDV_{\frac{1}{2}} &= -V \sum_{i=1}^N \lambda_i (\delta(q_i q_i^T) \mathbf{1}^T + \mathbf{1} \delta(q_i q_i^T)^T - 2q_i q_i^T) V_{\frac{1}{2}} \\ &= \sum_{i=1}^N \lambda_i q_i q_i^T \end{aligned} \quad (1300)$$

implies linear independence of those extreme directions. Then biorthogonal expansion is expressed

$$\text{dvec } D = Y Y^\dagger \text{dvec } D = Y \lambda (-VDV_{\frac{1}{2}}) \quad (1301)$$

where

$$Y \triangleq [\text{dvec}(\delta(q_i q_i^T) \mathbf{1}^T + \mathbf{1} \delta(q_i q_i^T)^T - 2q_i q_i^T), \ i=1 \dots N] \in \mathbb{R}^{N(N-1)/2 \times N} \quad (1302)$$

When  $D$  belongs to the EDM cone in the subspace of symmetric hollow matrices, unique coordinates  $Y^\dagger \text{dvec } D$  for this biorthogonal expansion must be the nonnegative eigenvalues  $\lambda$  of  $-VDV_{\frac{1}{2}}$ . This means  $D$  simultaneously belongs to the EDM cone and to the pointed polyhedral cone  $\text{dvec } \mathcal{K} = \text{cone}(Y)$ .  $\square$

### 6.4.3.3 open question

Result (1296) is analogous to that for the positive semidefinite cone (222), although the question remains open whether all faces of  $\mathbb{EDM}^N$  (whose dimension is less than dimension of the cone) are exposed like they are for the positive semidefinite cone.<sup>6.7</sup> (§2.9.2.3) [365]

## 6.5 Correspondence to PSD cone $\mathbb{S}_+^{N-1}$

Hayden, Wells, Liu, & Tarazaga [201, §2] assert one-to-one correspondence of EDMs with positive semidefinite matrices in the symmetric subspace. Because  $\text{rank}(VDV) \leq N-1$  (§5.7.1.1), that PSD cone corresponding to the EDM cone can only be  $\mathbb{S}_+^{N-1}$ . [9, §18.2.1] To clearly demonstrate this correspondence, we invoke inner-product form EDM definition

$$\begin{aligned} \mathbf{D}(\Phi) &= \begin{bmatrix} 0 \\ \delta(\Phi) \end{bmatrix} \mathbf{1}^T + \mathbf{1} \begin{bmatrix} 0 & \delta(\Phi)^T \end{bmatrix} - 2 \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathbf{0} & \Phi \end{bmatrix} \in \mathbb{EDM}^N \\ &\Leftrightarrow \\ &\Phi \succeq 0 \end{aligned} \quad (1105)$$

Then the EDM cone may be expressed

$$\mathbb{EDM}^N = \left\{ \mathbf{D}(\Phi) \mid \Phi \in \mathbb{S}_+^{N-1} \right\} \quad (1303)$$

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<sup>6.7</sup>Elementary example of face not exposed is given by the closed convex set in Figure 35 and in Figure 45.

Hayden & Wells' assertion can therefore be equivalently stated in terms of an inner-product form EDM operator

$$\mathbf{D}(\mathbb{S}_+^{N-1}) = \mathbf{EDM}^N \quad (1107)$$

$$\mathbf{V}_N(\mathbf{EDM}^N) = \mathbb{S}_+^{N-1} \quad (1108)$$

identity (1108) holding because  $\mathcal{R}(V_N) = \mathcal{N}(\mathbf{1}^T)$  (983), linear functions  $\mathbf{D}(\Phi)$  and  $\mathbf{V}_N(D) = -V_N^T D V_N$  (§5.6.2.1) being mutually inverse.

In terms of affine dimension  $r$ , Hayden & Wells claim particular correspondence between PSD and EDM cones:

- $r = N - 1$ : Symmetric hollow matrices  $-D$  positive definite on  $\mathcal{N}(\mathbf{1}^T)$  correspond to points relatively interior to the EDM cone.
- $r < N - 1$ : Symmetric hollow matrices  $-D$  positive semidefinite on  $\mathcal{N}(\mathbf{1}^T)$ , where  $-V_N^T D V_N$  has at least one 0 eigenvalue, correspond to points on the relative boundary of the EDM cone.
- $r = 1$ : Symmetric hollow nonnegative matrices rank-one on  $\mathcal{N}(\mathbf{1}^T)$  correspond to extreme directions (1298) of the EDM cone; *id est*, for some nonzero vector  $u$  (§A.3.1.0.7)

$$\left. \begin{array}{l} \text{rank } V_N^T D V_N = 1 \\ D \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N \times N} \end{array} \right\} \Leftrightarrow \begin{array}{l} D \in \mathbf{EDM}^N \\ D \text{ is an extreme direction} \end{array} \Leftrightarrow \left\{ \begin{array}{l} -V_N^T D V_N \equiv uu^T \\ D \in \mathbb{S}_h^N \end{array} \right. \quad (1304)$$

**6.5.0.0.1 Proof.** Case  $r = 1$  is easily proved: From the nonnegativity development in §5.8.1, extreme direction (1298), and Schoenberg criterion (995), we need show only sufficiency; *id est*, prove

$$\left. \begin{array}{l} \text{rank } V_N^T D V_N = 1 \\ D \in \mathbb{S}_h^N \cap \mathbb{R}_+^{N \times N} \end{array} \right\} \Rightarrow \begin{array}{l} D \in \mathbf{EDM}^N \\ D \text{ is an extreme direction} \end{array}$$

Any symmetric matrix  $D$  satisfying the rank condition must have the form, for  $z, q \in \mathbb{R}^N$  and nonzero  $z \in \mathcal{N}(\mathbf{1}^T)$ ,

$$D = \pm(\mathbf{1}q^T + q\mathbf{1}^T - 2zz^T) \quad (1305)$$

because (§5.6.2.1, confer §E.7.2.0.2)

$$\mathcal{N}(\mathbf{V}_N(D)) = \{\mathbf{1}q^T + q\mathbf{1}^T \mid q \in \mathbb{R}^N\} \subseteq \mathbb{S}^N \quad (1306)$$

Hollowness demands  $q = \delta(zz^T)$  while nonnegativity demands choice of positive sign in (1305). Matrix  $D$  thus takes the form of an extreme direction (1298) of the EDM cone.  $\blacklozenge$

The foregoing proof is not extensible in rank: An EDM with corresponding affine dimension  $r$  has the general form, for  $\{z_i \in \mathcal{N}(\mathbf{1}^T), i = 1 \dots r\}$  an independent set,

$$D = \mathbf{1}\delta\left(\sum_{i=1}^r z_i z_i^T\right)^T + \delta\left(\sum_{i=1}^r z_i z_i^T\right)\mathbf{1}^T - 2\sum_{i=1}^r z_i z_i^T \in \mathbf{EDM}^N \quad (1307)$$

The EDM so defined relies principally on the sum  $\sum z_i z_i^T$  having positive summand coefficients ( $\Leftrightarrow -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0$ )<sup>6.8</sup>. Then it is easy to find a sum incorporating negative coefficients while meeting rank, nonnegativity, and symmetric hollowness conditions but not positive semidefiniteness on subspace  $\mathcal{R}(V_{\mathcal{N}})$ ; *e.g.*, from page 418,

$$-V \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 5 \\ 1 & 5 & 0 \end{bmatrix} V \frac{1}{2} = z_1 z_1^T - z_2 z_2^T \quad (1308)$$

**6.5.0.0.2 Example.** *Extreme rays versus rays on the boundary.*

The EDM  $D = \begin{bmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{bmatrix}$  is an extreme direction of  $\mathbb{EDM}^3$  where  $u = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$  in (1304).

Because  $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$  has eigenvalues  $\{0, 5\}$ , the ray whose direction is  $D$  also lies on the relative boundary of  $\mathbb{EDM}^3$ .

In exception, EDM  $D = \kappa \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ , for any particular  $\kappa > 0$ , is an extreme direction of  $\mathbb{EDM}^2$  but  $-V_{\mathcal{N}}^T D V_{\mathcal{N}}$  has only one eigenvalue:  $\{\kappa\}$ . Because  $\mathbb{EDM}^2$  is a ray whose relative boundary (§2.6.1.4.1) is the origin, this conventional boundary does not include  $D$  which belongs to the relative interior in this dimension. (§2.7.0.0.1)  $\square$

### 6.5.1 Gram-form correspondence to $\mathbb{S}_+^{N-1}$

With respect to  $\mathbf{D}(G) = \delta(G)\mathbf{1}^T + \mathbf{1}\delta(G)^T - 2G$  (988) the linear Gram-form EDM operator, results in §5.6.1 provide [3, §2.6]

$$\mathbb{EDM}^N = \mathbf{D}(\mathbf{V}(\mathbb{EDM}^N)) \equiv \mathbf{D}(V_{\mathcal{N}} \mathbb{S}_+^{N-1} V_{\mathcal{N}}^T) \quad (1309)$$

$$V_{\mathcal{N}} \mathbb{S}_+^{N-1} V_{\mathcal{N}}^T \equiv \mathbf{V}(\mathbf{D}(V_{\mathcal{N}} \mathbb{S}_+^{N-1} V_{\mathcal{N}}^T)) = \mathbf{V}(\mathbb{EDM}^N) \triangleq -V \mathbb{EDM}^N V \frac{1}{2} = \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1310)$$

a one-to-one correspondence between  $\mathbb{EDM}^N$  and  $\mathbb{S}_+^{N-1}$ .

### 6.5.2 EDM cone by elliptope

Having defined the elliptope parametrized by scalar  $t > 0$

$$\mathcal{E}_t^N = \mathbb{S}_+^N \cap \{\Phi \in \mathbb{S}^N \mid \delta(\Phi) = t\mathbf{1}\} \quad (1185)$$

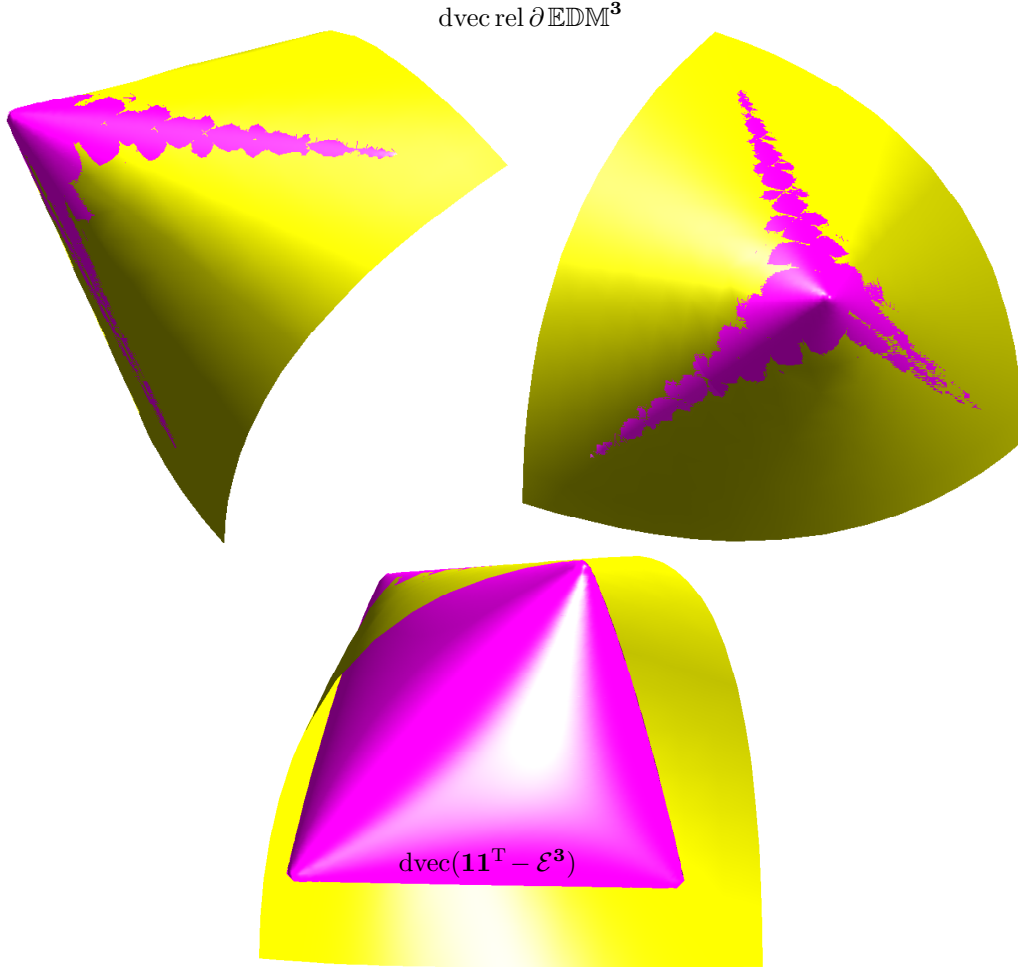
then following Alfakih [10] we have

$$\mathbb{EDM}^N = \overline{\text{cone}\{\mathbf{1}\mathbf{1}^T - \mathcal{E}_1^N\}} = \overline{\{t(\mathbf{1}\mathbf{1}^T - \mathcal{E}_1^N) \mid t \geq 0\}} \quad (1311)$$

Identification  $\mathcal{E}^N = \mathcal{E}_1^N$  equates the standard elliptope (§5.9.1.0.1, Figure 144) to our parametrized elliptope.

