On the Embeddability of Weighted Graphs in Euclidean Spaces

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Abstract

Given an incomplete edge-weighted graph, $G = (V, E, \omega)$, G is said to be embeddable in $\Re^r$, or r-embeddable, if the vertices of G can be mapped to points in $\Re^r$ such that every two adjacent vertices v_i , v_j of G are mapped to points x^i, $x^j \in \Re^r$ whose Euclidean distance is equal to the weight of the edge (v_i, v_j). Barvinok [3] proved that if G is r-embeddable for some r, then it is r^*-embeddable where $r^* = \lfloor(\sqrt{8|E|+1}-1)/2\rfloor$. In this paper we provide a constructive proof of this result by presenting an algorithm to construct such an r^*-embedding.

1 Introduction

Let $G = (V, E, \omega)$ be an incomplete undirected edge-weighted graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, edge set $E \subset V \times V$ and a nonnegative weight

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ω_{ij} for each $(v_i, v_j) \in E$. G is said to be r-embeddable if there exists a mapping $\phi : V \to \Re^r$ such that for every edge $(v_i, v_j) \in E$, the Euclidean distance $\|\phi(v_i) - \phi(v_j)\| = \omega_{ij}$; and, it is said to be *embeddable* if it is r-embeddable for some positive integer r.

The *Embeddability problem* (*r-embeddability problem*) is the problem of determining whether $G = (V, E, \omega)$ is embeddable (r-embeddable). In matrix theory literature, the r-embeddability problem is known as the *Euclidean distance matrix completion problem* (EDMCP$_r$). An $n \times n$ symmetric matrix $D = (d_{ij})$ with nonnegative elements and with zero diagonal is said to be a Euclidean distance matrix (EDM) if there exist points $x^1, x^2, \ldots, x^n \in \Re^r$ for some r such that

$$d_{ij} = \|x^i - x^j\|^2, \qquad i, j = 1, 2, \ldots, n.$$

The smallest such r is called the embedding dimension of D. Note that r is always $\leq n - 1$. Let A be an $n \times n$ symmetric partial matrix with some elements specified or *fixed* and the rest are unspecified or *free*. The problem of determining whether A can be completed to a EDM with embedding dimension r, by assigning certain values to its free elements, is called EDMCP$_r$; and, it is called EDMCP if the embedding dimension is unrestricted. The equivalence between the embeddability (r-embeddability) and EDMCP (EDMCP$_r$) is immediate if, in the matrix $A = A(\omega)$, the elements a_{ij} corresponding to $(v_i, v_j) \notin E$ are free, while elements a_{ij} corresponding to $(v_i, v_j) \in E$ are fixed as $a_{ij} = \omega_{ij}^2$. Thus $G = (V, E, \omega)$ is embeddable (r-embeddable) if and only if $A = A(\omega)$ can be completed to a EDM (EDM with embedding dimension r).

The r-embeddability problem or the ($EDMCP_r$) has received much attention in recent years because of its many applications in fields such as chemistry, statistics, archaeology, genetics, and geography [1]. In some applications (e.g. the molecular conformation problems in chemistry [4, 15]), the embedding dimension r is required to be 2 or 3, while in others (e.g. multidimensional scaling in statistics [12, 13]), only a small r is desired. It was shown by Saxe [20] that for any given positive integer r, the r-embeddability problem of an integer-weighted graph $G = (V, E, \omega)$ is NP-Hard. It remains so even if the weights ω_{ij} are restricted to 1 or 2 only. In [3], Barvinok proved that if $G = (V, E, \omega)$ is embeddable, then it is r^*-embeddable where $r^* = \lfloor(\sqrt{8|E| + 1} - 1)/2\rfloor$. His proof was based on the duality of semidefinite programming and on the "corank formula" for the strata of singular quadratic forms. However, no method was presented to construct such an r^*-embedding if G is embeddable. Another proof of Barvinok's result is given in [6].

