On the Nonnegative Rank of Euclidean Distance Matrices, II

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Abstract

Given a linear Euclidean distance matrix Q_n of size $n \times n$, it has been claimed that $\text{rank}_+(Q_n) = n$. The proof given in the previous LAA paper by Lin and Chu is incomplete. This note continues the investigation of this claim. The argument employed below is still not perfect, but shows at least that the claim is generically true. Additionally, this course of study leads to a few new discoveries which will be presented below.

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1. The feasible set

Let $\vartheta(Q_n)$ denote the pullback of Q_n to the unit simplex $\mathcal{D}_n$. It is known that $\text{rank}(Q_n) = 3$. Columns of $\vartheta(Q_n)$ therefore are "coplanar", whereas by their common plane we refer to a 2-dimensional affine subspace $\mathscr{A}_n \in \mathbb{R}^n$. Denote $\mathscr{T}_n := \mathscr{A}_n \bigcap \mathcal{D}_n$ which is said to be feasible with respect to the inequality system (2) described below. Obviously, columns of $\vartheta(Q_n)$ are embedded in $\mathscr{T}_n$. We first elaborate on how to see this 2-dimensional feasible set $\mathscr{T}_n$ in $\mathbb{R}^n$ via its isomorphic image over $\mathbb{R}^2$.

We begin with a fixed point, say, $\vartheta(\mathbf{q}_1)$, and two coordinate axes, say, $\mathbf{b}_1 := \vartheta(\mathbf{q}_2) - \vartheta(\mathbf{q}_1)$ and $\mathbf{b}_2 := \vartheta(\mathbf{q}_3) - \vartheta(\mathbf{q}_1)$. All points in the 2-dimensional affine subspace, including those in $\mathscr{T}_n$, can be represented as

$$\vartheta(\mathbf{q}_1) + \alpha\mathbf{b}_1 + \beta\mathbf{b}_2$$

by some real scalars α and β. Denote the $n \times 2$ basis matrix by

$$B := [\mathbf{b}_1, \mathbf{b}_2]. \tag{1}$$

We seek feasible α and β such that

$$\vartheta(\mathbf{q}_1) + B \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \geq 0. \tag{2}$$

Because B is of full column rank, it defines an isomorphism by which we may identify the set $\mathscr{T}_n$ with the collection $\mathscr{P}_n$ of all feasible pairs (α, β). The former is a set residing in $\mathbb{R}^n$ which is hard to see, but the latter is a polygon residing in $\mathbb{R}^2$.

Note that the inequality system (2) involves exactly n lines. The set $\mathscr{P}_n$ is generically a convex polygon. In particular, we should have

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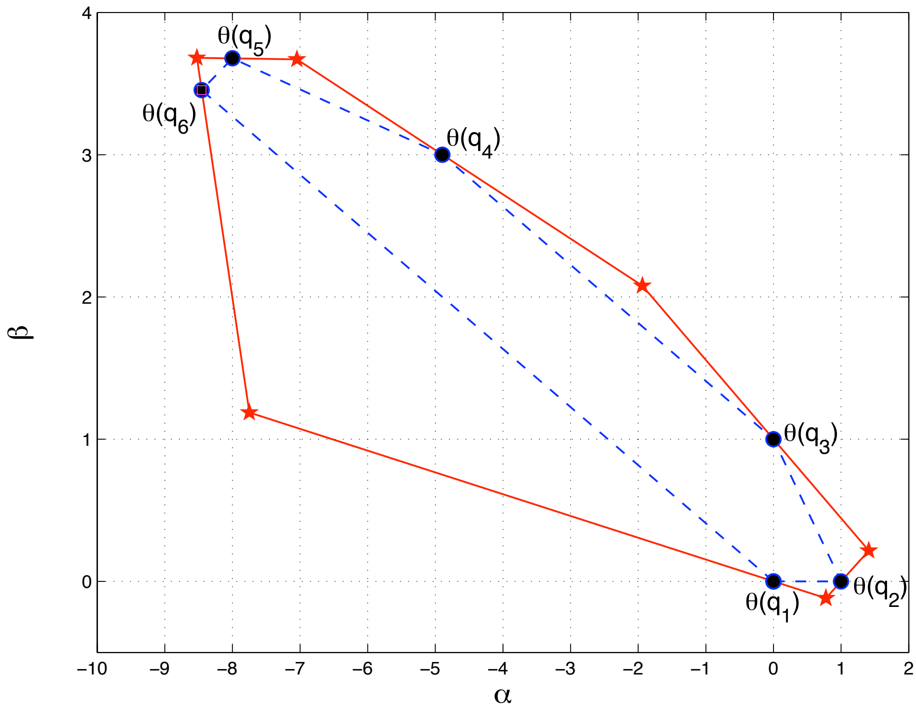