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<sup>6.8</sup> ( $\Leftarrow$ ) For  $a_i \in \mathbb{R}^{N-1}$ , let  $z_i = V_{\mathcal{N}}^T a_i$ .



$$\mathbb{EDM}^N = \overline{\text{cone}\{\mathbf{1}\mathbf{1}^T - \mathcal{E}^N\}} = \overline{\{t(\mathbf{1}\mathbf{1}^T - \mathcal{E}^N) \mid t \geq 0\}} \quad (1311)$$

Figure 155: Three views of translated negated ellipsope  $\mathbf{1}\mathbf{1}^T - \mathcal{E}_1^3$  (confer Figure 144) shrouded by truncated EDM cone. Fractal on EDM cone relative boundary is numerical artifact belonging to intersection with ellipsope relative boundary. The fractal is trying to convey existence of a neighborhood about the origin where the translated ellipsope boundary and EDM cone boundary intersect.



**6.5.2.0.1 Expository.** *Normal cone, tangent cone, ellipptope.*

Define  $\mathcal{T}_{\mathcal{E}}(\mathbf{11}^T)$  to be the *tangent cone* to the ellipptope  $\mathcal{E}$  at point  $\mathbf{11}^T$ ; *id est*,

$$\mathcal{T}_{\mathcal{E}}(\mathbf{11}^T) \triangleq \overline{\{t(\mathcal{E} - \mathbf{11}^T) \mid t \geq 0\}} \quad (1312)$$

The normal cone  $\mathcal{K}_{\mathcal{E}}^{\perp}(\mathbf{11}^T)$  to the ellipptope at  $\mathbf{11}^T$  is a closed convex cone defined (§E.10.3.2.1, Figure 191)

$$\mathcal{K}_{\mathcal{E}}^{\perp}(\mathbf{11}^T) \triangleq \{B \mid \langle B, \Phi - \mathbf{11}^T \rangle \leq 0, \Phi \in \mathcal{E}\} \quad (1313)$$

The *polar cone* of any set  $\mathcal{K}$  is the closed convex cone (*confer* (296))

$$\mathcal{K}^{\circ} \triangleq \{B \mid \langle B, A \rangle \leq 0, \text{ for all } A \in \mathcal{K}\} \quad (1314)$$

The normal cone is well known to be the polar of the tangent cone,

$$\mathcal{K}_{\mathcal{E}}^{\perp}(\mathbf{11}^T) = \mathcal{T}_{\mathcal{E}}(\mathbf{11}^T)^{\circ} \quad (1315)$$

and *vice versa*; [215, §A.5.2.4]

$$\mathcal{K}_{\mathcal{E}}^{\perp}(\mathbf{11}^T)^{\circ} = \mathcal{T}_{\mathcal{E}}(\mathbf{11}^T) \quad (1316)$$

From Deza & Laurent [120, p.535] we have the EDM cone

$$\mathbb{EDM} = -\mathcal{T}_{\mathcal{E}}(\mathbf{11}^T) \quad (1317)$$

The polar EDM cone is also expressible in terms of the ellipptope. From (1315) we have

$$\mathbb{EDM}^{\circ} = -\mathcal{K}_{\mathcal{E}}^{\perp}(\mathbf{11}^T) \quad (1318)$$

★

In §5.10.1 we proposed the expression for EDM  $D$

$$D = t\mathbf{11}^T - \mathfrak{E} \in \mathbb{EDM}^N \quad (1186)$$

where  $t \in \mathbb{R}_+$  and  $\mathfrak{E}$  belongs to the parametrized ellipptope  $\mathcal{E}_t^N$ . We further propose, for any particular  $t > 0$

$$\mathbb{EDM}^N = \overline{\text{cone}\{t\mathbf{11}^T - \mathcal{E}_t^N\}} \quad (1319)$$

**Proof (pending).** ■

**6.5.2.0.2 Exercise.** *EDM cone from ellipptope.*

Relationship of the translated negated ellipptope with the EDM cone is illustrated in Figure 155. Prove whether it holds that

$$\mathbb{EDM}^N = \overline{\lim_{t \rightarrow \infty} t\mathbf{11}^T - \mathcal{E}_t^N} \quad (1320)$$

▼

## 6.6 Vectorization & projection interpretation

In §E.7.2.0.2 we learn:  $-VDV$  can be interpreted as orthogonal projection [7, §2] of vectorized  $-D \in \mathbb{S}_h^N$  on the subspace of geometrically centered symmetric matrices

$$\begin{aligned} \mathbb{S}_c^N &= \{G \in \mathbb{S}^N \mid G\mathbf{1} = \mathbf{0}\} \\ &= \{G \in \mathbb{S}^N \mid \mathcal{N}(G) \supseteq \mathbf{1}\} = \{G \in \mathbb{S}^N \mid \mathcal{R}(G) \subseteq \mathcal{N}(\mathbf{1}^T)\} \\ &= \{VYV \mid Y \in \mathbb{S}^N\} \subset \mathbb{S}^N \\ &\equiv \{V_{\mathcal{N}}AV_{\mathcal{N}}^T \mid A \in \mathbb{S}^{N-1}\} \end{aligned} \quad (1078)$$

because elementary auxiliary matrix  $V$  is an orthogonal projector (§B.4.1). Yet there is another useful projection interpretation:

Revising the fundamental matrix criterion for membership to the EDM cone (971),<sup>6.9</sup>

$$\left. \begin{aligned} \langle zz^T, -D \rangle \geq 0 \quad \forall zz^T \mid \mathbf{1}^T zz^T = \mathbf{0} \\ D \in \mathbb{S}_h^N \end{aligned} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (1321)$$

this is equivalent, of course, to the Schoenberg criterion

$$\left. \begin{aligned} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \\ D \in \mathbb{S}_h^N \end{aligned} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (995)$$

because  $\mathcal{N}(\mathbf{1}^T) = \mathcal{R}(V_{\mathcal{N}})$ . When  $D \in \text{EDM}^N$ , correspondence (1321) means  $-z^T D z$  is proportional to a nonnegative coefficient of orthogonal projection (§E.6.4.2, Figure 157) of  $-D$  in isometrically isomorphic  $\mathbb{R}^{N(N+1)/2}$  on the range of each and every vectorized (§2.2.2.1) symmetric dyad (§B.1) in the nullspace of  $\mathbf{1}^T$ ; *id est*, on each and every member of

$$\begin{aligned} \mathcal{T} &\triangleq \{\text{svec}(zz^T) \mid z \in \mathcal{N}(\mathbf{1}^T) = \mathcal{R}(V_{\mathcal{N}})\} \subset \text{svec } \partial \mathbb{S}_+^N \\ &= \{\text{svec}(V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T) \mid v \in \mathbb{R}^{N-1}\} \end{aligned} \quad (1322)$$

whose dimension is

$$\dim \mathcal{T} = N(N-1)/2 \quad (1323)$$

The set of all symmetric dyads  $\{zz^T \mid z \in \mathbb{R}^N\}$  constitute the extreme directions of the positive semidefinite cone (§2.8.1, §2.9)  $\mathbb{S}_+^N$ , hence lie on its boundary. Yet only those dyads in  $\mathcal{R}(V_{\mathcal{N}})$  are included in the test (1321), thus only a subset  $\mathcal{T}$  of all vectorized extreme directions of  $\mathbb{S}_+^N$  is observed.

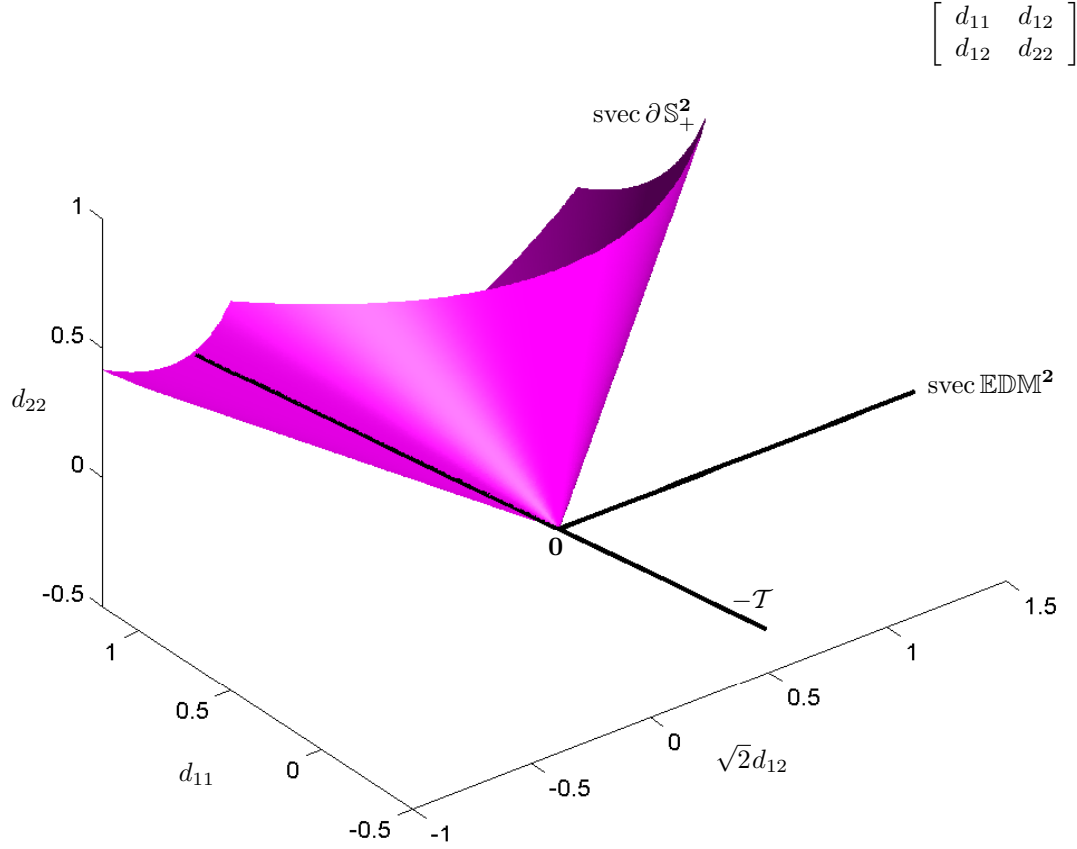
In the particularly simple case  $D \in \text{EDM}^2 = \{D \in \mathbb{S}_h^2 \mid d_{12} \geq 0\}$ , for example, only one extreme direction of the PSD cone is involved:

$$zz^T = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (1324)$$

Any nonnegative scaling of vectorized  $zz^T$  belongs to the set  $\mathcal{T}$  illustrated in Figure 156 and Figure 157.

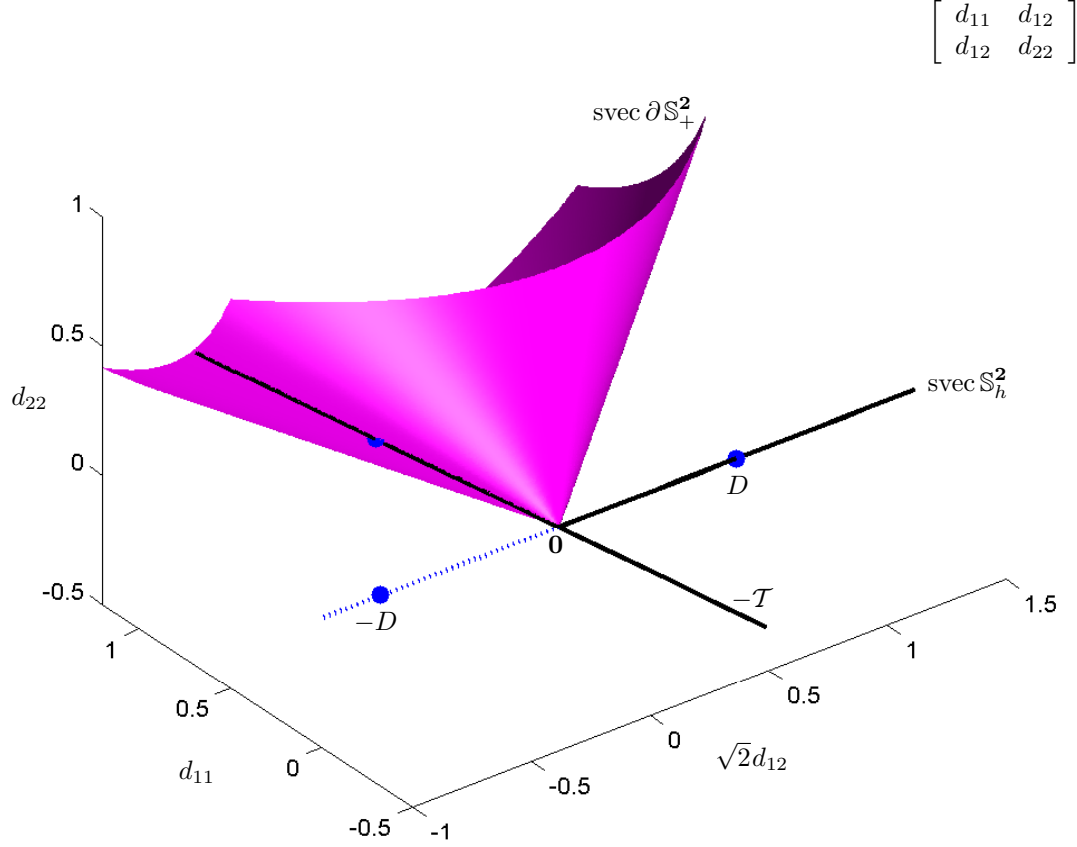
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<sup>6.9</sup>  $\mathcal{N}(\mathbf{1}^T) = \mathcal{N}(\mathbf{1}^T)$  and  $\mathcal{R}(zz^T) = \mathcal{R}(z)$



$$\mathcal{T} \triangleq \left\{ \text{svec}(zz^T) \mid z \in \mathcal{N}(\mathbf{1}\mathbf{1}^T) = \kappa \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \kappa \in \mathbb{R} \right\} \subset \text{svec } \partial \mathbb{S}_+^2$$