In this note we present a constructive proof of Barvinok's result. i.e., we present an algorithm to construct such an r^*-embedding if G is embeddable. This algorithm consists of two steps. In step 1, EDMCP is formulated as a semidefinite programming problem. This problem is then solved, using an interior-point method, to determine whether $G = (V, E, \omega)$ is embeddable or not. If it is embeddable, due to the nature of the interior-point methods, an r-embedding with large r is usually obtained. In step 2, a rounding procedure, exploiting the facial structure of the set of optimal solutions of the semidefinite program, is used to construct an r^*-embedding starting from the r-embedding obtained in step 1.

2 Problem Formulation

Given an edge-weighted graph $G(V, E, \omega)$, let H be its adjacency matrix and let

$$A = A(\omega) = (a_{ij}) = \begin{cases} \omega_{ij}^2 & \text{if } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

Note that wlog all free elements of A are originally set to zero. Consider the following problem

$$\mu^* := \begin{array}{cc} \min & f(D) = \|H \circ (D - A)\|_F^2 \\ \text{subject to} & D \in \mathcal{E}, \end{array} \tag{1}$$

where $\| \ \|_F$ denote the Frobenius norm defined as $\| A \|_F = \sqrt{\operatorname{trace} A^T A}$, $(\circ)$ denotes the *Hadamard* product or the element-wise product, and $\mathcal{E}$ denotes the cone of EDMs. Let D^* be the optimal solution of (1). Then, it immediately follows that $G = (V, E, \omega)$ is embeddable if and only if $f(D^*)$ is zero. Furthermore, (1) can be posed as a semidefinite programming problem be exploiting the relation between the cone $\mathcal{E}$ and $\mathcal{P}$, the cone of positive semidefinite matrices. This relation is established in the following subsection.

2.1 Distance Geometry

It is well known, e.g. [21, 7, 9, 22], that a symmetric matrix D with nonnegative elements and with zero diagonal is a EDM if and only if D is negative semidefinite on

$$M := \left\{ x \in \Re^n : x^T e = 0 \right\},$$

the orthogonal complement of e, the vector of all ones. Let $\mathcal{S}_n$ denote the space of symmetric matrices of order n. Define the *centered* and *hollow* subspaces of $\mathcal{S}_n$ as

$$\begin{array}{rcl} \mathcal{S}_C & := & \{B \in \mathcal{S}_n : Be = 0\}, \\ \mathcal{S}_H & := & \{D \in \mathcal{S}_n : \mathrm{diag(D)} = 0\}, \end{array} \tag{2}$$

where $\operatorname{diag}(D)$ denotes the column vector formed from the diagonal of D. Following [5], define the two linear operators acting on $\mathcal{S}_n$

$$\mathcal{K}(B) \quad := \quad \operatorname{diag}(B)\, e^T + e \operatorname{diag}(B)^T - 2B, \tag{3}$$

and

$$\mathcal{T}(D) \quad := \quad -\tfrac{1}{2} JDJ, \tag{4}$$

where $J = I - \dfrac{ee^T}{n}$ is the orthogonal projection matrix onto subspace M.

Theorem 2.1 *The linear operators satisfy*

$$\mathcal{K}(\mathcal{S}_C) = \mathcal{S}_H,$$
$$\mathcal{T}(\mathcal{S}_H) = \mathcal{S}_C,$$

and $\mathcal{K}_{|\mathcal{S}_C}$ *and* $\mathcal{T}_{|\mathcal{S}_H}$ *are inverses of each other.*

Proof. See [8, 10].

□

It can easily be verified that

$$\mathcal{K}^*(D) \quad = \quad 2\,(\mathrm{Diag(De)} - \mathrm{D}) \tag{5}$$

is the adjoint operator of $\mathcal{K}$, where Diag(De) denotes the diagonal matrix formed from the vector De. Thus, a hollow matrix D is EDM if and only if $B = \mathcal{T}(D)$ is positive semidefinite, to be denoted as $B \succeq 0$. Equivalently, D is EDM if and only if $D = \mathcal{K}(B)$, for some B with $Be = 0$ and $B \succeq 0$. In this case, the embedding dimension r is given by the rank of B. If $B = XX^T$ for some $n \times r$ matrix X, then the rows of X are the coordinates of the points $x^1, x^2, \ldots, x^n$ that generate D. Furthermore, since $Be = 0$, it follows that the origin coincides with the centroid of these points. For these and other basic results on EDM see e.g. [8, 9, 10, 11, 21].

