Some Properties of Euclidean Distance Matrices and Elliptic Matrices

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SOME PROPERTIES OF EUCLIDEAN DISTANCE MATRICES AND ELLIPTIC MATRICES*

by

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1.- INTRODUCTION

Euclidean Distance Matrices ($EDMs$) have been studied lately not only for their intrinsic interest, but also because of their important applications in statistics and molecular conformations in Chemistry among others.

Many important result have been established about the structure of the cone of $EDMs$, however some interesting questions have not yet been answered.

In this paper we deal with the relation between EDMs and special elliptic matrices [HT] [F]. Special elliptic matrices have only one simple positive eigenvalue and zero entries on the diagonal. In the papers mentioned above it is proved that every EDM is special elliptic.

For every EDM D, $Dx = e$ always has a solution as happen for most of the special elliptic matrices, the parameter $e^t x$, where x is a solution of this system, plays an important role in the results obtained. This parameter allows us to say whether or not a special elliptic matrix is EDM. This same parameter was studied in [THW] to characterize Circum-Euclidean Distance Matrices.

The border of EDMs is characterized in terms of the maximum Rayleigh quotient on the subspace M (the orthogonal complement to the subspace generated by the vector of all ones).

We also study the eigenvalue eigenvector structure determined by the rank deficient matrices in the border of the the cone of EDMs as well as properties of the borders of both sets.

The organization of the paper is as follows: In section 2 we present basic results and definitions. Results about eigenvalue-eigenvector structure are in section 3 and properties of the border of EDMs in the next section. In section 5 we present a characterization of EDMs and we also characterize the border of this cone. In the last section we look at some simple but interesting examples.

2.- PRELIMINARIES

The set of symmetric matrices of order n will be denoted by S_n. In this space we will consider special subsets that we now describe. First of all, $\mathcal{H}_n$ will denote the matrices in S_n such that the diagonal entries are zero (hollow matrices). We will denote by Ω_n the set of symmetric positive semidefinite matrices. A matrix D is elliptic if it has a simple positive eigenvalue and the other $n-1$ are nonpositive; it is special elliptic if it is elliptic

and hollow. We are interested in most of this paper in the nonnegative special elliptic matrices that we will denote by $\mathcal{E}_n^+$, i.e., the nonnegative special elliptic matrices.
A matrix D is called a Euclidean Distance Matrix if there are n points $x_1, \ldots, x_n \in R^r$ such that

$$d_{ij} = ||x_i - x_j||_2^2.$$

Observe that the entries of D are square distances. The set of all EDMs of order n form a convex cone that we denote by Λ_n.
There are well known relations between the sets Ω_n, Λ_n and $\mathcal{E}_n^+$ that we have introduced. The EDMs are the image under a linear transformation of the cone Ω_n [G] [JT]. Given $B \in \Omega_n$ we define the linear transformation

$$\kappa(B) = be^t + eb^t - 2B$$

where e is the vector of all ones with appropriate dimension and b is a vector with the diagonal entries of B.
It is well known that $D = \kappa(B) \in \Lambda_n$ if $B \in \Omega_n$, moreover, every EDM can be obtained in this way. If κ is restricted to faces of Ω_n, then

$$\Omega_n(s) = \{X \in \Omega_n / Xs = 0\}$$

with $s^t e = 1$, the function κ is one to one and the inverse transformation is given by

$$\tau_s(D) = -\frac{1}{2}(I - es^t)D(I - se^t)$$

(for more details see section 2 of [JT]).

Schoemberg proved in [S] that D is EDM if and only if D is negative semidefinite on $M = \{x/x^t e = 0\}$, the orthogonal complement of the subspace generated by e. The linear transformation τ_s given above is strongly related to this result (see also [G]).
On the other hand, it has been pointed out that every EDM is special elliptic [HT] [F], in other words

$$\Lambda_n \subseteq \mathcal{E}_n^+$$

It is also known that special elliptic matrices can be generated as the image of Ω_n using a nonlinear function. In Theorem 2.2 of [F], Fiedler proved that all special elliptic matrices can be generated as follows: Given A, $B \in \Omega_n$ and B with rank one satisfying $diag(A) = diag(B)$, then

$$C = B - A$$

is in $\mathcal{E}_n$ (if different from zero). The converse is also true.