Figure 156: Truncated boundary of positive semidefinite cone  $\mathbb{S}_+^2$  in isometrically isomorphic  $\mathbb{R}^3$  (via  $\text{svec}$  (56)) is, in this dimension, constituted solely by its extreme directions. Truncated cone of Euclidean distance matrices  $\mathbb{EDM}^2$  in isometrically isomorphic subspace  $\mathbb{R}^3$ . Relative boundary of EDM cone is constituted solely by matrix  $\mathbf{0}$ . Halfline  $\mathcal{T} = \{\kappa^2 [1 \ -\sqrt{2} \ 1]^T \mid \kappa \in \mathbb{R}\}$  on PSD cone boundary depicts that lone extreme ray (1324) on which orthogonal projection of  $-D$  must be positive semidefinite if  $D$  is to belong to  $\mathbb{EDM}^2$ .  $\text{aff cone } \mathcal{T} = \text{svec } \mathbb{S}_c^2$ . (1329) Dual EDM cone is halfspace in  $\mathbb{R}^3$  whose bounding hyperplane has inward-normal  $\text{svec } \mathbb{EDM}^2$ .



$P_{\text{svec } zz^T}(\text{svec}(-D)) = \frac{\langle zz^T, -D \rangle}{\langle zz^T, zz^T \rangle} zz^T$  is projection of vectorized  $-D$  on range of vectorized  $zz^T$ .

$$D \in \text{EDM}^N \Leftrightarrow \begin{cases} \langle zz^T, -D \rangle \geq 0 & \forall zz^T \mid \mathbf{1}\mathbf{1}^T zz^T = \mathbf{0} \\ D \in \mathbb{S}_h^N \end{cases} \quad (1321)$$

Figure 157: Given-matrix  $D$  is assumed to belong to symmetric hollow subspace  $\mathbb{S}_h^2$ ; a line in this dimension. Negative  $D$  is found along  $\mathbb{S}_h^2$ . Set  $\mathcal{T}$  (1322) has only one ray member in this dimension; not orthogonal to  $\mathbb{S}_h^2$ . Orthogonal projection of  $-D$  on  $\mathcal{T}$  (indicated by half dot) has nonnegative projection coefficient. Matrix  $D$  must therefore be an EDM.

### 6.6.1 Face of PSD cone $\mathbb{S}_+^N$ containing $V$

In any case, set  $\mathcal{T}$  (1322) constitutes the vectorized extreme directions of an  $N(N-1)/2$ -dimensional face of the PSD cone  $\mathbb{S}_+^N$  containing auxiliary matrix  $V$ ; a face isomorphic with  $\mathbb{S}_+^{N-1} = \mathbb{S}_+^{\text{rank } V}$  (§2.9.2.3).

To show this, we must first find the smallest face that contains auxiliary matrix  $V$  and then determine its extreme directions. From (221),

$$\begin{aligned} \mathcal{F}(\mathbb{S}_+^N \ni V) &= \{W \in \mathbb{S}_+^N \mid \mathcal{N}(W) \supseteq \mathcal{N}(V)\} = \{W \in \mathbb{S}_+^N \mid \mathcal{N}(W) \supseteq \mathbf{1}\} \\ &= \{VYV \succeq 0 \mid Y \in \mathbb{S}^N\} \equiv \{V_{\mathcal{N}} B V_{\mathcal{N}}^T \mid B \in \mathbb{S}_+^{N-1}\} \\ &\simeq \mathbb{S}_+^{\text{rank } V} = -V_{\mathcal{N}}^T \text{EDM}^N V_{\mathcal{N}} \end{aligned} \quad (1325)$$

where the equivalence  $\equiv$  is from §5.6.1 while isomorphic equality  $\simeq$  with transformed EDM cone is from (1108). Projector  $V$  belongs to  $\mathcal{F}(\mathbb{S}_+^N \ni V)$  because  $V_{\mathcal{N}} V_{\mathcal{N}}^\dagger V_{\mathcal{N}}^{\dagger T} V_{\mathcal{N}}^T = V$  (§B.4.3). Each and every rank-one matrix belonging to this face is therefore of the form:

$$V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \quad (1326)$$

Because  $\mathcal{F}(\mathbb{S}_+^N \ni V)$  is isomorphic with a positive semidefinite cone  $\mathbb{S}_+^{N-1}$ , then  $\mathcal{T}$  constitutes the vectorized extreme directions of  $\mathcal{F}$ , the origin constitutes the extreme points of  $\mathcal{F}$ , and auxiliary matrix  $V$  is some convex combination of those extreme points and directions by the *extremes theorem* (§2.8.1.1.1).  $\blacklozenge$

In fact the smallest face, that contains auxiliary matrix  $V$ , of the PSD cone  $\mathbb{S}_+^N$  is the intersection with the geometric center subspace (2113) (2114);

$$\begin{aligned} \mathcal{F}(\mathbb{S}_+^N \ni V) &= \text{cone} \left\{ V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \\ &= \mathbb{S}_c^N \cap \mathbb{S}_+^N \\ &\equiv \{X \succeq 0 \mid \langle X, \mathbf{1}\mathbf{1}^T \rangle = 0\} \end{aligned} \quad (1327) \quad (1684)$$

In isometrically isomorphic  $\mathbb{R}^{N(N+1)/2}$

$$\text{svec } \mathcal{F}(\mathbb{S}_+^N \ni V) = \text{cone } \mathcal{T} \quad (1328)$$

related to  $\mathbb{S}_c^N$  by

$$\text{aff cone } \mathcal{T} = \text{svec } \mathbb{S}_c^N \quad (1329)$$

### 6.6.2 EDM criteria in $\mathbf{1}\mathbf{1}^T$

(confer §6.4, (1002)) Laurent specifies an ellipsope trajectory condition for EDM cone membership: [251, §2.3]

$$D \in \text{EDM}^N \Leftrightarrow [1 - e^{-\alpha d_{ij}}] \in \text{EDM}^N \quad \forall \alpha > 0 \quad (1180a)$$

From the parametrized ellipsope  $\mathcal{E}_t^N$  in §6.5.2 and §5.10.1 we propose

$$D \in \mathbb{EDM}^N \Leftrightarrow \left. \begin{array}{l} t \in \mathbb{R}_+ \\ \mathfrak{E} \in \mathcal{E}_t^N \end{array} \right\} \ni D = t\mathbf{1}\mathbf{1}^T - \mathfrak{E} \quad (1330)$$

Chabrillac & Crouzeix [77, §4] prove a different criterion they attribute to Finsler, 1937 [156]. We apply it to EDMs: for  $D \in \mathbb{S}_h^N$  (1128)

$$\begin{aligned} -V_N^T D V_N \succ 0 &\Leftrightarrow \exists \kappa > 0 \ni -D + \kappa \mathbf{1}\mathbf{1}^T \succ 0 \\ &\Leftrightarrow \\ D \in \mathbb{EDM}^N &\text{ with corresponding affine dimension } r = N - 1 \end{aligned} \quad (1331)$$

This *Finsler criterion* has geometric interpretation in terms of the vectorization & projection already discussed in connection with (1321). With reference to Figure 156, the offset  $\mathbf{1}\mathbf{1}^T$  is simply a direction orthogonal to  $\mathcal{T}$  in isomorphic  $\mathbb{R}^3$ . Intuitively, translation of  $-D$  in direction  $\mathbf{1}\mathbf{1}^T$  is like orthogonal projection on  $\mathcal{T}$  insofar as similar information can be obtained.

When the Finsler criterion (1331) is applied despite lower affine dimension, the constant  $\kappa$  can go to infinity making the test  $-D + \kappa \mathbf{1}\mathbf{1}^T \succeq 0$  impractical for numerical computation. Chabrillac & Crouzeix invent a criterion for the semidefinite case, but is no more practical: for  $D \in \mathbb{S}_h^N$

$$\begin{aligned} D \in \mathbb{EDM}^N \\ \Leftrightarrow \\ \exists \kappa_p > 0 \ni \forall \kappa \geq \kappa_p, -D - \kappa \mathbf{1}\mathbf{1}^T \text{ [sic] has exactly one negative eigenvalue} \end{aligned} \quad (1332)$$

## 6.7 A geometry of completion

*It is not known how to proceed if one wishes to restrict the dimension of the Euclidean space in which the configuration of points may be constructed.*

—Michael W. Trosset, 2000 [371, §1]

Given an incomplete noiseless EDM, intriguing is the question of whether a list in  $X \in \mathbb{R}^{n \times N}$  (76) may be reconstructed and under what circumstances reconstruction is unique. [3] [5] [6] [7] [9] [18] [70] [221] [233] [250] [251] [252]

If one or more entries of a particular EDM are fixed, then geometric interpretation of the feasible set of completions is the intersection of the EDM cone  $\mathbb{EDM}^N$  in isomorphic subspace  $\mathbb{R}^{N(N-1)/2}$  with as many hyperplanes as there are fixed symmetric entries.<sup>6.10</sup> Assuming a nonempty intersection, then the number of completions is generally infinite, and those corresponding to particular affine dimension  $r < N - 1$  belong to some generally nonconvex subset of that intersection (*confer* §2.9.2.9.2) that can be as small as a point.

<sup>6.10</sup>Depicted in Figure 158a is an intersection of the EDM cone  $\mathbb{EDM}^3$  with a single hyperplane representing the set of all EDMs having one fixed symmetric entry. This representation is practical because it is easily combined with or replaced by other convex constraints; *e.g.*, slab inequalities in (789) that admit bounding of noise processes.

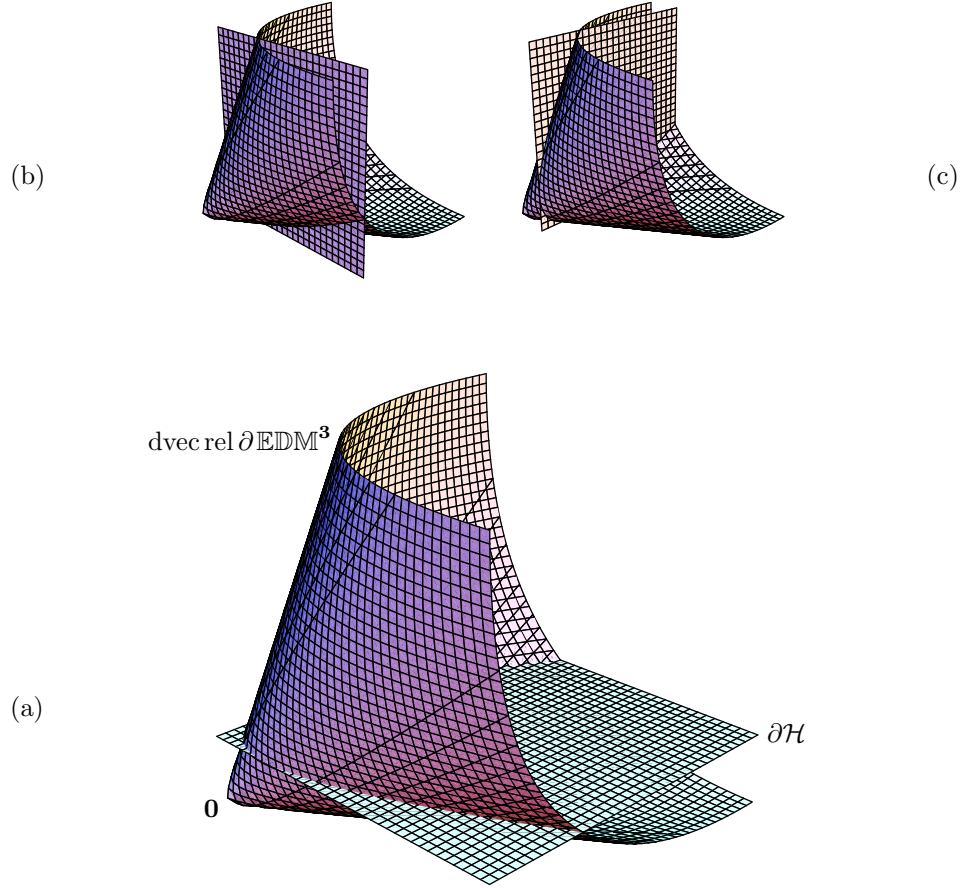


Figure 158: **(a)** In isometrically isomorphic subspace  $\mathbb{R}^3$ , intersection of  $\text{EDM}^3$  with hyperplane  $\partial \mathcal{H}$  representing one fixed symmetric entry  $d_{23} = \kappa$  (both drawn truncated, rounded vertex is artifact of plot). EDMs in this dimension corresponding to affine dimension 1 comprise relative boundary of EDM cone (§6.5). Since intersection illustrated includes a nontrivial subset of cone's relative boundary, then it is apparent there exist infinitely many EDM completions corresponding to affine dimension 1. In this dimension it is impossible to represent a unique nonzero completion corresponding to affine dimension 1, for example, using a single hyperplane because any hyperplane supporting relative boundary at a particular point  $\Gamma$  contains an entire ray  $\{\zeta \Gamma \mid \zeta \geq 0\}$  belonging to  $\text{rel } \partial \text{EDM}^3$  by Lemma 2.8.0.0.1. **(b)**  $d_{13} = \kappa$ . **(c)**  $d_{12} = \kappa$ .