Let V be an $n \times (n-1)$ matrix such that

$$V^T e = 0\,, \quad V^T V = I\,, \tag{6}$$

where $I \in \mathcal{S}_{n-1}$ is the identity matrix. Hence, the subspace M can be represented as the range of V. J, the orthogonal projection matrix onto M, is then given by $J := VV^T = I - \dfrac{ee^T}{n}$. Now introduce the composite operators

$$\mathcal{K}_V(X) \quad := \quad \mathcal{K}(VXV^T), \tag{7}$$

and

$$\mathcal{T}_V(D) \quad := \quad V^T\mathcal{T}(D)V = -\tfrac{1}{2}V^TDV, \tag{8}$$

Lemma 2.1

$$\mathcal{K}_V(\mathcal{S}_{n-1}) = \mathcal{S}_H,$$
$$\mathcal{T}_V(\mathcal{S}_H) = \mathcal{S}_{n-1},$$

and $\mathcal{K}_V$ and $\mathcal{T}_V$ are inverses of each other on these two spaces.

It follows from (5) that

$$\mathcal{K}_V^*(D) \quad = \quad V^t\mathcal{K}^*(D)V \tag{9}$$

is the adjoint operator of $\mathcal{K}_V$. The following corollary summarizes the relationships between $\mathcal{E}$, the cone of Euclidean distance matrices of order n, and $\mathcal{P}_{n-1}$, the cone of positive semidefinite matrices of order $n-1$.

Corollary 2.1 *Suppose that V is defined as in (6). Then:*

$$\begin{aligned} \mathcal{K}_V(\mathcal{P}_{n-1}) &= \mathcal{E}, \\ \mathcal{T}_V(\mathcal{E}) &= \mathcal{P}_{n-1}. \end{aligned}$$

Proof. We saw earlier that D is EDM if and only if $D = \mathcal{K}(B)$ with $Be = 0$ and $B \succeq 0$. Let $X = V^tBV$, then since $Be = 0$ we have $B = VXV^t$. Therefore, $VXV^t \succeq 0$ if and only if $X \succeq 0$; and the result follows using (7) and Lemma 2.1.

□

Thus (1) is equivalent to the following semidefinite programming problem

$$(EDMCP) \quad \begin{array}{rll} \mu^* := & \min & f(X) = \|H \circ \mathcal{K}_V(X - B)\|_F^2 \\ & & X \succeq 0. \end{array}$$

where $B = \mathcal{T}_V(A)$. The optimal EDM D^* can be recovered from the optimal solution X^* of EDMCP using $D^* = \mathcal{K}_V(X^*)$. Two comments are in order.

First, the EDMCP is a convex problem which can be solved in polynomial time with an arbitrary precision. Second, the EDMCP_r is intractable since restricting the rank of X to r destroys the convexity of the problem. EDMCP is solved using a Primal-Dual Interior- Point algorithm introduced in [2]. Due to the nature of Interior-Point methods, optimal solutions of large ranks are often obtained. Rounding this optimal solution into another one with a lower rank necessitates the study of the set of optimal solution of EDMCP in the next section

3 Set of Optimal Solutions of EDMCP

Let X^* be the optimal solution of EDMCP and assume that $\mu^* = f(X^*) = 0$. i.e., graph $G = (V, E, \omega)$ is embeddable. $f(X^1) = f(X^2) = 0$ if and only if $Z = X^1 - X^2$ belong to the nullspace of $\mathcal{A}(X)$, where $\mathcal{A}(X) = H \circ \mathcal{K}_V(X)$. Thus, Ω, the set of optimal solutions of EDMCP, is given by

$$\Omega = \{X \in \mathcal{S}_{n-1} : X \succeq 0, \;\; X = X^* + Z, \text{ where } \mathcal{A}(Z) = 0\},$$