A small modification generates the set $\mathcal{E}_n^+$ in a similar way. We will replace B by the matrix $\bar{a}\bar{a}^t$, where $\bar{a} = (\sqrt{a_{11}}, \ldots, \sqrt{a_{nn}})^t$. Then

$$X = \bar{a}\bar{a}^t - A$$

is a continuous function of A from Ω_n to $\mathcal{E}_n^+$. Because of convexity of Ω_n and the continuity of this function, $\mathcal{E}_n^+$ is a connected set.

3.- EIGENVALUE-EIGENVECTOR STRUCTURE

In this section we want to point out some properties concerning the structure of eigenvalues and eigenvectors of EDMs. The first result is a consequence of the spectral structure of the matrix $E = ee^t - I$, the center direction of the EDM cone.

Lemma 3.1: Given $D \in \mathcal{H}_n$, for every eigenvector x of D with eigenvalue λ such that $x^t e = 0$, x is an eigenvector of the family

$$D(t) = tD + (1-t)E \qquad t \in \mathbf{R}$$

with eigenvalue $t(\lambda + 1) - 1$.

Proof: Suppose that $Dx = \lambda x$ and $x^t e = 0$, then

$$\begin{aligned} D(t)x &= tDx + (1-t)Ex \\ &= t\lambda x + (1-t)(ee^t - I)x \\ &= t\lambda x - (1-t)x \\ &= [t\lambda - (1-t)]x \\ &= [t(\lambda+1) - 1)]x. \ \blacksquare \end{aligned}$$

Remark: First of all observe that e is an eigenvector of E. Also it is easy to see that $D(t)$ is singular for $t = \frac{1}{\lambda+1}$. Finally Lemma 3.1 holds for any matrix $D \in S_n$ but because of our interest the lemma is stated only for hollow matrices.

Theorem 3.1: If $D \in \Lambda_n$ and is rank deficient, then every vector in the null space of D is an eigenvector of $D(t)$. Moreover the corresponding eigenvalue is $\lambda = t - 1$.

Proof: Because $D(t)$ is an symmetric matrix, the range and the null space are orthogonal, and for EDMs e always belongs to the range of the matrix [THW]. $\blacksquare$

Remark: The result is true for any matrix that has e in its range. This is the case for almost all hollow matrices.

Lemma 3.2: Given $D \in \mathcal{H}_n$, then $De = \lambda e$ if and only if the eigenvectors of $D(t)$ are the same for every t.

Proof: The condition is necessary because the eigenvectors of D different from e are also eigenvectors of E (they are orthogonal to e). It is also sufficient because $D(0) = E$ and then e is an eigenvector of the family which implies that it is an eigenvector of $D = D(1)$.

This special class of EDMs was studied by Hayden and Tarazaga in [HT].

Because of the conic structure of Λ_n, $D(t)$ exits the cone at some positive t (also at some negative t) under certain conditions, for example $||D||_F = ||E||_F$ and $D \neq E$. We can propose now a kind of converse result for our last theorem.

Theorem 3.2: Let $D \in \Lambda_n$ ($D \neq E$) with rank n and $||D||_F = ||E||_F$ and suppose that $span(x_1, \ldots, x_k)$ is the maximal invariant subspace associated with λ, the minimum eigenvalue in absolute value, and $e^t x_i = 0$ $i = 1, \ldots, k$. Then there exists a $\bar{t} > 1$ such that $span(x_1, \ldots, x_k) \subset N(D(\bar{t}))$. Moreover if $D(\bar{t}) \in \Lambda_n$, then $span(x_1, \ldots, x_k) = N(D(\bar{t}))$.

Proof: By Theorem 3.1, x_i, $i = 1, \ldots, k$, are eigenvectors of $D(t)$ with eigenvalue $t\lambda - (1-t)$ and clearly this value vanishes for $\bar{t} = \frac{1}{\lambda+1}$. But $|\lambda| < 1$ since $\|D\|_F = \|E\|_F$ and if λ is negative, then $\bar{t} = \frac{1}{\lambda+1} > 1$.