Figure 1: Feasible domain for (α, β) when $n = 6$ and $r = 1$

$$\vartheta(Q_n) = \underbrace{[\vartheta(\mathbf{q}_1), \ldots, \vartheta(\mathbf{q}_1)]}_{A} + BC, \tag{3}$$

where $A \in \mathbb{R}^{n\times n}$ and $C \in \mathbb{R}^{2\times n}$ is of this special form

$$C = \begin{bmatrix} 0 & 1 & 0 & \times & \ldots \\ 0 & 0 & 1 & \times & \ldots \end{bmatrix},$$

where $\times$ stands for some nonzero scalars. Obviously each column $\mathbf{c}_i$ of C is a feasible point in $\mathscr{P}_n$. By our isomorphism, each column vector $\vartheta(\mathbf{q}_i)$ is uniquely represented by the point $\mathbf{c}_i$ in $\mathscr{P}_n$. An example for the case $n = 6$ is depicted in Figure 1 in which the feasible set $\mathscr{P}_n$ is enclosed by solid lines, each $\mathbf{c}_i$ is marked by a solid bullet, and the region bordered by dashed lines represents the convex hull spanned by $\vartheta(Q_6)$.

Of particular importance is that because the i entry of $\vartheta(\mathbf{q}_i)$ for $i = 1, \ldots, n$ is zero, each $\mathbf{c}_i$ satisfies precisely one equation in the inequality system (2). In other words, each $\mathbf{c}_i$ is a point on precisely one side of the polygon $\mathscr{P}_n$. A careful examination of the slopes of these lines from the definition of Q_n shows that these lines can be ordered, starting with the side passing through the origin and going counterclockwise. It then can be argued that $\mathscr{P}_n$ is a convex n-tope. Because $\mathbf{c}_i$'s reside on the boundary of the 2-dimensional polygon $\mathscr{P}_n$, it is now clear that the convex hull of $\{\mathbf{c}_1, \ldots, \mathbf{c}_n\}$ cannot be enclosed by any convex n-gon, except by itself or the polytope $\mathscr{P}_n$. Any other n-gon in the (α, β)-plane containing $\{\mathbf{c}_1, \ldots, \mathbf{c}_n\}$ will necessarily contain infeasible point.

2. Constructing nonnegative factorizations

Based on the above understanding, we can actually construct a few nontrivial nonnegative factorizations for Q_n numerically. We outline three construction schemes in this section.

The first approach is to calculate the vertices of $\mathscr{T}_n$ in $\mathbb{R}^n$ which, in turn, offers a mechanism for computing a nonnegative factorization of Q_n. All it matters is to calculate the vertices of the polytope $\mathscr{P}_n$ and transform these vertices in $\mathbb{R}^2$ via B back to $\mathscr{T}_n$ in $\mathbb{R}^n$.

Specifically, let columns of $U = [\mathbf{u}_1, \ldots, \mathbf{u}_n]$ denote the vertices of $\mathscr{T}_n$. Then

$$\mathbf{u}_i = \vartheta(\mathbf{q}_1) + B \begin{bmatrix} \alpha_i \\ \beta i \end{bmatrix}, \quad i = 1, \ldots, n, \tag{4}$$

where $\begin{bmatrix} \alpha_i \\ \beta i \end{bmatrix}$ is a simultaneous solution to the linear system

$$\begin{bmatrix} b_{i,1} & b_{i,2} \\ b_{i+1,1} & b_{i+1,2} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta i \end{bmatrix} = \begin{bmatrix} \vartheta(\mathbf{q}_1)_i \\ \vartheta(\mathbf{q}_1)_{i+1} \end{bmatrix}, \tag{5}$$

with the interpretation that $[b_{n+1,1}, b_{n+1,2}] = [b_{1,1}, b_{1,2}]$ and $\vartheta(\mathbf{q}_1)_{n+1} = \vartheta(\mathbf{q}_1)_1$. By construction, we immediately see that U must be of the structure

$$U = \begin{bmatrix} 0 & \times & \times & \ldots & & \times & 0 \\ 0 & 0 & \times & \ldots & & & \times \\ \times & 0 & 0 & & & & \times \\ \times & \times & 0 & & & & \\ \vdots & & & \ddots & \ddots & & \\ & & & & & 0 & \times \\ \times & & & & & 0 & 0 \end{bmatrix}. \tag{6}$$

In other words, each vertex of $\mathscr{T}_n$ has exactly two zero entries and, thus, must reside on precisely one and distinct "ridge" of the simplex $\mathcal{D}_n$. As $\operatorname{conv}(\mathscr{T}_n) \supset \operatorname{conv}(\vartheta(Q_n))$, we obtain a nonnegative factorization

$$\vartheta(Q_n) = UV, \tag{7}$$

where each column of V has exactly two nonzero entries representing a convex combination of two columns of U. With appropriate scaling, we obtain a nonnegative factorization $Q_n = U_n V_n$ for the linear EDM Q_n.