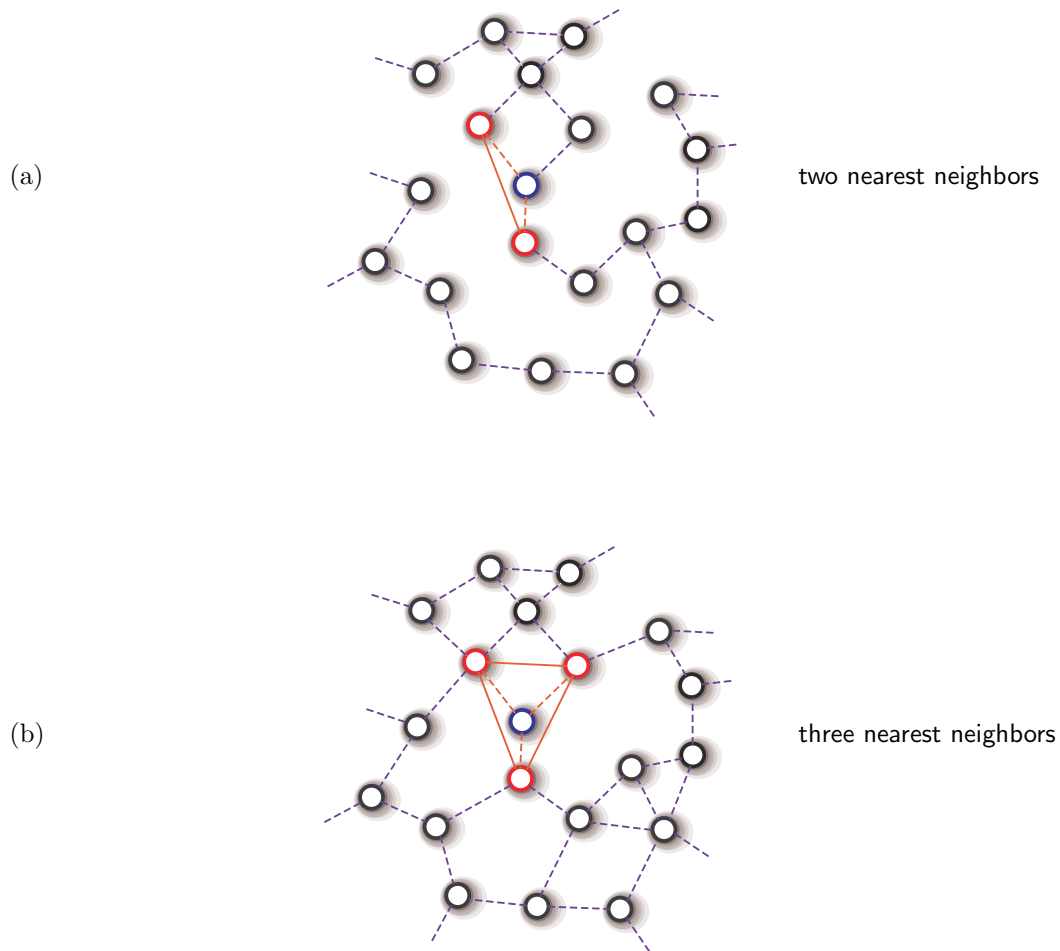


Figure 159: One dimensionless EDM subgraph completion (solid) superimposed on (but not obscuring) neighborhood graph (dashed). Local view of a few dense samples  $\circ$  from relative interior of some arbitrary Euclidean manifold whose affine dimension appears two-dimensional in this neighborhood. All line segments measure absolute distance. Dashed line segments help visually locate nearest neighbors; suggesting, best number of nearest neighbors can be greater than value of embedding dimension after topological transformation (*confer* [228, §2]). Solid line segments represent completion of EDM subgraph from available distance data for an arbitrarily chosen sample and its nearest neighbors. Each distance from EDM subgraph becomes distance-square in corresponding EDM submatrix.



**6.7.0.0.1 Example.** *Maximum variance unfolding.*

[411]

A process minimizing affine dimension (§2.1.5) of certain kinds of Euclidean *manifold* by topological transformation can be posed as a completion problem (*confer* §E.10.2.1.2). Weinberger & Saul, who originated the technique, specify an applicable manifold in three dimensions by analogy to an ordinary sheet of paper (*confer* §2.1.6); imagine, we find it deformed from flatness in some way introducing neither holes, tears, or selfintersections. [411, §2.2] The physical process is intuitively described as *unfurling*, *unfolding*, *diffusing*, *decompacting*, or *unraveling*. In particular instances, the process is a sort of flattening by stretching until taut (but not by crushing); *e.g.*, unfurling a three-dimensional Euclidean body resembling a billowy national flag reduces that manifold's affine dimension to  $r=2$ .

Data input to the proposed process originates from distances between neighboring relatively dense samples of a given manifold. Figure 159 realizes a densely sampled neighborhood; called, *neighborhood graph*. Essentially, the algorithmic process preserves local isometry between *nearest neighbors* allowing distant neighbors to excuse expansively by “maximizing variance” (Figure 7). The common number of nearest neighbors to each sample is a data-dependent algorithmic parameter whose minimum value connects the graph. The dimensionless *EDM subgraph* between each sample and its nearest neighbors is completed from available data and included as input; one such EDM subgraph completion is drawn superimposed upon the neighborhood graph in Figure 159.<sup>6.11</sup> The consequent dimensionless EDM graph comprising all the subgraphs is incomplete, in general, because the neighbor number is relatively small; incomplete even though it is a superset of the neighborhood graph. Remaining distances (those not graphed at all) are squared then made variables within the algorithm; it is this variability that admits unfurling.

To demonstrate, consider untying the *trefoil knot* drawn in Figure 160a. A corresponding EDM  $D = [d_{ij}, i, j = 1 \dots N]$  employing only two nearest neighbors is banded having the incomplete form

$$D = \begin{bmatrix} 0 & \check{d}_{12} & \check{d}_{13} & ? & \cdots & ? & \check{d}_{1,N-1} & \check{d}_{1N} \\ \check{d}_{12} & 0 & \check{d}_{23} & \check{d}_{24} & \ddots & ? & ? & \check{d}_{2N} \\ \check{d}_{13} & \check{d}_{23} & 0 & \check{d}_{34} & \ddots & ? & ? & ? \\ ? & \check{d}_{24} & \check{d}_{34} & 0 & \ddots & \ddots & ? & ? \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & ? \\ ? & ? & ? & \ddots & \ddots & 0 & \check{d}_{N-2,N-1} & \check{d}_{N-2,N} \\ \check{d}_{1,N-1} & ? & ? & ? & \ddots & \check{d}_{N-2,N-1} & 0 & \check{d}_{N-1,N} \\ \check{d}_{1N} & \check{d}_{2N} & ? & ? & ? & \check{d}_{N-2,N} & \check{d}_{N-1,N} & 0 \end{bmatrix} \quad (1333)$$

where  $\check{d}_{ij}$  denotes a given fixed distance-square. The unfurling algorithm can be expressed

<sup>6.11</sup>Local reconstruction of point position, from the EDM submatrix corresponding to a complete dimensionless EDM subgraph, is unique to within an isometry (§5.6, §5.12).

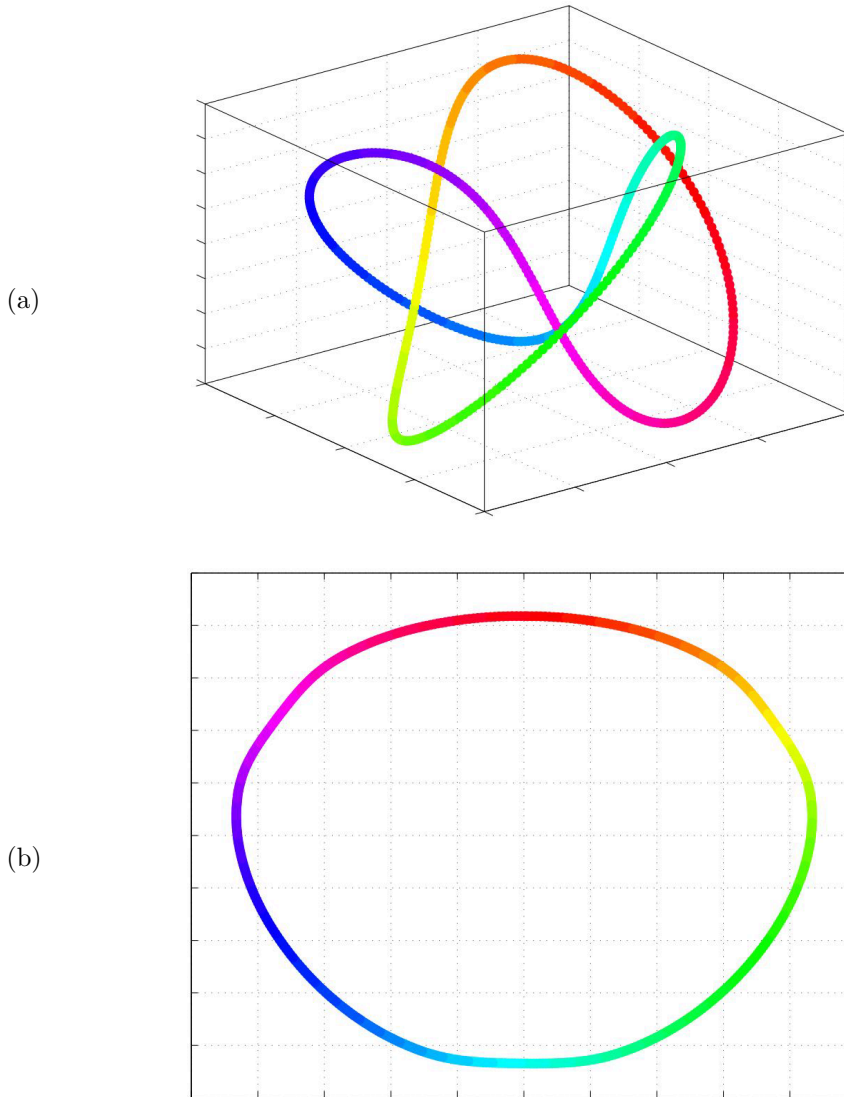


Figure 160: **(a)** *Trefoil knot* in  $\mathbb{R}^3$  from Weinberger & Saul [411]. **(b)** Topological transformation algorithm employing four nearest neighbors and  $N = 539$  samples reduces affine dimension of knot to  $r=2$ . Choosing instead two nearest neighbors would make this embedding more circular.

as an optimization problem; constrained total distance-square maximization:

$$\begin{aligned}
 & \underset{D}{\text{maximize}} && \langle -V, D \rangle \\
 & \text{subject to} && \langle D, e_i e_j^T + e_j e_i^T \rangle_{\frac{1}{2}} = \check{d}_{ij} \quad \forall (i, j) \in \mathcal{I} \\
 & && \text{rank}(VDV) = 2 \\
 & && D \in \mathbb{EDM}^N
 \end{aligned} \tag{1334}$$

where  $e_i \in \mathbb{R}^N$  is the  $i^{\text{th}}$  member of the standard basis, where set  $\mathcal{I}$  indexes the given distance-square data like that in (1333), where  $V \in \mathbb{R}^{N \times N}$  is the geometric centering matrix (§B.4.1), and where

$$\langle -V, D \rangle = \text{tr}(-VDV) = 2 \text{tr} G = \frac{1}{N} \sum_{i,j} d_{ij} \tag{1000}$$

where  $G$  is the Gram matrix producing  $D$  assuming  $G\mathbf{1} = \mathbf{0}$ .

If the (rank) constraint on affine dimension is ignored, then problem (1334) becomes convex, a corresponding solution  $D^*$  can be found, and a nearest rank-2 solution is then had by ordered eigenvalue decomposition of  $-VD^*V$  followed by *spectral projection* (§7.1.3) on  $\begin{bmatrix} \mathbb{R}_+^2 \\ \mathbf{0} \end{bmatrix} \subset \mathbb{R}^N$ . This two-step process is necessarily suboptimal. Yet because the decomposition for the trefoil knot reveals only two dominant eigenvalues, the spectral projection is nearly benign. Such a reconstruction of point position (§5.12) utilizing four nearest neighbors is drawn in Figure 160b; a low-dimensional embedding of the trefoil knot.