Clearly $span(x_1, \ldots, x_k) \subseteq N(D(\bar{t}))$. Now assuming $D(\bar{t}) \in \Lambda_n$, suppose there exists a $y \notin span(x_1, \ldots, x_k)$ such that

$$D(\bar{t})y = 0$$

We can generate the family $\bar{D}(s) = sD(\bar{t}) + (1-s)E$ and we obtain that

$$\begin{aligned} D(s) &= s(\frac{1}{\lambda+1}D + (1 - \frac{1}{\lambda+1})E) + (1-s)E \\ &= \frac{s}{\lambda+1}D + \frac{s\lambda}{\lambda+1}E + (1-s)E \\ &= \frac{s}{\lambda+1}D + \frac{\lambda+1-s}{\lambda+1}E \end{aligned} \qquad .$$

Now

$$\bar{D}(\frac{1}{\bar{t}}) = \bar{D}(1+\lambda) = D,$$

which implies that

$$\begin{aligned} Dx_i =&(1 - \frac{1}{\bar{t}})x_i = \lambda x_i \qquad i = 1, \ldots, k \\ Dy =&(1 - \frac{1}{\bar{t}})y = \lambda y. \end{aligned}$$

In the last equality we use the fact that $y^t e = 0$ since $y \in N(D(\bar{t}))$ and $D(\bar{t}) \in \Lambda_n$. This is a clear contradiction to the maximality property of $span(x_1, \ldots, x_k)$. ■

We want to point out that if $D(\bar{t})$ is rank deficient, then a matrix $D(t)$ in the interior of Λ_n, has the structure of the null space of the matrix $D(\bar{t})$ that intersects with the boundary of Λ_n. It is interesting to note that this is a well known and simple property of the cone of positive semidefinite matrices Ω_n. No similar relations can be established between the range of D and the range of the family $D(t)$.

4.- PROPERETIES OF THE BORDER OF Λ_n.

It is known that Λ_n is a subset of the set of nonnegative special elliptic matrices $\mathcal{E}_n^+$ as shown in [HT] and [F]. In this section to investigate more about the relation between these two sets to determine if they share part of their borders. The border of Λ_n has been studied in [THW] and [HWLT], and clearly rank deficient matrices form the border of special elliptic matrices. Our first result is related to matrices in the border of Λ_n with rank less than or equal to $n-2$.

Theorem 4.1: Give $\bar{D} \in \Lambda_n$ with rank$(\bar{D}) \leq n-2$ and D in the interior of Λ_n, then the matrices

$$D(t) = t\bar{D} + (1-t)D$$

have at least two positive eigenvalues for $t > 1$ and arbitrarily close to 1.

Proof: Since D is in the interior of Λ_n, rank$(D) = n$ and $D = D^+ + D^-$ with rank$(D^+) = 1$ and rank$(D^-) = n-1$ (D^+ and $-D^-$ belongs to Ω_n)

If $\bar{\lambda}_1 \geq \bar{\lambda}_2 \geq \ldots \bar{\lambda}_n$ are the eigenvalue of $\bar{D}$, then $t\bar{\lambda}_1 \geq t\bar{\lambda}_2 \geq \ldots \geq t\bar{\lambda}_n$ are the eigenvalue of $t\bar{D}$ for $t \in \mathbf{R}$. Note that at least $\bar{\lambda}_2 = \bar{\lambda}_3 = 0$ since rank$(\bar{D}) \leq n-2$.

Now consider the matrices

$$\tilde{D}(t) = t\bar{D} + (1-t)D^-$$

and

$$\hat{D}(t) = \tilde{D} + (1-t)D^+$$

for values of $t > 1$. If we order the eigenvalues of $\tilde{D}$ in the same way and consider that $(1-t)D^-$ is positive definite on M and the null space of $\bar{D}$ is included in M, then using Corollary 4.3.3 of [HJ] we have

$$\lambda_k(\bar{D}(t) < \lambda_k(t\bar{D} + (1-t)D^-) = \lambda_k(\tilde{D}(t))$$

which implies that $\widetilde{D}$ has three eigenvalues greater than zero.