We remark that in the above construction, the nonnegative matrix U_n obtained via the vertices of $\mathscr{F}_n$ is of rank 3 in general. While V_4 is of rank 3 always, it has been observed and conjectured that V_{2m-1} is of full rank $2m-1$ generically and V_{2m} could be of rank $2m$ or $2m-1$ for $m \geq 3$. In the special case when $n = 4$, we note the unique fact that each column of either U_4 or $V_4^\top$ has exactly two zeros and two nonzeros. Thus, columns of $\vartheta(U_4)$ and $\vartheta(V_4^\top)$ represent the same set of vertices of $\mathscr{T}_4$. Such a coincidence does not hold for $n > 4$.

The second approach is to take advantage of the above observation for the case $n = 4$. Write

$$Q_n = \left[\begin{array}{c|c} Q_4 & \widehat{Q}_{n,4} \\ \hline \widehat{Q}_{n,4}^\top & \widetilde{Q}_{n,4} \end{array}\right], \tag{8}$$

with $\widetilde{Q}_{n,4} \in \mathbb{R}^{(n-4)\times(n-4)}$. Consider the submatrix $[Q_4, \widehat{Q}_{n,4}]$ only. Clearly, if $Q_4 = U_4 V_4$ where columns of $\vartheta(U_4)$ (or $\vartheta(V_4^\top)$) are the four vertices of $\mathscr{T}_4$, then there exist nonnegative matrices $W_4, Z_4 \in \mathbb{R}^{4\times(n-4)}$ such that

$$\widehat{Q}_{n,4} = U_4 W_4 = V_4^\top Z_4 \in \mathbb{R}^{4\times(n-4)}. \tag{9}$$

In this way, we obtain two nontrivial standard nonnegative factorizations of Q_n via the relationship

$$Q_n = \left[\begin{array}{c|c} U_4 & \mathbf{0} \\ \hline \mathbf{0}^\top & I_{n-4} \end{array}\right] \left[\begin{array}{c|c} V_4 & W_4 \\ \hline \widehat{Q}_{n,4}^\top & \widetilde{Q}_{n,4} \end{array}\right] = \left[\begin{array}{c|c} U_4 & \widehat{Q}_{n,4} \\ \hline Z_4^\top & \widetilde{Q}_{n,4} \end{array}\right] \left[\begin{array}{c|c} V_4 & \mathbf{0} \\ \hline \mathbf{0}^\top & I_{n-4} \end{array}\right], \tag{10}$$

respectively. In the former case, the nonnegative factors U is of rank $n-1$ and V if of rank 4.

The second scheme for constructing nonnegative factorizations in the first form of (10) can be generalized. Still taking advantage of the coplanar property if $Q_k = U_k V_k$ where columns of $\vartheta(U_k)$ are the k vertices of $\mathscr{T}_k$ when $k > 4$, we know that there exists a nonnegative matrices $W_k \in \mathbb{R}^{k\times(n-k)}$ such that

$$Q_n = \left[\begin{array}{c|c} U_k & \mathbf{0} \\ \hline \mathbf{0}^\top & I_{n-k} \end{array}\right] \left[\begin{array}{c|c} V_k & W_k \\ \hline \widehat{Q}_n^\top & \widetilde{Q}_{n,4} \end{array}\right], \tag{11}$$

with

$$\widehat{Q}_{n,k} = U_k W_k \in \mathbb{R}^{k\times(n-k)} \tag{12}$$

denoting the upper right corner of Q_n in a way similar to the partition in (8). In this case, the nonnegative factor U is of rank $n-k+3$ and V is of rank no greater than k. Take note that a similar generalization of the second form in (10) is not as obvious because generally columns of $\vartheta(V_k^\top)$ are not coplanar and, thus, it is not guaranteed that the equation

$$V_k^\top Z_k = \widehat{Q}_{n,k} \tag{13}$$

can be solved for a nonnegative Z_k. See the next section, however, for further remarks.

3. New discoveries

This section contains a few newer observations made during the course of this study. Theoretical justification remains lacking at this point.

The columns of a rank-3 matrix generally are not coplanar. The original purpose of the pullback map was to conveniently introduce the intersection with a hyperplane in $\mathbb{R}^n$ and, hence, induce the coplanar property of $\vartheta(Q_n)$. It has been observed recently, however, that the linear EDM is so special that the columns of Q_n are automatically coplanar to begin with. I still do not have a nice analytic proof of this property yet. If this observation is true, then notion of feasible set discussed in Section 1 becomes obsolete and the construction schemes of nonnegative factorizations can be further simplified.