This problem (1334) can, of course, be written equivalently in terms of Gram matrix  $G$ , facilitated by (1006); *videlicet*, for  $\Phi_{ij}$  as in (974)

$$\begin{aligned}
 & \underset{G \in \mathbb{S}_c^N}{\text{maximize}} && \langle I, G \rangle \\
 & \text{subject to} && \langle G, \Phi_{ij} \rangle = \check{d}_{ij} \quad \forall (i, j) \in \mathcal{I} \\
 & && \text{rank } G = 2 \\
 & && G \succeq 0
 \end{aligned} \tag{1335}$$

The advantage to converting EDM to Gram is: Gram matrix  $G$  is a bridge between point list  $X$  and EDM  $D$ ; constraints on any or all of these three variables may now be introduced. (Example 5.4.2.2.8) Confinement to the geometric center subspace  $\mathbb{S}_c^N$  (implicit constraint  $G\mathbf{1} = \mathbf{0}$ ) keeps  $G$  independent of its translation-invariant subspace  $\mathbb{S}_c^{N\perp}$  (§5.5.1.1, Figure 162) so as not to become numerically unbounded.

A problem dual to *maximum variance unfolding problem* (1335) (less the Gram rank constraint) has been called the *fastest mixing Markov process*. That dual has simple interpretations in graph and circuit theory and in mechanical and thermal systems, explored in [357], and has direct application to quick calculation of *PageRank* by search engines [247, §4]. Optimal Gram rank turns out to be tightly bounded above by minimum multiplicity of the second smallest eigenvalue of a dual optimal variable.  $\square$

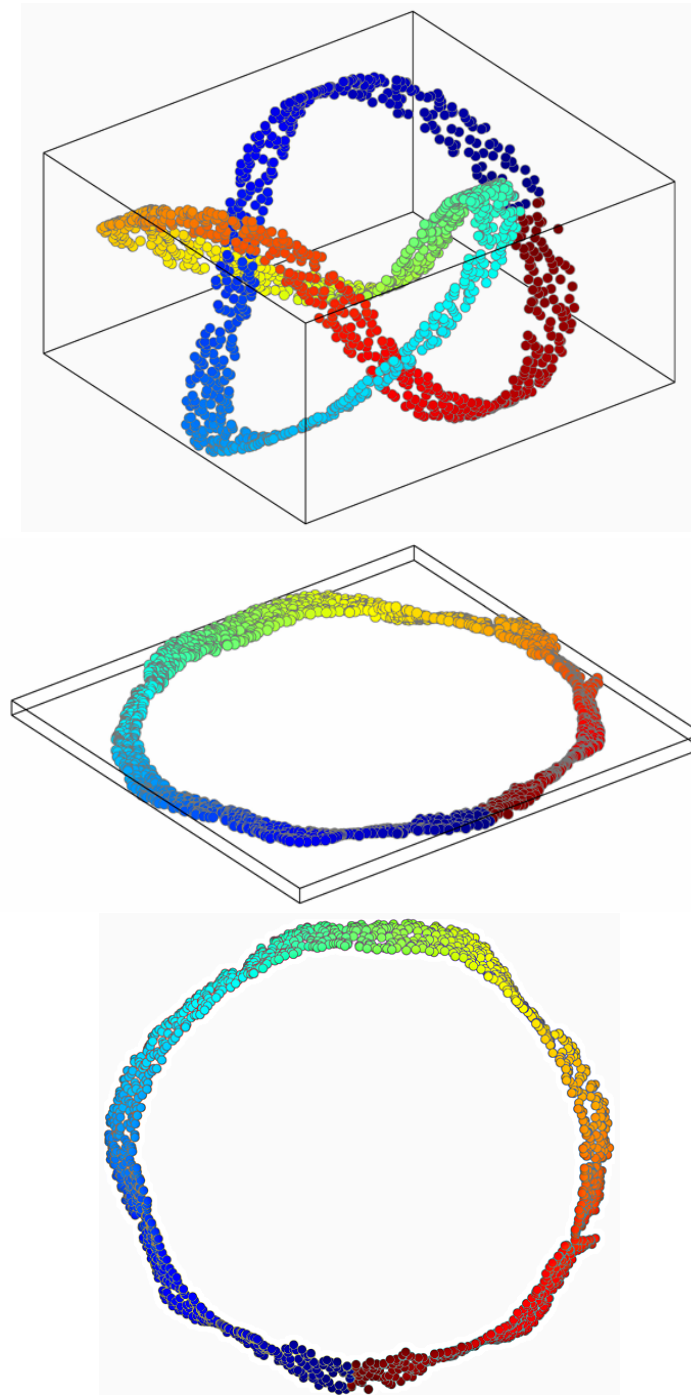


Figure 161: *Trefoil ribbon* (Kilian Weinberger). Same topological transformation algorithm as in Figure 160b with five nearest neighbors and  $N = 1617$  samples.

## 6.8 Dual EDM cone

### 6.8.1 Ambient $\mathbb{S}^N$

We consider finding the ordinary dual EDM cone in ambient space  $\mathbb{S}^N$  where  $\mathbb{EDM}^N$  is pointed, closed, convex, but not full-dimensional. The set of all EDMs in  $\mathbb{S}^N$  is a closed convex cone because it is the intersection of halfspaces about the origin in vectorized variable  $D$  (§2.4.1.1.1, §2.7.2):

$$\mathbb{EDM}^N = \bigcap_{\substack{z \in \mathcal{N}(\mathbf{1}^T) \\ i=1 \dots N}} \left\{ D \in \mathbb{S}^N \mid \langle e_i e_i^T, D \rangle \geq 0, \langle e_i e_i^T, D \rangle \leq 0, \langle z z^T, -D \rangle \geq 0 \right\} \quad (1336)$$

By definition (296), dual cone  $\mathcal{K}^*$  comprises each and every vector inward-normal to a hyperplane supporting convex cone  $\mathcal{K}$ . The dual EDM cone in the ambient space of symmetric matrices is therefore expressible as the aggregate of every conic combination of inward-normals from (1336):

$$\begin{aligned} \mathbb{EDM}^{N*} &= \text{cone}\{e_i e_i^T, -e_j e_j^T \mid i, j = 1 \dots N\} - \text{cone}\{z z^T \mid \mathbf{1}^T z z^T = 0\} \\ &= \left\{ \sum_{i=1}^N \zeta_i e_i e_i^T - \sum_{j=1}^N \xi_j e_j e_j^T \mid \zeta_i, \xi_j \geq 0 \right\} - \text{cone}\{z z^T \mid \mathbf{1}^T z z^T = 0\} \\ &= \{\delta(u) \mid u \in \mathbb{R}^N\} - \text{cone}\left\{V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1}, (\|v\| = 1)\right\} \subset \mathbb{S}^N \\ &= \{\delta^2(Y) - V_{\mathcal{N}} \Psi V_{\mathcal{N}}^T \mid Y \in \mathbb{S}^N, \Psi \in \mathbb{S}_+^{N-1}\} \end{aligned} \quad (1337)$$

The EDM cone is not selfdual in ambient  $\mathbb{S}^N$  because its affine hull belongs to a proper subspace

$$\text{aff } \mathbb{EDM}^N = \mathbb{S}_h^N \quad (1338)$$

The ordinary dual EDM cone cannot, therefore, be pointed. (§2.13.1.1)

When  $N=1$ , the EDM cone is the point at the origin in  $\mathbb{R}$ . Auxiliary matrix  $V_{\mathcal{N}}$  is empty  $[\emptyset]$ , and dual cone  $\mathbb{EDM}^*$  is the real line.

When  $N=2$ , the EDM cone is a nonnegative real line in isometrically isomorphic  $\mathbb{R}^3$ ; there  $\mathbb{S}_h^2$  is a real line containing the EDM cone. Dual cone  $\mathbb{EDM}^{2*}$  is the particular halfspace in  $\mathbb{R}^3$  whose boundary has inward-normal  $\mathbb{EDM}^2$ . Diagonal matrices  $\{\delta(u)\}$  in (1337) are represented by a hyperplane through the origin  $\{\underline{d} \mid [0 \ 1 \ 0] \underline{d} = 0\}$  while the term  $\text{cone}\{V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T\}$  is represented by the halfline  $\mathcal{T}$  in Figure 156 belonging to the positive semidefinite cone boundary. The dual EDM cone is formed by translating the hyperplane along the negative semidefinite halfline  $-\mathcal{T}$ ; the union of each and every translation. (confer §2.10.2.0.1)

When cardinality  $N$  exceeds 2, the dual EDM cone can no longer be polyhedral simply because the EDM cone cannot. (§2.13.1.1)

### 6.8.1.1 EDM cone and its dual in ambient $\mathbb{S}^N$

Consider the two convex cones

$$\begin{aligned}
 \mathcal{K}_1 &\triangleq \mathbb{S}_h^N \\
 \mathcal{K}_2 &\triangleq \bigcap_{y \in \mathcal{N}(\mathbf{1}^T)} \left\{ A \in \mathbb{S}^N \mid \langle yy^T, -A \rangle \geq 0 \right\} \\
 &= \left\{ A \in \mathbb{S}^N \mid -z^T V A V z \geq 0 \quad \forall zz^T (\succeq 0) \right\} \\
 &= \left\{ A \in \mathbb{S}^N \mid -V A V \succeq 0 \right\}
 \end{aligned} \tag{1339}$$

so

$$\mathcal{K}_1 \cap \mathcal{K}_2 = \mathbb{EDM}^N \tag{1340}$$

Dual cone  $\mathcal{K}_1^* = \mathbb{S}_h^{N\perp} \subseteq \mathbb{S}^N$  (72) is the subspace of diagonal matrices. From (1337) via (313),

$$\mathcal{K}_2^* = -\text{cone} \left\{ V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \subset \mathbb{S}^N \tag{1341}$$

Gaffke & Mathar [161, §5.3] observe that projection on  $\mathcal{K}_1$  and  $\mathcal{K}_2$  have simple closed forms: Projection on subspace  $\mathcal{K}_1$  is easily performed by symmetrization and zeroing the main diagonal or *vice versa*, while projection of  $H \in \mathbb{S}^N$  on  $\mathcal{K}_2$  is<sup>6.12</sup>

$$P_{\mathcal{K}_2} H = H - P_{\mathbb{S}_+^N}(V H V) \tag{1342}$$

**Proof.** First, we observe membership of  $H - P_{\mathbb{S}_+^N}(V H V)$  to  $\mathcal{K}_2$  because

$$P_{\mathbb{S}_+^N}(V H V) - H = \left( P_{\mathbb{S}_+^N}(V H V) - V H V \right) + (V H V - H) \tag{1343}$$

The term  $P_{\mathbb{S}_+^N}(V H V) - V H V$  necessarily belongs to the (dual) positive semidefinite cone by Theorem E.9.2.0.1.  $V^2 = V$ , hence

$$-V \left( H - P_{\mathbb{S}_+^N}(V H V) \right) V \succeq 0 \tag{1344}$$

by Corollary A.3.1.0.5.

Next, we require

$$\langle P_{\mathcal{K}_2} H - H, P_{\mathcal{K}_2} H \rangle = 0 \tag{1345}$$

Expanding,

$$\langle -P_{\mathbb{S}_+^N}(V H V), H - P_{\mathbb{S}_+^N}(V H V) \rangle = 0 \tag{1346}$$

$$\langle P_{\mathbb{S}_+^N}(V H V), (P_{\mathbb{S}_+^N}(V H V) - V H V) + (V H V - H) \rangle = 0 \tag{1347}$$

$$\langle P_{\mathbb{S}_+^N}(V H V), (V H V - H) \rangle = 0 \tag{1348}$$

Product  $V H V$  belongs to the geometric center subspace; (§E.7.2.0.2)

$$V H V \in \mathbb{S}_c^N = \{ Y \in \mathbb{S}^N \mid \mathcal{N}(Y) \supseteq \mathbf{1} \} \tag{1349}$$

---

<sup>6.12</sup>  $P_{\mathbb{S}_+^N}(V H V) = \mathbf{0}$  for  $H \in \mathbb{EDM}^N$ .

Diagonalize  $VHV \triangleq Q\Lambda Q^T$  (§A.5) whose nullspace is spanned by the eigenvectors corresponding to 0 eigenvalues by Theorem A.7.3.0.1. Projection of  $VHV$  on the PSD cone (§7.1) simply zeroes negative eigenvalues in diagonal matrix  $\Lambda$ . Then

$$\mathcal{N}(P_{\mathbb{S}_+^N}(VHV)) \supseteq \mathcal{N}(VHV) (\supseteq \mathcal{N}(V)) \quad (1350)$$

from which it follows:

$$P_{\mathbb{S}_+^N}(VHV) \in \mathbb{S}_c^N \quad (1351)$$

so  $P_{\mathbb{S}_+^N}(VHV) \perp (VHV - H)$  because  $VHV - H \in \mathbb{S}_c^{N\perp}$ .