Now using the fact that $(1-t)D^+$ has rank one and is negative semidefinite for $t > 1$, and Theorem 4.3.4 of [HJ] we have

$$\lambda_{k+1}(\tilde{D}(t)) \leq \lambda_k(\tilde{D}(t) + (1-t)D^+) = \lambda_k(\hat{D}(t))$$

which implies, using $k = 1$ and $k = 2$, that $\hat{D}(t) = D(t)$ has at least two positive eigenvalues. ∎

We will look now at the case in which $\bar{D}$ has rank $n-1$.

Theorem 4.2: Suppose $\bar{D} \in \Lambda_n$ has $\text{rank}(\bar{D}) = n-1$ and that $\bar{D}x = 0$. If D is in the interior of Λ_n and x is an eigenvector of D with eigenvalue λ, then all matrices of the family

$$D(t) = t\bar{D} + (1-t)D$$

have at least two positive eigenvalues for $t > 1$ and arbitrarily close to 1.

Proof: Using the same argument as in Lemma 3.1, we have that x is an eigenvector of the family

$$D(t) = t\bar{D} + (1-t)D$$

with eigenvalue $(1-t)\lambda$. But λ is negative since x is not the Peron-Frobenius eigenvector of $\bar{D}$. Hence this eigenvalue is positive for $t > 1$ and distinct from the Perron-Frobenius eigenvalue. ∎

We do not know of an example that would show that the hypothesis that D be in the interior of Λ_n is necessary.

Up to now in this section we have proved that part of the frontier of Λ_n is the same for $\mathcal{E}_n^+$ and it is a natural frontier, in the sense that at least one eigenvalue vanishes when we exit the cone.

We now want to look for properties on the boundary of Λ_n when the border elements are full rank matrices. But in this case we need an indicator different from zero eigenvalues. In [THW], Tarazaga, Hayden and Wells proved that if $D \in \Lambda_n$, then the linear system

$$Dx = e$$

always has a solution and morever the parameter $x^t e$ discriminates between spheric ($x^t e > 0$) and nonspheric ($x^t e = 0$) matrices. Gower [G] also introduced a related result. Our next result explores the behavior of this parameter for the family

$$D(t) = \bar{D}t + (1-t)D$$

where $\bar{D}$ is a full rank matrix in the border and D is in the interior of Λ_n. Observe that $\bar{D}$ is not spheric.

We will consider the function

$$f(t) = e^t D(t)^{-1} e = e^t x_{D(t)}.$$

For simplicity we will not write the subindex of x. From [THW] we know that $f(t) > 0$ for $0 \leq t < 1$ and $f(1) = 0$.

Lemma 4.1: $f'(1) < 0$.

Proof: Let us compute the derivate,

$$f(t+h) - f(t) = e^t \big(D^{-1}(t+h) - D^{-1}(t) \big) e.$$

Using the identity $A^{-1} - B^{-1} = B^{-1}(B-A)A^{-1}$ we obtain

$$\begin{aligned} f(t+h) - f(t) &= e^t D^{-1}(t) \big[D(t) - D(t+h) \big] D^{-1}(t+h) e \\ &= e^t D^{-1}(t) \big[\bar{D}t + (1-t)D - \big(\bar{D}(t+h) + [1-(t+h)]D \big] D^{-1}(t+h) e \\ &= e^t D^{-1}(t) \big[h(D - \bar{D}) \big] D^{-1}(t+h) e \end{aligned}$$

Dividing by h and taking the limit as $h \to 0$ we obtain

$$\begin{aligned} f'(1) &= e^t \bar{D}^{-1} \big[D - \bar{D} \big] \bar{D}^{-1} e \\ &= e^t \bar{D}^{-1} D \bar{D}^{-1} e - e^t \bar{D}^{-1} e \\ &= \bar{x}^t D \bar{x} < 0. \ \blacksquare \end{aligned}$$

Theorem 4.3: Given $\bar{D}$ on the border of Λ_n with rank n and D in the interior, we have the following for the family of matrices

$$D(t) = t\bar{D} + (1-t)D$$

a) $f(t) > 0$, for $0 \leq t < 1$
b) $f(1) = 0$
c) $f(t) < 0$ for $t > 1$ and arbitrarily close to 1.

Proof: a) and b) are consequence of Theorem 3.4 of [THW] . Part c) is a consequence of Lemma 4.1. $\blacksquare$

5.- CHARACTERIZATION OF Λ_n AND THE RELATION WITH ELLIPTIC MATRICES.