Ω is a convex set; and in general it is non-polyhedral. If graph G is complete. i.e., if all off-diagonal elements of H are ones, it readily follows that $f(X)$ is a strictly convex function and Ω is a single point. On the other hand, if G is disconnected then EDMCP can be solved more simply as two or more smaller subproblems; one for each connected component of G. Thus assume that G is connected. Since G is also assumed to be incomplete, X^* is not a singleton set. Next we study the facial structure of Ω. (See also the theses [17, 18] and the papers [19, 16, 14] for characterizations for general sets).

Definition 3.1 *A matrix $X \in \Omega$ is said to be an extreme point if X can not be represented as a proper convex combination of two distinct points X^1 and X^2 in Ω.*

Lemma 3.1 *Let X, $Z \in \mathcal{S}_{n-1}$ and let X be positive definite and Z be indefinite. Then, there exist two positive numbers α_1 and α_2 such that $X + \alpha_1 Z$ and $X - \alpha_2 Z$ are both positive semidefinite with rank $\leq n-2$.*

Proof. Let $X = Q\Lambda Q^T$ be the spectral decomposition of X. Then,

$$X + \alpha Z = Q\Lambda^{1/2}(I + \alpha Z')\Lambda^{1/2}Q^T$$

where $Z' = \Lambda^{-1/2}Q^T Z Q\Lambda^{-1/2}$. Let $\nu_1 \leq \nu_2 \leq \ldots \leq \nu_n$ be the eigenvalues of Z'. The assertion follows by setting $\alpha_1 = 1/|\nu_1|$ and $\alpha_2 = 1/\nu_n$

$\square$

Lemma 3.2 *Let the weighted graph $G = (V, E, \omega)$ be connected and let Z be a nonzero symmetric matrix in the null space of $\mathcal{A}$. Then Z is indefinite.*

Proof. Assume to the contrary that Z is definite; and wlog assume that $Z \succeq 0$. Then $D = (d_{ij}) = \mathcal{K}_V(Z)$ is a EDM. Since G is connected, there exists a *path* between node v_1 and node v_n. Hence there exist indices $i_1, i_2, \ldots, i_{n-2}$ such that $H_{1,i_1} = H_{i_1,i_2} = \cdots = H_{i_{n-2},n} = 1$. Since $\mathcal{A}(Z) = H \circ \mathcal{K}_V(Z) = H \circ D = 0$, it follows that $d_{1,i_1} = d_{i_1,i_2} = \cdots = d_{i_{n-2},n} = 0$. Thus $D = 0$ and consequently $Z = 0$.

$\square$

Corollary 3.1 *Let the weighted graph $G = (V, E, \omega)$ be connected. Then Ω is bounded.*

Next we present a characterization of the extreme points of Ω.

Theorem 3.1 *$X \in \Omega$ is not an extreme point if and only if there exists a nonzero symmetric matrix Z in the nullspace of $\mathcal{A}$, such that the nullspace of Z contains the nullspace of X.*

Proof. Let $Z \neq 0$ be in the nullspace of $\mathcal{A}$ such that $\mathcal{N}(X) \subseteq \mathcal{N}(Z)$, where $\mathcal{N}(.)$ denotes the null space. Let $\operatorname{rank}(X) = k$ and let $X = Q\Lambda Q^T$ be the spectral decomposition of X. Then, wlog we can assume that $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_k, 0, \ldots, 0)$ where λ_i are positive for all $i = 1, 2, \ldots, k$. Hence, $X = W\operatorname{diag}(\lambda_1, \ldots, \lambda_k)W^T$ where $W = [Q_{.1}Q_{.2}\cdots Q_{.k}]$ ($Q_{.j}$ denotes the jth column of Q). Since $\mathcal{N}(X) \subseteq \mathcal{N}(Z)$, $Z = WZ'W^T$. From Lemmas 3.1 and 3.2 there exists a positive number $\alpha = \min\{\alpha_1, \alpha_2\}$, such that $X^1 = X - \alpha Z \succeq 0$ and $X^2 = X + \alpha Z \succeq 0$. Furthermore, X^1 and X^2 belong to Ω since $Z \in \mathcal{N}(\mathcal{A})$. Hence, X is not an extreme point of Ω.