Finally, we must have  $P_{\mathcal{K}_2}H - H = -P_{\mathbb{S}_+^N}(VHV) \in \mathcal{K}_2^*$ . Dual cone  $\mathcal{K}_2^* = -\mathcal{F}(\mathbb{S}_+^N \ni V)$  is the negative of the positive semidefinite cone's smallest face that contains auxiliary matrix  $V$ . (§6.6.1) Thus  $P_{\mathbb{S}_+^N}(VHV) \in \mathcal{F}(\mathbb{S}_+^N \ni V) \Leftrightarrow \mathcal{N}(P_{\mathbb{S}_+^N}(VHV)) \supseteq \mathcal{N}(V)$  (§2.9.2.3) which was already established in (1350).  $\blacklozenge$

From results in §E.7.2.0.2 we know: matrix product  $VHV = P_{\mathbb{S}_c^N}H$  is the orthogonal projection of  $H \in \mathbb{S}^N$  on the geometric center subspace  $\mathbb{S}_c^N$ . Thus the projection product

$$P_{\mathcal{K}_2}H = H - P_{\mathbb{S}_+^N}P_{\mathbb{S}_c^N}H \quad (1352)$$

**6.8.1.1.1 Lemma.** *Projection on PSD cone  $\cap$  geometric center subspace.*

$$P_{\mathbb{S}_+^N \cap \mathbb{S}_c^N} = P_{\mathbb{S}_+^N}P_{\mathbb{S}_c^N} \quad (1353)$$

$\diamond$

**Proof.** For each and every  $H \in \mathbb{S}^N$ , projection of  $P_{\mathbb{S}_c^N}H$  on the positive semidefinite cone remains in the geometric center subspace

$$\begin{aligned} \mathbb{S}_c^N &= \{G \in \mathbb{S}^N \mid G\mathbf{1} = \mathbf{0}\} \\ &= \{G \in \mathbb{S}^N \mid \mathcal{N}(G) \supseteq \mathbf{1}\} = \{G \in \mathbb{S}^N \mid \mathcal{R}(G) \subseteq \mathcal{N}(\mathbf{1}^T)\} \quad (1078) \\ &= \{VYV \mid Y \in \mathbb{S}^N\} \subset \mathbb{S}^N \end{aligned}$$

That is because: eigenvectors of  $P_{\mathbb{S}_c^N}H$ , corresponding to 0 eigenvalues, span its nullspace  $\mathcal{N}(P_{\mathbb{S}_c^N}H)$ . (§A.7.3.0.1) To project  $P_{\mathbb{S}_c^N}H$  on the positive semidefinite cone, its negative eigenvalues are zeroed. (§7.1.2) The nullspace is thereby expanded while eigenvectors originally spanning  $\mathcal{N}(P_{\mathbb{S}_c^N}H)$  remain intact. Because the geometric center subspace is invariant to projection on the PSD cone, then the rule for projection on a convex set in a subspace governs (§E.9.5, projectors do not commute) and statement (1353) follows directly.  $\blacklozenge$

From the lemma it follows

$$\{P_{\mathbb{S}_+^N}P_{\mathbb{S}_c^N}H \mid H \in \mathbb{S}^N\} = \{P_{\mathbb{S}_+^N \cap \mathbb{S}_c^N}H \mid H \in \mathbb{S}^N\} \quad (1354)$$

Then from (2141)

$$-(\mathbb{S}_c^N \cap \mathbb{S}_+^N)^* = \{H - P_{\mathbb{S}_+^N}P_{\mathbb{S}_c^N}H \mid H \in \mathbb{S}^N\} \quad (1355)$$

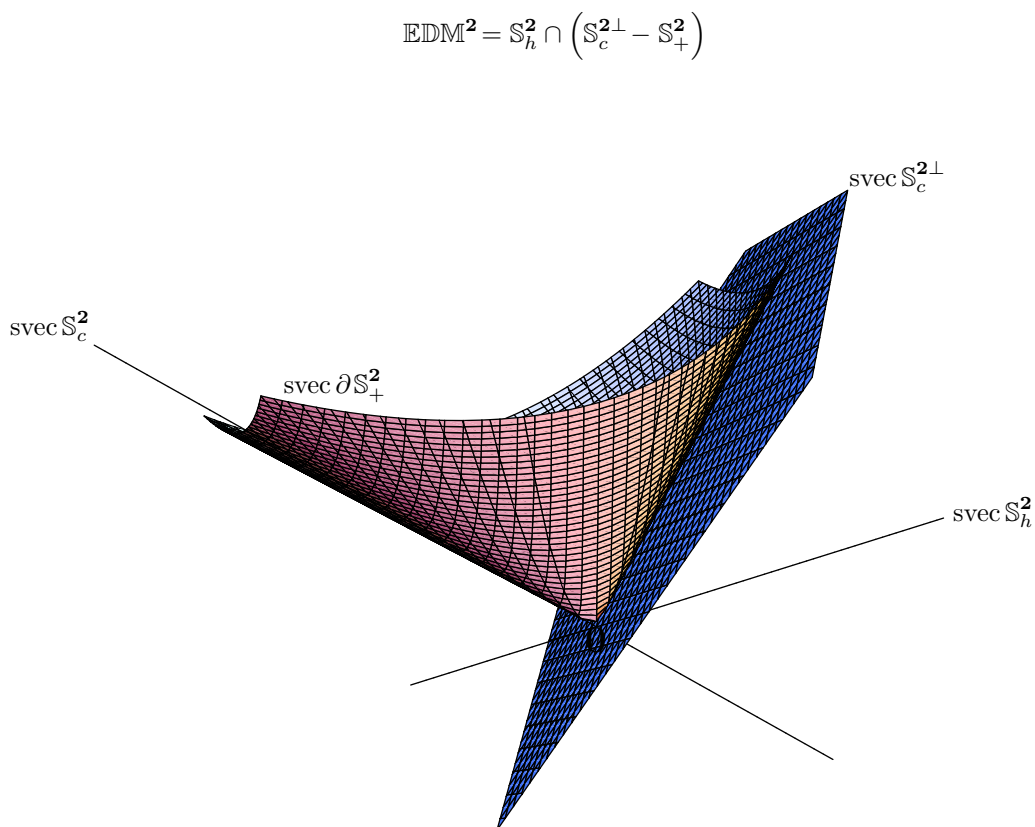


Figure 162: A plane in isometrically isomorphic  $\mathbb{R}^3$ , orthogonal complement  $\mathbb{S}_c^{2\perp}$  (2115) (§B.2) of geometric center subspace (tiled fragment drawn) apparently supports PSD cone (rounded vertex is plot artifact). Line  $\text{svec } \mathbb{S}_c^2 = \text{aff cone } \mathcal{T}$  (1329), intersecting  $\text{svec } \partial \mathbb{S}_+^2$  and drawn in Figure 156, runs along PSD cone boundary. (confer Figure 143)



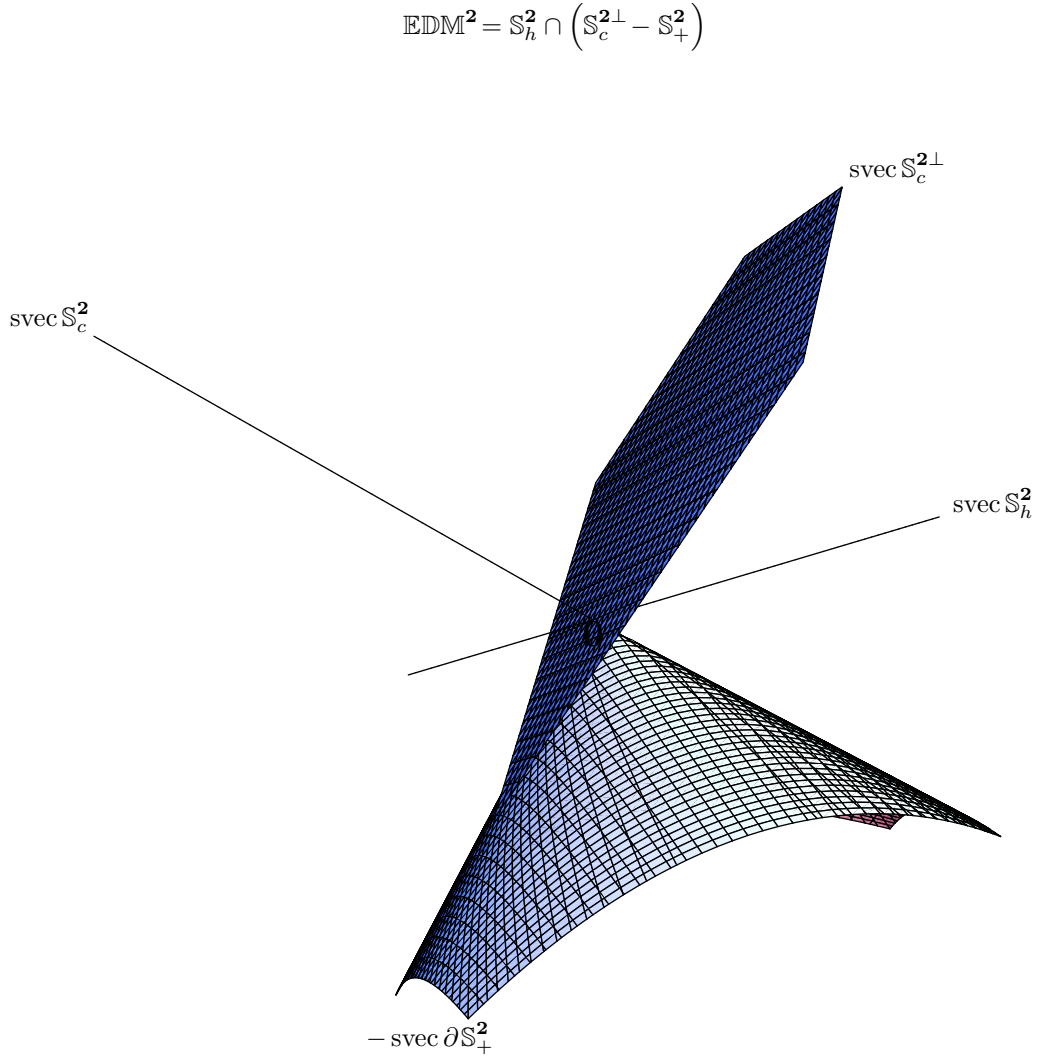


Figure 163: EDM cone construction in isometrically isomorphic  $\mathbb{R}^3$  by adding polar PSD cone to  $\text{svec } \mathbb{S}_c^{2\perp}$ . Difference  $\text{svec}(\mathbb{S}_c^{2\perp} - \mathbb{S}_+^2)$  is halfspace partially bounded by  $\text{svec } \mathbb{S}_c^{2\perp}$ . EDM cone is nonnegative halfline along  $\text{svec } \mathbb{S}_h^2$  in this dimension.

From (313) we get closure of a vector sum

$$\mathcal{K}_2 = -(\mathbb{S}_c^N \cap \mathbb{S}_+^N)^* = \mathbb{S}_c^{N\perp} - \mathbb{S}_+^N \quad (1356)$$

therefore the equality [106]

$$\text{EDM}^N = \mathcal{K}_1 \cap \mathcal{K}_2 = \mathbb{S}_h^N \cap (\mathbb{S}_c^{N\perp} - \mathbb{S}_+^N) \quad (1357)$$

whose veracity is intuitively evident, in hindsight, [93, p.109] from the most fundamental EDM definition (976).<sup>6.13</sup> A realization of this construction in low dimension is illustrated in Figure 162 and Figure 163.

The dual EDM cone follows directly from (1357) by standard properties of cones (§2.13.1.1):

$$\text{EDM}^{N*} = \overline{\mathcal{K}_1^* + \mathcal{K}_2^*} = \mathbb{S}_h^{N\perp} - \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1358)$$

which bears strong resemblance to (1337).

### 6.8.1.2 nonnegative orthant contains $\text{EDM}^N$

That  $\text{EDM}^N$  is a proper subset of the nonnegative orthant is not obvious from (1357). We wish to verify

$$\text{EDM}^N = \mathbb{S}_h^N \cap (\mathbb{S}_c^{N\perp} - \mathbb{S}_+^N) \subset \mathbb{R}_+^{N \times N} \quad (1359)$$

While there are many ways to prove this, it is sufficient to show that all entries of the extreme directions of  $\text{EDM}^N$  must be nonnegative; *id est*, for any particular nonzero vector  $z = [z_i, i=1 \dots N] \in \mathcal{N}(\mathbf{1}^T)$  (§6.4.3.2),

$$\delta(zz^T)\mathbf{1}^T + \mathbf{1}\delta(zz^T)^T - 2zz^T \geq \mathbf{0} \quad (1360)$$

where the inequality denotes entrywise comparison. The inequality holds because the  $i, j^{\text{th}}$  entry of an extreme direction is squared:  $(z_i - z_j)^2$ .