In this section we obtain a characterization of EDMs and we describe the border of Λ_n.

Lemma 5.1: If D is special elliptic satisfying $Dx = e$ and $x^te > 0$, then D is in Λ_n. Moreover D is spheric.

Proof: Because of the characterization mentioned in section 2 [S] we must prove that for $y \in M$,

$$y^tDy \leq 0.$$

Suppose that there exist $y \in M$ $(y^te = 0)$ such that

$$y^tDy > 0.$$

Then for any vector $z = \alpha x + \beta y$ with α and β real,

$$\begin{aligned} z^tDz &= (\alpha x + \beta y)D(\alpha x + \beta y) \\ &= \alpha^2 x^tDx + 2\alpha\beta x^tDy + \beta^2 y^tDy \\ &= \alpha^2 x^tDx + 2\alpha\beta (Dx)^ty + \beta^2 y^tDy \end{aligned}$$

Since $Dx = e$, the second term is zero and since $x^tDx = x^te > 0$, the first is greater than zero, which implies

$$z^tDz > 0$$

when $z \neq 0$ $((\alpha, \beta) \neq (0,0))$.
But this implies that D is positive definite in the plane generated by x and y, which contradicts the fact that D is special elliptic. ■
A different technique is needed for the case in which the solution of $Dx = e$ satisfies $x^te = 0$.
Given a matrix D (elliptic for our purposes) we consider the matrix

$$\widehat{D} = \begin{pmatrix} 0 & e^t \\ e & D \end{pmatrix}$$

It is clear that for any vector x such that $Dx = e$ and $x^te = 0$, the vector $(-1, x)^t$ is in the null space of $\widehat{D}$. Also if $Dx = 0$, then $(0, x)^t$ is in the null space of $\hat{D}$.

Lemma 5.2: Suppose D is elliptic and $Dx = e$ with $x^te = 0$. Then D is in Λ_n and moreover is on the boundary.

Proof: Suppose $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{n-1} \leq 0 < \lambda_n$ are the ordered eigenvalues of D. By the eigenvalues interlacing theorem

$$\lambda_{n-1} \leq \widehat{\lambda}_n \leq \lambda_n.$$

But $(-1, x)$ is in the null space of $\hat{D}$. Thus $\hat{\lambda}_n = 0$ which implies that $\hat{D}$ is elliptic. Using [HW], D is EDM, but according to [THW], D is not spheric which implies it is on the boundary of Λ_n.

These two preliminaries results allow us to state the following.

Theorem 5.1: If D is special elliptic satisfying $Dx = e$, then D is EDM if and only if $x^t e \geq 0$.

Proof: The sufficiency of $x^t e \geq 0$ is a consequence of the previous lemmas. The condition is necessary from [THW]. ∎

Note that for some matrices D on the boundary of $\mathcal{E}_n^+$, the system $Dx = e$ has no solution. Matrices such as

$$D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

are on the boundary of $\mathcal{E}_3^+$ and $Dx = e$ has no solution.

Finally, we wish to observe the behavior of the maximum of the Rayleigh quotient of EDMs on the subspace M. First, consider the interior of Λ_n.

Lemma 5.3: If D is in the interior of Δ_n, then

$$\max_{\substack{x \in M \\ x \neq 0}} \frac{x^t D x}{x^t x} < 0.$$

Proof: The minimal embedding dimension of D, a distance matrix in the interior of Δ_n, is $n-1$. Then using Corollary 3.1 of [THW], there exists λ such that

$$-\frac{1}{2} D + \lambda e e^t$$

which is positive definite, and hence full rank.

On the other hand, we know that since D is negative semidefinite on M,

$$\frac{x^t D x}{x^t x} \leq 0.$$

Now suppose that there exists $\bar{x} \in M$ such that

$$\frac{\bar{x}^t D \bar{x}}{\bar{x}^t \bar{x}} = 0.$$

Then

$$\frac{\bar{x}^t(-\frac{1}{2}D + \lambda ee^t)\bar{x}}{\bar{x}^t\bar{x}} = -\frac{1}{2}\frac{\bar{x}^tD\bar{x}}{\bar{x}^t\bar{x}} + \frac{\lambda(e^t\bar{x})^2}{\bar{x}^t\bar{x}} = 0$$

which contradict the fact that $-\frac{1}{2}D + \lambda ee^t$ is full rank. ■

Now let us look at the boundary of Λ_n to see what happens.