To prove the converse, assume that $X \in \Omega$ is not an extreme point. Then there exist two points $X^1 \neq X^2$ in Ω such that $X = \frac{1}{2}X^1 + \frac{1}{2}X^2$. Let $Z = \frac{1}{2}(X^1 - X^2)$. Then clearly $Z \neq 0$ and $Z \in \mathcal{N}(\mathcal{A})$. Furthermore, $X^1 = X + Z$ and $X^2 = X - Z$. Let $\operatorname{rank}(X) = k$ and let $X = Q\Lambda Q^T$, $\Lambda = \operatorname{diag}(\lambda)$, be the spectral decomposition of X. As before, wlog assume that the first k elements of λ are positive. Hence, the last $(n-k)$ rows and columns of the matrix Q^TXQ are zeros. Then since $X + Z \succeq 0$ and $X - Z \succeq 0$, it follows that the last $n-k$ rows and columns of Q^TZQ must also be zeros. Hence, $\mathcal{N}(X) \subseteq \mathcal{N}(Z)$.

$\square$

Corollary 3.2 *X is an extreme point of Ω if and only if there does not exist a nonzero symmetric matrix Y such that $H \circ \mathcal{K}_V(WYW^T) = 0$, where the columns of W form an orthonormal basis for the range of X.*

Corollary 3.3 *Let the weighted graph $G = (V, E, \omega)$ be connected. Let X, of rank k, be an extreme point of Ω. Then $k \leq \lfloor (\sqrt{8|E|+1} - 1)/2 \rfloor$.*

Proof. The system $H \circ \mathcal{K}_V(WYW^T) = 0$ has $|E|$ equations, one for each $H_{ij} = 1$, $i < j$; and $\frac{1}{2}k(k+1)$ variables since Y is symmetric. Thus if $k(k+1) > 2|E|$ this system has a solution and X is not an extreme point of Ω.

$\square$

Next we present an algorithm which rounds any point of Ω into an extreme point which by Corollary 3.3 has a rank $k \leq \lfloor (\sqrt{8|E|+1} - 1)/2 \rfloor$. (An algorithm that does this (purifying step) for general semidefinite programs is given in the thesis [17].)

Algorithm 3.1 .

Input: *Tolerance ϵ ; H, the adjacency matrix of Graph $G = (V, E, \omega)$;*

$r^* = \lfloor (\sqrt{8|E|+1} - 1)/2 \rfloor$; $A = (a_{ij}) = \begin{cases} \omega_{ij}^2 & \text{if } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$

Step 1: *solve the corresponding EDMCP to obtain μ^* and X^**

If $\mu^* > \epsilon$, stop. G is not embeddable in any dimension.

If $\mu^* \leq \epsilon$, r= rank (X^*), go to step 2.

Step 2: while $r > r^*$

Solve $H \circ \mathcal{K}_V(WYW^T) = 0$ to get Y.

$Z = WYW^T$, compute α_1 from Lemma 3.1

$X^* \leftarrow X^* + \alpha_1 Z$.

r= rank (X^*).

endwhile

Output: *$B = VX^*V^T$, let $B = PP^T$ then the rows of P give the coordinates of the vertices of G embedded in dimension $r \leq r^*$.*

Note that α_2 and $X^* \leftarrow X^* - \alpha_2 Z$ can be used in Step 2 as well. Also, note that after each iteration in step 2, the rank of X^* decreases by at least one.