The generalization of the second approach outlined in Section 2 generally cannot be applied to second type of factorization in (10) for $k > 4$ because the equation (13) is not always solvable. Further numerical experiments, however, reveal some additional details which are yet to be understood analytically. That is, it is observed numerically that (13) is not solvable only if k is odd. But if k is even, then both equations (12) and (13) are solvable for nonnegative matrices $W_k, Z_k \in \mathbb{R}^{k\times(n-k)}$, respectively. In the latter case, we obtain a nonnegative factorization

$$Q_n = \left[\begin{array}{c|c} U_k & \widehat{Q}_{n,k} \\ \hline Z_k^\top & \widetilde{Q}_{n,k} \end{array}\right] \left[\begin{array}{c|c} V_k & \mathbf{0} \\ \hline \mathbf{0}^\top & I_{n-4} \end{array}\right]. \tag{14}$$

Obviously, the second type of factorization in (10) is a special case of (14) with $k = 4$ which is even. It is not clear why the evenness of k will entail such a factorization, but the oddness will not.

If $Q_n = UV$ is a nonnegative factorization, then by symmetry $Q_n = V^\top U^\top$ is also a nonnegative factorization. This dual relationship has an interesting implication in that our previous geometric argument about the nonnegative rank of Q_n is not sufficient. It shows that it is entirely possible, despite of the facts of coplanar property and zero patterns inherent in Q_n, that columns of Q_n (or even of $\vartheta(Q_n)$ after the pullback) could be enclosed by polytopes whose vertices are *not* coplanar at all.

4. The nonnegative rank

All the schemes discussed above construct a nonnegative factorization for Q_n with n rank-1 *nonnegative components*. Though it was claimed in Lin and Chu's LAA paper that $\text{rank}_+(Q_n) = n$, their proof there has overlooked the possibility that the nonnegative factor U might be composed of vertices outside the 2-dimensional affine subspace containing Q_n. So how can the claim be absolved?

The case $n = 4$ is all clear. We can prove either geometrically or algebraically that $\text{rank}_+(Q_4) = 4$. We adopt an induction argument as follows. Assuming that it is known that $\text{rank}_+(Q_n) = n$ *almost surely* in the sense that points in $\mathbb{R}$ such that their corresponding EDM has nonnegative rank strictly less than n form a subset of measure zero. We want to show that $\text{rank}_+(Q_{n+1}) = n + 1$ almost surely. To prove by contradiction, we may assume a factorization

$$Q_{n+1} = \left[\begin{array}{c} U \\ \hline \mathbf{z}^\top \end{array}\right] \left[\begin{array}{c|c} V & \mathbf{w} \end{array}\right], \tag{15}$$

where $U, V \in \mathbb{R}^{n\times n}$ and $\mathbf{w}, \mathbf{z} \in \mathbb{R}$ are nonnegative matrices and vectors, respectively. As Q_n is nested in Q_{n+1} by ways of

$$Q_{n+1} = \left[\begin{array}{c|c} Q_n & \widehat{Q}_{n+1,n} \\ \hline \widehat{Q}_{n+1,n}^\top & 0 \end{array}\right] \tag{16}$$

with $\widehat{Q}_{n+1,n} \in \mathbb{R}^n$, we see from (15) that the product UV must be one of the nonnegative factorizations of Q_n and the relationships

$$\begin{cases} U\mathbf{w} &= \widehat{Q}_{n+1,n}, \\ V^\top \mathbf{z} &= \widehat{Q}_{n+1,n} \end{cases} \tag{17}$$

must hold. The qualification that $\mathbf{z}^\top \mathbf{w} = 0$, together with the proviso that both $\mathbf{w}$ and $\mathbf{z}$ are nonnegative, implies additional equations $w_i z_i = 0, i = 1, \ldots, n$. There are a total of $3n$ equations for $2n$ unknowns, implying an overdetermined system even before taking into account of the additional requirement of a nonnegative solution. Additionally, the system (17) implicates an implicit constraint that the range spaces of U and $V^\top$ must intersect at a nontrivial point. By the transversality theorem, we know that the system is not solvable for almost all $\widehat{Q}_{n+1,n} \in \mathbb{R}^n$. In other words, almost surely we *could not* have $\text{rank}_+(Q_{n+1}) = n$.

Alternatively, by permuting columns of U and rows of V simultaneously if necessary, we may assume that the first k entries of $\mathbf{w}$ are the only nonzero (positive) unknowns in $\mathbf{w}$. The true value of k is not essential at this point, though it should be such that $2 \le k \le n - 2$. Then $\mathbf{z}$ can carry at most $n - k$ unknowns. By this reduction, there are only n unknowns to be determined from $2n$ linear equations. Still the linear system (17) is overdetermined.

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