We observe that the dyad  $2zz^T \in \mathbb{S}_+^N$  belongs to the positive semidefinite cone, the doublet

$$\delta(zz^T)\mathbf{1}^T + \mathbf{1}\delta(zz^T)^T \in \mathbb{S}_c^{N\perp} \quad (1361)$$

to the orthogonal complement (2115) of the geometric center subspace, while their difference is a member of the symmetric hollow subspace  $\mathbb{S}_h^N$ . ♦

Here is an algebraic method to prove nonnegativity: Suppose we are given  $A \in \mathbb{S}_c^{N\perp}$  and  $B = [B_{ij}] \in \mathbb{S}_+^N$  and  $A - B \in \mathbb{S}_h^N$ . Then we have, for some vector  $u$ ,  $A = u\mathbf{1}^T + \mathbf{1}u^T = [A_{ij}] = [u_i + u_j]$  and  $\delta(B) = \delta(A) = 2u$ . Positive semidefiniteness of  $B$  requires nonnegativity  $A - B \geq \mathbf{0}$  because

$$(e_i - e_j)^T B (e_i - e_j) = (B_{ii} - B_{ij}) - (B_{ji} - B_{jj}) = 2(u_i + u_j) - 2B_{ij} \geq 0 \quad (1362)$$

♦

<sup>6.13</sup> Formula (1357) is not a matrix criterion for membership to the EDM cone, it is not an EDM definition, and it is not an equivalence between EDM operators or an isomorphism. Rather, it is a recipe for constructing the EDM cone whole from large Euclidean bodies: the positive semidefinite cone, orthogonal complement of the geometric center subspace, and symmetric hollow subspace.

### 6.8.1.3 Dual Euclidean distance matrix criterion

Conditions necessary for membership of a matrix  $D^* \in \mathbb{S}^N$  to the dual EDM cone  $\mathbb{EDM}^{N*}$  may be derived from (1337):  $D^* \in \mathbb{EDM}^{N*} \Rightarrow D^* = \delta(y) - V_N A V_N^T$  for some vector  $y$  and positive semidefinite matrix  $A \in \mathbb{S}_+^{N-1}$ . This in turn implies  $\delta(D^* \mathbf{1}) = \delta(y)$ . Then, for  $D^* \in \mathbb{S}^N$

$$D^* \in \mathbb{EDM}^{N*} \Leftrightarrow \delta(D^* \mathbf{1}) - D^* \succeq 0 \quad (1363)$$

where, for any symmetric matrix  $D^*$

$$\delta(D^* \mathbf{1}) - D^* \in \mathbb{S}_c^N \quad (1364)$$

To show sufficiency of the matrix criterion in (1363), recall Gram-form EDM operator

$$\mathbf{D}(G) = \delta(G) \mathbf{1}^T + \mathbf{1} \delta(G)^T - 2G \quad (988)$$

where Gram matrix  $G$  is positive semidefinite by definition, and recall the selfadjointness property of the main-diagonal linear operator  $\delta$  (§A.1):

$$\langle D, D^* \rangle = \langle \delta(G) \mathbf{1}^T + \mathbf{1} \delta(G)^T - 2G, D^* \rangle = \langle G, \delta(D^* \mathbf{1}) - D^* \rangle 2 \quad (1006)$$

Assuming  $\langle G, \delta(D^* \mathbf{1}) - D^* \rangle \geq 0$  (1574), then we have known membership relation (§2.13.2.0.1)

$$D^* \in \mathbb{EDM}^{N*} \Leftrightarrow \langle D, D^* \rangle \geq 0 \quad \forall D \in \mathbb{EDM}^N \quad (1365)$$

◆

Elegance of this matrix criterion (1363) for membership to the dual EDM cone derives from lack of any other assumptions except that  $D^*$  be symmetric:<sup>6.14</sup> Linear Gram-form EDM operator  $\mathbf{D}(Y)$  (988) has adjoint, for  $Y \in \mathbb{S}^N$

$$\mathbf{D}^T(Y) \triangleq (\delta(Y \mathbf{1}) - Y) 2 \quad (1366)$$

Then from (1365) and (989) we have: [93, p.111]

$$\begin{aligned} \mathbb{EDM}^{N*} &= \{D^* \in \mathbb{S}^N \mid \langle D, D^* \rangle \geq 0 \quad \forall D \in \mathbb{EDM}^N\} \\ &= \{D^* \in \mathbb{S}^N \mid \langle \mathbf{D}(G), D^* \rangle \geq 0 \quad \forall G \in \mathbb{S}_+^N\} \\ &= \{D^* \in \mathbb{S}^N \mid \langle G, \mathbf{D}^T(D^*) \rangle \geq 0 \quad \forall G \in \mathbb{S}_+^N\} \\ &= \{D^* \in \mathbb{S}^N \mid \delta(D^* \mathbf{1}) - D^* \succeq 0\} \end{aligned} \quad (1367)$$

the dual EDM cone expressed in terms of the adjoint operator. A dual EDM cone determined this way is illustrated in Figure 165.

#### 6.8.1.3.1 Exercise. Dual EDM spectral cone.

Find a spectral cone as in §5.11.2 corresponding to  $\mathbb{EDM}^{N*}$ .

▼

<sup>6.14</sup>Recall: Schoenberg criterion (995) for membership to the EDM cone requires membership to the symmetric hollow subspace.

$$D^\circ = \delta(D^\circ \mathbf{1}) + (D^\circ - \delta(D^\circ \mathbf{1})) \in \mathbb{S}_h^{N\perp} \oplus \mathbb{S}_c^N \cap \mathbb{S}_+^N = \mathbb{EDM}^{N^\circ}$$

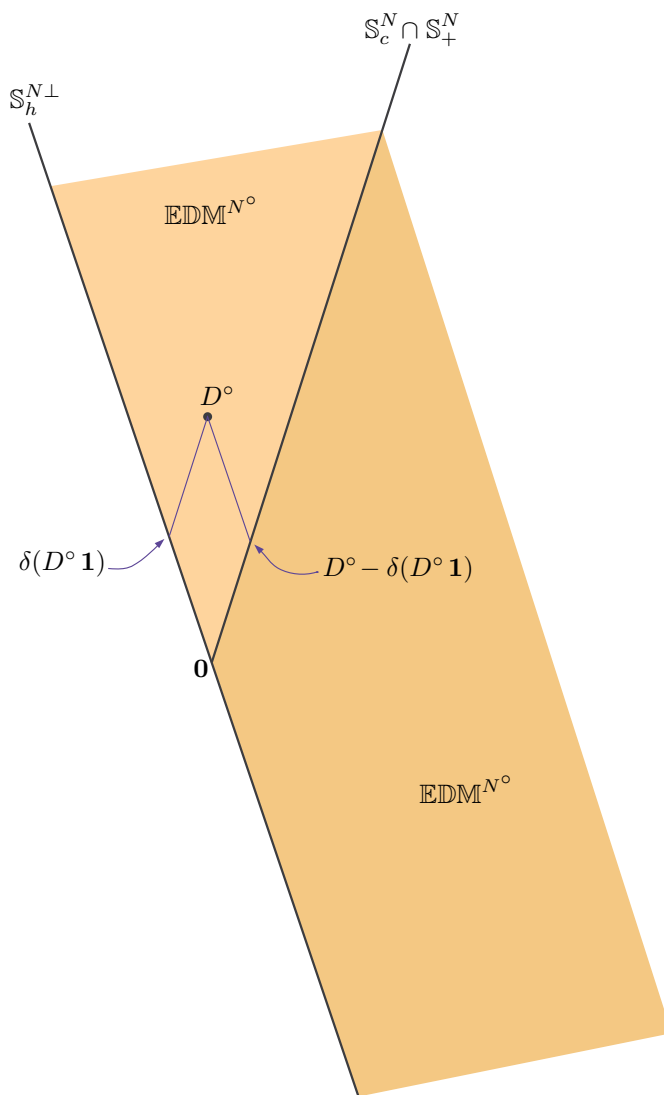


Figure 164: [Hand-drawn abstraction](#) of polar EDM cone  $\mathbb{EDM}^{N^\circ}$  (drawn truncated). Any member  $D^\circ$  of polar EDM cone can be decomposed into two linearly independent nonorthogonal components:  $\delta(D^\circ \mathbf{1})$  and  $D^\circ - \delta(D^\circ \mathbf{1})$ .

#### 6.8.1.4 Nonorthogonal components of dual EDM

Now we tie construct (1358) for the dual EDM cone together with the matrix criterion (1363) for dual EDM cone membership. For any  $D^* \in \mathbb{S}^N$  it is obvious:

$$\delta(D^* \mathbf{1}) \in \mathbb{S}_h^{N\perp} \quad (1368)$$

any diagonal matrix belongs to the subspace of diagonal matrices (67). We know when  $D^* \in \text{EDM}^{N*}$

$$\delta(D^* \mathbf{1}) - D^* \in \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1369)$$

this adjoint expression (1366) belongs to that face (1327) of the positive semidefinite cone  $\mathbb{S}_+^N$  in the geometric center subspace. Any nonzero dual EDM

$$D^* = \delta(D^* \mathbf{1}) - (\delta(D^* \mathbf{1}) - D^*) \in \mathbb{S}_h^{N\perp} \ominus \mathbb{S}_c^N \cap \mathbb{S}_+^N = \text{EDM}^{N*} \quad (1370)$$

can therefore be expressed as the difference of two linearly independent (when vectorized) nonorthogonal components (Figure 143, Figure 164).

#### 6.8.1.5 Affine dimension complementarity

From §6.8.1.3 we have, for some  $A \in \mathbb{S}_+^{N-1}$  (confer (1369))

$$\delta(D^* \mathbf{1}) - D^* = V_{\mathcal{N}} A V_{\mathcal{N}}^T \in \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1371)$$

if and only if  $D^*$  belongs to the dual EDM cone. Call  $\text{rank}(V_{\mathcal{N}} A V_{\mathcal{N}}^T)$  *dual affine dimension*. Empirically, we find a complementary relationship in affine dimension between the projection of some arbitrary symmetric matrix  $H$  on the polar EDM cone,  $\text{EDM}^{N^\circ} = -\text{EDM}^{N*}$ , and its projection on the EDM cone; *id est*, the optimal solution of 6.15

$$\begin{aligned} & \underset{D^\circ \in \mathbb{S}^N}{\text{minimize}} && \|D^\circ - H\|_F \\ & \text{subject to} && D^\circ - \delta(D^\circ \mathbf{1}) \succeq 0 \end{aligned} \quad (1372)$$

has dual affine dimension complementary to affine dimension corresponding to the optimal solution of

$$\begin{aligned} & \underset{D \in \mathbb{S}_h^N}{\text{minimize}} && \|D - H\|_F \\ & \text{subject to} && -V_{\mathcal{N}}^T D V_{\mathcal{N}} \succeq 0 \end{aligned} \quad (1373)$$

Precisely,

$$\text{rank}(D^{\circ*} - \delta(D^{\circ*} \mathbf{1})) + \text{rank}(V_{\mathcal{N}}^T D^* V_{\mathcal{N}}) = N - 1 \quad (1374)$$

**6.15** This polar projection can be solved quickly (without semidefinite programming) via Lemma 6.8.1.1.1; rewriting,

$$\begin{aligned} & \underset{D^\circ \in \mathbb{S}^N}{\text{minimize}} && \|(D^\circ - \delta(D^\circ \mathbf{1})) - (H - \delta(D^\circ \mathbf{1}))\|_F \\ & \text{subject to} && D^\circ - \delta(D^\circ \mathbf{1}) \succeq 0 \end{aligned}$$

which is the projection of affinely transformed optimal solution  $H - \delta(D^{\circ*} \mathbf{1})$  on  $\mathbb{S}_c^N \cap \mathbb{S}_+^N$ ;

$$D^{\circ*} - \delta(D^{\circ*} \mathbf{1}) = P_{\mathbb{S}_+^N} P_{\mathbb{S}_c^N} (H - \delta(D^{\circ*} \mathbf{1}))$$

Foreknowledge of an optimal solution  $D^{\circ*}$  as argument to projection suggests recursion.

and  $\text{rank}(D^{\circ*} - \delta(D^{\circ*} \mathbf{1})) \leq N - 1$  because vector  $\mathbf{1}$  is always in the nullspace of rank's argument. This is similar to the known result for projection on the selfdual positive semidefinite cone and its polar:

$$\text{rank } P_{-\mathbb{S}_+^N} H + \text{rank } P_{\mathbb{S}_+^N} H = N \quad (1375)$$

When low affine dimension is a desirable result of projection on the EDM cone, projection on the polar EDM cone should be performed instead. Convex polar problem (1372) can be solved for  $D^{\circ*}$  by transforming to an equivalent Schur-form semidefinite program (§3.5.2). Interior-point methods for numerically solving semidefinite programs tend to produce high-rank solutions. (§4.1.2) Then  $D^* = H - D^{\circ*} \in \text{EDM}^N$  by Corollary E.9.2.2.1, and  $D^*$  will tend to have low affine dimension. This approach breaks when attempting projection on a cone subset discriminated by affine dimension or rank, because then we have no complementarity relation like (1374) or (1375) (§7.1.4.1).