Lemma 5.4: If D is in the border of Δ_n, then

$$\max_{\substack{x\in M\\ x\neq o}} \frac{x^tDx}{x^tx} = 0.$$

Proof: If D is rank deficient, then there exist $x(\neq 0) \in N(D) \subset M$ such that $Dx = 0$ which implies that

$$\frac{x^tDx}{x^tx} = 0.$$

Suppose now that $rank(D) = n$ and D is on the boundary. This implies that D is not spheric and by Theorem 3.4 of [THW] there exists x such that

$$Dx = \beta e$$

with $\beta > 0$ and $e^tx = 0$. But now

$$x^tDx = x^t(\beta e) = \beta x^te = 0$$

and so the result holds. ■

We can now state the following result.

Theorem 5.2: Given $D \in \Lambda_n$, the Rayleigh quotient satisfies

$$\max_{\substack{x\in M\\ x\neq o}} \frac{x^tDx}{x^tx} \leq 0.$$

Moreover, D is on the boundary of Λ_n if and only if

$$\max_{\substack{x\in M\\ x\neq o}} \frac{x^tDx}{x^tx} = 0.$$

Proof: The condition is necessary because of Lemma 5.4 and it is sufficient because of Lemma 5.3. ■

We close this section by pointing out that this characterization of the border of Λ_n is completely equivalent to the characterization of the border of the cone of positive semidefinite matrices if we use the minimum Rayleigh quotient for the whole space.

6.- SOME EXAMPLES

Let us look at some examples in low dimension. We will see what nice geometry we have for $n = 3$ and how complicated it turns out to be for larger dimension.

Case n = 3

Let us consider the typical nonnegative hollow matrix

$$A = \begin{pmatrix} 0 & \alpha & \beta \\ \alpha & 0 & \gamma \\ \beta & \gamma & 0 \end{pmatrix}$$

with $\alpha, \beta, \gamma \geq 0$.

If we define E_{ij} to be the matrix with 1 in positions (i,j) and (j,i) and zeros in all remaining positions, then we have

$$A = \alpha E_{12} + \beta E_{13} + \gamma E_{23}$$

We can consider $(\alpha, \beta, \gamma)^t$ as a vector in $\mathbf{R^3}$. Each of the extremal directions correspond to the canonical vector in this space $\mathbf{R^3}$ and the matrix E corresponds to the vector e.
It is easy to compute the determinant of A

$$det(A) = 2\alpha\beta\gamma \geq 0$$

Thus if A is nonsingular, it has to have two negative eigenvalues. Also if $A \neq 0$ and A is singular, then it has one positive and one negative eigenvalue, equal in absolute value since the trace of A is 0. This allows us to establish the following results.

Theorem 6.1: Every nonnegative hollow matrix in $\mathbf{R^{3\times 3}}$ is special elliptic.

Corollary 6.1: $\mathcal{E}_3^+$ is a convex cone.

Proof: $\mathcal{E}_3^+$ is an orthant.

Also Λ_3 has a special structure. First, observe that the boundary of Λ_3 consists of matrices with embedding dimension one. If $D \in \Lambda_3$ and has embedding dimension one, then using Theorem 3.3 of [HWLT] we have that

$$\cos(D, E) = \sqrt{\frac{2}{3}},$$

which means that Λ_n is a circular cone.

The cone Λ_3 is as wide as possible, touching the faces of the orthant with the distance matrices

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

These matrices correspond to three point configurations where two of them collapse.

For this particular example, $\cos(X, E)$ decides whether or not X, a nonnegative special elliptic matrix, is a distance matrix:

$$X \text{ is EDM if and only if } \cos(X, E) \geq \sqrt{\tfrac{2}{3}}.$$

This nice relation is similar to the one that characterizes the positive semidefinite matrices of order 2. When we increase the dimension all of this simple structure deteriorates as we show next.