Example:

Let $G = (V, E, \omega)$ be the 5-cycle with weights 1, 1, 2, 2, 2; and let $\epsilon = 10^{-9}$. Then

$$H = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}; \quad A = \begin{pmatrix} 0 & 1 & 0 & 0 & 4 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 4 & 0 \\ 0 & 0 & 4 & 0 & 4 \\ 4 & 0 & 0 & 4 & 0 \end{pmatrix}$$

Thus $r^* = 2$. Solving the EDMCP we get $\mu^* = 9.9 \times 10^{-10}$, X^* and $D^* = \mathcal{K}_V(X^*)$ as follows

$$X^* = \begin{pmatrix} 0.6557 & 0.3433 & -0.5383 & -0.6333 \\ 0.3433 & 1.0310 & -0.1666 & -0.5687 \\ -0.5383 & -0.1666 & 2.6358 & 0.5408 \\ -0.6333 & -0.5687 & 0.5408 & 2.4459 \end{pmatrix}$$

$$D^* = \begin{pmatrix} 0 & 1.0000 & 1.8768 & 4.6143 & 4.0000 \\ 1.0000 & 0 & 1.0000 & 4.3681 & 4.3681 \\ 1.8768 & 1.0000 & 0 & 4.0000 & 4.6143 \\ 4.6143 & 4.3681 & 4.0000 & 0 & 4.0000 \\ 4.0000 & 4.3681 & 4.6143 & 4.0000 & 0 \end{pmatrix}$$

Here r = rank(X^*)=4. After the first iteration of the algorithm we get:

$$X^* = \begin{pmatrix} 0.5602 & 0.6484 & -0.6611 & -0.8080 \\ 0.6484 & 1.7367 & 0.2013 & -0.4211 \\ -0.6611 & 0.2013 & 2.6660 & 0.5190 \\ -0.8080 & -0.4211 & 0.5190 & 2.3721 \end{pmatrix}$$

$$D^* = \begin{pmatrix} 0 & 1.0000 & 3.6757 & 4.9511 & 4.0000 \\ 1.0000 & 0 & 1.0000 & 4.5483 & 4.5483 \\ 3.6757 & 1.0000 & 0 & 4.0000 & 4.9511 \\ 4.9511 & 4.5483 & 4.0000 & 0 & 4.0000 \\ 4.0000 & 4.5483 & 4.9511 & 4.0000 & 0 \end{pmatrix}$$

where $\alpha_1 = 0.9496$. Here r= 3. After the second iteration we get:

$$X^* = \begin{pmatrix} 0.8218 & 0.7857 & -0.9130 & -1.4906 \\ 0.7857 & 1.7497 & 0.8238 & -1.6228 \\ -0.9130 & 0.8238 & 3.8979 & 1.3203 \\ -1.4906 & -1.6228 & 1.3203 & 2.7428 \end{pmatrix}$$

$$D^* = \begin{pmatrix} 0 & 1.0000 & 3.4932 & 7.7380 & 4.0000 \\ 1.0000 & 0 & 1.0000 & 6.5457 & 6.5457 \\ 3.4932 & 1.0000 & 0 & 4.0000 & 7.7380 \\ 7.7380 & 6.5457 & 4.0000 & 0 & 4.0000 \\ 4.0000 & 6.5457 & 7.7380 & 4.0000 & 0 \end{pmatrix}$$

where $\alpha_1 = 2.7805$. Here r= 2. Factorizing $B = VXV^T = PP^T$ yields the following 2-dimensional embedding

$$\begin{aligned} x^1 &= (-0.7284, -0.9345)^T \\ x^2 &= (-1.0844, -0.0000)^T \\ x^3 &= (-0.7284, \quad 0.9345)^T \\ x^4 &= (\quad 1.2706, \quad 1.0000)^T \\ x^5 &= (\quad 1.2706, -1.0000)^T \end{aligned}$$

Thus we obtained a 2-dimensional embedding for G. However, for these weights, G has also a 1-dimensional embedding namely

$$x_1 = x_4 = 0, \quad x_2 = 1, \quad x_3 = 1, \quad x_5 = -2$$

which we are not able to obtain. This should come as no surprise since it is NP-hard to find the extreme points of Ω with the smallest rank.

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