#### 6.8.1.6 EDM cone is not selfdual

In §5.6.1.1, via Gram-form EDM operator

$$\mathbf{D}(G) = \delta(G) \mathbf{1}^T + \mathbf{1} \delta(G)^T - 2G \in \text{EDM}^N \iff G \succeq 0 \quad (988)$$

we established clear connection between the EDM cone and that face (1327) of positive semidefinite cone  $\mathbb{S}_+^N$  in the geometric center subspace:

$$\text{EDM}^N = \mathbf{D}(\mathbb{S}_c^N \cap \mathbb{S}_+^N) \quad (1095)$$

$$\mathbf{V}(\text{EDM}^N) = \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1096)$$

where

$$\mathbf{V}(D) = -VDV^{\frac{1}{2}} \quad (1084)$$

In §5.6.1 we established

$$\mathbb{S}_c^N \cap \mathbb{S}_+^N = V_{\mathcal{N}} \mathbb{S}_+^{N-1} V_{\mathcal{N}}^T \quad (1082)$$

Then from (1363), (1371), and (1337) we can deduce

$$\delta(\text{EDM}^{N*} \mathbf{1}) - \text{EDM}^{N*} = V_{\mathcal{N}} \mathbb{S}_+^{N-1} V_{\mathcal{N}}^T = \mathbb{S}_c^N \cap \mathbb{S}_+^N \quad (1376)$$

which, by (1095) and (1096), means the EDM cone can be related to the dual EDM cone by an equality:

$$\text{EDM}^N = \mathbf{D}(\delta(\text{EDM}^{N*} \mathbf{1}) - \text{EDM}^{N*}) \quad (1377)$$

$$\mathbf{V}(\text{EDM}^N) = \delta(\text{EDM}^{N*} \mathbf{1}) - \text{EDM}^{N*} \quad (1378)$$

This means projection  $-\mathbf{V}(\text{EDM}^N)$  of the EDM cone on the geometric center subspace  $\mathbb{S}_c^N$  (§E.7.2.0.2) is a linear transformation of the dual EDM cone:  $\text{EDM}^{N*} - \delta(\text{EDM}^{N*} \mathbf{1})$ . Secondly, it means the EDM cone is not selfdual in  $\mathbb{S}^N$ .

### 6.8.1.7 Schoenberg criterion is discretized membership relation

We show the Schoenberg criterion

$$\left. \begin{array}{l} -V_{\mathcal{N}}^T D V_{\mathcal{N}} \in \mathbb{S}_+^{N-1} \\ D \in \mathbb{S}_h^N \end{array} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (995)$$

to be a discretized membership relation (§2.13.4) between a closed convex cone  $\mathcal{K}$  and its dual  $\mathcal{K}^*$  like

$$\langle y, x \rangle \geq 0 \text{ for all } y \in \mathcal{G}(\mathcal{K}^*) \Leftrightarrow x \in \mathcal{K} \quad (365)$$

where  $\mathcal{G}(\mathcal{K}^*)$  is any set of generators whose conic hull constructs closed convex dual cone  $\mathcal{K}^*$ :

The Schoenberg criterion is the same as

$$\left. \begin{array}{l} \langle zz^T, -D \rangle \geq 0 \quad \forall zz^T \mid \mathbf{1}\mathbf{1}^T zz^T = \mathbf{0} \\ D \in \mathbb{S}_h^N \end{array} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (1321)$$

which, by (1322), is the same as

$$\left. \begin{array}{l} \langle zz^T, -D \rangle \geq 0 \quad \forall zz^T \in \left\{ V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \\ D \in \mathbb{S}_h^N \end{array} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (1379)$$

where the  $zz^T$  constitute a set of generators  $\mathcal{G}$  for the positive semidefinite cone's smallest face  $\mathcal{F}(\mathbb{S}_+^N \ni V)$  (§6.6.1) that contains auxiliary matrix  $V$ . From the aggregate in (1337) we get the ordinary membership relation, assuming only  $D \in \mathbb{S}^N$  [215, p.58]

$$\langle D^*, D \rangle \geq 0 \quad \forall D^* \in \text{EDM}^{N*} \Leftrightarrow D \in \text{EDM}^N \quad (1380)$$

$$\langle D^*, D \rangle \geq 0 \quad \forall D^* \in \{ \delta(u) \mid u \in \mathbb{R}^N \} - \text{cone} \left\{ V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \Leftrightarrow D \in \text{EDM}^N$$

Discretization (365) yields:

$$\langle D^*, D \rangle \geq 0 \quad \forall D^* \in \{ e_i e_i^T, -e_j e_j^T, -V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid i, j = 1 \dots N, v \in \mathbb{R}^{N-1} \} \Leftrightarrow D \in \text{EDM}^N \quad (1381)$$

Because  $\langle \{ \delta(u) \mid u \in \mathbb{R}^N \}, D \rangle \geq 0 \Leftrightarrow D \in \mathbb{S}_h^N$ , we can restrict observation to the symmetric hollow subspace without loss of generality. Then for  $D \in \mathbb{S}_h^N$

$$\langle D^*, D \rangle \geq 0 \quad \forall D^* \in \left\{ -V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \Leftrightarrow D \in \text{EDM}^N \quad (1382)$$

this discretized membership relation becomes (1379); identical to the Schoenberg criterion.

Hitherto a correspondence between the EDM cone and a face of a PSD cone, the Schoenberg criterion is now accurately interpreted as a discretized membership relation between the EDM cone and its ordinary dual.

### 6.8.2 Ambient $\mathbb{S}_h^N$

When instead we consider the ambient space of symmetric hollow matrices (1338), then still we find the EDM cone is not selfdual for  $N > 2$ . The simplest way to prove this is as follows:

Given a set of generators  $\mathcal{G} = \{\Gamma\}$  (1298) for the pointed closed convex EDM cone, the *discretized membership theorem* in §2.13.4.2.1 asserts that members of the dual EDM cone in the ambient space of symmetric hollow matrices can be discerned via discretized membership relation:

$$\begin{aligned} \text{EDM}^{N*} \cap \mathbb{S}_h^N &\triangleq \{D^* \in \mathbb{S}_h^N \mid \langle \Gamma, D^* \rangle \geq 0 \quad \forall \Gamma \in \mathcal{G}(\text{EDM}^N)\} \\ &= \{D^* \in \mathbb{S}_h^N \mid \langle \delta(zz^T)\mathbf{1}^T + \mathbf{1}\delta(zz^T)^T - 2zz^T, D^* \rangle \geq 0 \quad \forall z \in \mathcal{N}(\mathbf{1}^T)\} \\ &= \{D^* \in \mathbb{S}_h^N \mid \langle \mathbf{1}\delta(zz^T)^T - zz^T, D^* \rangle \geq 0 \quad \forall z \in \mathcal{N}(\mathbf{1}^T)\} \end{aligned} \quad (1383)$$

By comparison

$$\text{EDM}^N = \{D \in \mathbb{S}_h^N \mid \langle -zz^T, D \rangle \geq 0 \quad \forall z \in \mathcal{N}(\mathbf{1}^T)\} \quad (1384)$$

the term  $\delta(zz^T)^T D^* \mathbf{1}$  foils any hope of selfdualness in ambient  $\mathbb{S}_h^N$ . ♦

To find the dual EDM cone in ambient  $\mathbb{S}_h^N$  per §2.13.9.4 we prune the aggregate in (1337) describing the ordinary dual EDM cone, removing any member having nonzero main diagonal:

$$\begin{aligned} \text{EDM}^{N*} \cap \mathbb{S}_h^N &= \text{cone} \left\{ \delta^2(V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T) - V_{\mathcal{N}} v v^T V_{\mathcal{N}}^T \mid v \in \mathbb{R}^{N-1} \right\} \\ &= \{ \delta^2(V_{\mathcal{N}} \Psi V_{\mathcal{N}}^T) - V_{\mathcal{N}} \Psi V_{\mathcal{N}}^T \mid \Psi \in \mathbb{S}_+^{N-1} \} \end{aligned} \quad (1385)$$

When  $N=1$ , the EDM cone and its dual in ambient  $\mathbb{S}_h$  each comprise the origin in isomorphic  $\mathbb{R}^0$ ; thus, selfdual in this dimension. (*confer*(104))

When  $N=2$ , the EDM cone is the nonnegative real line in isomorphic  $\mathbb{R}$ . (Figure 156)  $\text{EDM}^{2*}$  in  $\mathbb{S}_h^2$  is identical, thus selfdual in this dimension. This result is in agreement with (1383), verified directly: for all  $\kappa \in \mathbb{R}$ ,  $z = \kappa \begin{bmatrix} 1 \\ -1 \end{bmatrix}$  and

$$\delta(zz^T) = \kappa^2 \begin{bmatrix} 1 \\ 1 \end{bmatrix} \Rightarrow d_{12}^* \geq 0.$$

The first case adverse to selfdualness  $N=3$  may be deduced from Figure 152; the EDM cone is a circular cone in isomorphic  $\mathbb{R}^3$  corresponding to no rotation of Lorentz cone (178) (the selfdual circular cone). Figure 165 illustrates the EDM cone and its dual in ambient  $\mathbb{S}_h^3$ ; no longer selfdual.

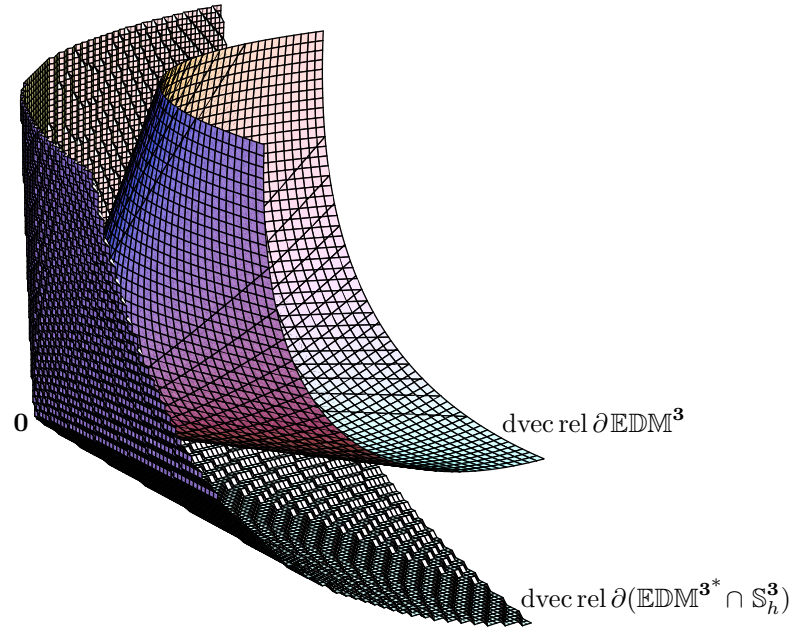
#### 6.8.2.0.1 Exercise. Positive semidefinite cone from EDM cone.

What, if any, is the inversion of semidefinite and distance cone equality (1357)? That is to say, can  $\mathbb{S}_+$  be expressed only in terms of  $\text{EDM}$ ,  $\mathbb{S}_h$ , and  $\mathbb{S}_c$ ? ▼

#### 6.8.2.0.2 Exercise. Rank complementarity for EDM cone.

Prove (1374). ▼





$$D^* \in \text{EDM}^{N^*} \Leftrightarrow \delta(D^* \mathbf{1}) - D^* \succeq 0 \quad (1363)$$

Figure 165: Ordinary dual EDM cone projected on  $\mathbb{S}_h^3$  shrouds  $\text{EDM}^3$ ; drawn tiled in isometrically isomorphic  $\mathbb{R}^3$ . (It so happens: intersection  $\text{EDM}^{N^*} \cap \mathbb{S}_h^N$  (§2.13.9.3) is identical to projection of dual EDM cone on  $\mathbb{S}_h^N$ .)

## 6.9 Theorem of the alternative

In §2.13.2.1.1 we showed how alternative systems of generalized inequality can be derived from closed convex cones and their duals. This section is, therefore, a fitting postscript to the discussion of the dual EDM cone.

**6.9.0.0.3 Theorem.** *EDM alternative.* [179, §1]  
Given  $D \in \mathbb{S}_h^N$

$$\begin{aligned} & D \in \text{EDM}^N \\ & \text{or in the alternative} \\ & \exists z \text{ such that } \begin{cases} \mathbf{1}^T z = 1 \\ Dz = \mathbf{0} \end{cases} \end{aligned} \quad (1386)$$

In words, either  $\mathcal{N}(D)$  intersects hyperplane  $\{z \mid \mathbf{1}^T z = 1\}$  or  $D$  is an EDM; the alternatives are incompatible.  $\diamond$

When  $D$  is an EDM [275, §2]

$$\mathcal{N}(D) \subset \mathcal{N}(\mathbf{1}^T) = \{z \mid \mathbf{1}^T z = 0\} \quad (1387)$$

Because [179, §2] (§E.0.1)

$$\begin{aligned} DD^\dagger \mathbf{1} &= \mathbf{1} \\ \mathbf{1}^T D^\dagger D &= \mathbf{1}^T \end{aligned} \quad (1388)$$

then

$$\mathcal{R}(\mathbf{1}) \subset \mathcal{R}(D) \quad (1389)$$

## 6.10 Postscript

We provided an equality (1357) relating the convex cone of Euclidean distance matrices to the convex cone of positive semidefinite matrices. Projection on a positive semidefinite cone, constrained by an upper bound on rank, is easy and well known; [140] simply, a matter of truncating a list of eigenvalues. Projection on a positive semidefinite cone with such a rank constraint is, in fact, a convex optimization problem. (§7.1.4)

In the past, it was difficult to project on the EDM cone under a constraint on rank or affine dimension. A surrogate method was to invoke the Schoenberg criterion (995) and then project on a positive semidefinite cone under a rank constraint bounding affine dimension from above. But a solution acquired that way is necessarily suboptimal.

In §7.3.3 we present a method for projecting directly on the EDM cone under a constraint on rank or affine dimension.