Case $\mathbf{n} = 4$

In this case convex combinations of the extreme direction E_{ij} $j \geq i$ which generate the two dimensional faces of the orthant, show different behavior. For example, $tE_{12} + (1-t)E_{13}$ for $0 \leq t \leq 1$ generates the matrices

$$\begin{pmatrix} 0 & t & 1-t & 0 \\ t & 0 & 0 & 0 \\ 1-t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

with rank two and which thus belong to $\mathcal{E}_4^+$ for $0 \leq t \leq 1$.

However, a completely different situation arises when we consider matrices $tE_{12}+(1-t)E_{34}$ for $0 \leq t \leq 1$ which generate

$$\begin{pmatrix} 0 & t & 0 & 0 \\ t & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-t \\ 0 & 0 & 1-t & 0 \end{pmatrix}.$$

Here we have two positive eigenvalues for each matrix with $0 < t < 1$.

Now since E is the central direction of $\Lambda_n \subseteq \mathcal{E}_n^+$, we want to investigate the behavior of the family

$$X(t) = tE_{ij} + (1-t)E$$

for any extreme matrix E_{ij}.

Since every E_{ij} can be obtained from E_{12} using the appropriate permutation P,

$$E_{ij} = P^t E_{12} P$$

we will look at the case

$$X(t) = tE_{12} + (1-t)E.$$

The determinant of $X(t)$ is

$$\det(X(t)) = \det \begin{vmatrix} 0 & 1 & 1-t & 1-t \\ 1 & 0 & 1-t & 1-t \\ 1-t & 1-t & 0 & 1-t \\ 1-t & 1-t & 1-t & 0 \end{vmatrix} = (1-t)^2(4t-3)$$

The first observation is that the matrix is singular only for $t = 1$ or $t = \frac{3}{4}$ in the interval $[0,1]$. Second we have that $X(t)$ is elliptic for $t \in [0, \frac{3}{4}]$ because $X(0)$ is elliptic and $det(X(t)) \neq 0$ does not allow eigenvalues to change sign. It is also elliptic for $t = 1$. But for $t \in (\frac{3}{4}, 1)$ $X(t)$ has a positive determinant and at least one positive eigenvalue, the Perron-Frobenius one. Also since $X(t)$ is not singular, it has two positive eigenvalues and hence $X(t)$ is not elliptic in $(\frac{3}{4}, 1)$.

Finally, we consider the polyhedral cone generated by E, E_{12} and the following matrices

$$X = \frac{1}{3}E_{12} + \frac{1}{3}E_{13} + \frac{1}{3}E_{14} = \begin{pmatrix} 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 \end{pmatrix}$$

$$Y = \frac{1}{3}E_{12} + \frac{1}{3}E_{23} + \frac{1}{3}E_{24} = \begin{pmatrix} 0 & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \end{pmatrix}$$

It is easy to see that X and Y are distance matrices corresponding to the configuration in which three points collapse.

Now the four two dimensional faces of the polyhedral cone generated by E, E_{12}, X, and Y consist of elliptic matrices. The faces generated by

$$\alpha E_{12} + \beta X \qquad \alpha, \beta \geq 0$$

and

$$\alpha E_{12} + \beta Y \qquad \alpha, \beta \geq 0$$

are elliptic since the matrices have rank 2 and are hollow. The faces

$$\alpha X + \beta E \qquad \alpha, \beta \geq 0$$

and

$$\alpha Y + \beta E \qquad \alpha, \beta \geq 0$$

are included in $\Lambda_4 \qquad (X, Y, E \in \Lambda_4)$.

However, the matrices

$$X(t) = tE_{12} + (1-t)E,$$

$t \in (\frac{3}{4}, 1)$, are not elliptic, but they are contained in the polyhedral cone. In other words, the polyhedral cone generated by E_{12}, E, X and Y has an elliptic boundary but there is a hole of nonelliptic matrices inside.

These computations show that the structure of $\mathcal{E}_4^+$ inside the nonnegative orthant is highly complicated.

The structure of Λ_4 is also more complex. Matrices with embedding rank one do not form a constant angle with E. From [HWLT] we know that if D has embedding dimension one, then

$$\sqrt{\frac{2}{3}} \geq cos(D, E) \geq \frac{1}{\sqrt{2}}$$

even though the cone is convex and is included in $\mathcal{E}_4^+$. In other words the more complicated shape of $\mathcal{E}_4^+$ takes place outside of Λ_4.

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