Two Theorems On Euclidean Distance Matrices and Gale Transform

Abdo Y. Alfakih [*]and Henry Wolkowicz [†]

University of Waterloo
Department of Combinatorics and Optimization
Waterloo, Ontario N2L 3G1, Canada
Research Report CORR 2001-06

January 28, 2001

Keywords: Euclidean distance matrices, semidefinite matrices, correlation matrices, tangent cones, Gale transform.

AMS Subject Classification: 51K05, 15A48, 52B35.

Abstract

We present a characterization of those Euclidean distance matrices D which can be expressed as $D = \lambda(E - C)$ for some nonnegative scalar λ and some correlation matrix C, where E is the matrix of all ones. This shows that the cones

$$\text{cone }(E - \mathcal{E}_n) \neq \overline{\text{cone }(E - \mathcal{E}_n)} = \mathcal{D}_n,$$

where $\mathcal{E}_n$ is the elliptope (set of correlation matrices) and $\mathcal{D}_n$ is the (closed convex) cone of Euclidean distance matrices.

The characterization is given using the Gale transform of the points generating D. We also show that given points $p^1, p^2, \ldots, p^n \in \Re^r$, for any scalars $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that

$$\sum_{j=1}^{n} \lambda_j \, p^j = 0, \qquad \sum_{j=1}^{n} \lambda_j = 0,$$

*E-mail: aalfakih@orion.uwaterloo.ca

†Research supported by Natural Sciences Engineering Research Council Canada. E-mail hwolkowicz@uwaterloo.ca

we have

$$\sum_{j=1}^{n} \lambda_j \, ||p^i - p^j||^2 = \alpha \text{ for all } i = 1, \ldots, n,$$

for some scalar α independent of i.

1 Introduction

An $n \times n$ matrix $D = (d_{ij})$ is said to be a *Euclidean distance matrix (EDM)* if there exist n points $p^1, p^2, \ldots, p^n$ in some Euclidean space $\Re^r$, such that $||p^i - p^j||^2 = d_{ij}$ for all $i, j = 1, \ldots, n$ where $||\ .\ ||$ is the Euclidean norm. It is well known, e.g. [5, 8], that D with zero diagonal is EDM if and only if D is negative semidefinite on the orthogonal complement of e, the vector of all ones. Hence, the set of $n \times n$ EDM matrices is a closed convex cone, to be denoted by $\mathcal{D}_n$.

Let $\mathcal{E}_n$ denote the set of $n \times n$ correlation matrices. i.e., the set of all positive semidefinite symmetric matrices whose diagonal is equal to e. It is also well known [3] that $\mathcal{D}_n$ is the tangent cone of $\mathcal{E}_n$ at E, the matrix of all ones, i.e.,

$$\mathcal{D}_n = \overline{\text{cone } (E - \mathcal{E}_n)} = \overline{\{\lambda(E - C) : \lambda \geq 0, C \in \mathcal{E}_n\}}, \tag{1}$$

where $\bar{\cdot}$ denotes closure.

In this paper, we present a characterization of EDM matrices D that can be represented as $D = \lambda(E - C)$, where λ is a nonnegative scalar and C is a correlation matrix. This characterization is given using the Gale transform of the points p^i, $i = 1, \ldots, n$ that generate D. (This transform is a powerful technique used in the theory of polytopes [4, 6].) The Gale transform of a set P of n points in $\Re^r$ is another set of n points in $\Re^{(n-1-r)}$. These new points reflect the affine dependencies of the set P.

The characterization shows that closure is essential in (1), i.e. the cone generated by the compact convex set $E - \mathcal{E}_n$ is not closed. In general, it is hard to show whether the cone generated by a closed convex set is closed. One usually needs special structure such as the set does not contain the origin, (e.g. [7]).

Applications of Euclidean distance matrices include among others, molecular conformation theory, protein folding, and the statistical theory of multidimensional scaling, see e.g. [1] for a list of applications.

2 Preliminaries

Positive semidefiniteness of a symmetric matrix C is denoted by $C \succeq 0$; e and E denote, respectively, the vector and the matrix of all ones. The $n \times n$ identity matrix is denoted by I_n. The diagonal of a matrix A is denoted by $\text{diag}\, A$, and its null space by $\mathcal{N}(A)$. Finally, $\| \, . \, \|$ denotes the Euclidean norm.

An $n \times n$ matrix $D = (d_{ij})$ is said to be a *Euclidean distance matrix (EDM)* if there exist points $p^1, p^2, \ldots, p^n$ in some Euclidean space $\Re^r$ such that $\|p^i - p^j\|^2 = d_{ij}$ for all $i, j = 1, \ldots, n$. The dimension of the smallest such Euclidean space containing $p^1, p^2, \ldots, p^n$ is called the *embedding dimension* of D. It is well known that the matrix D with zero diagonal is EDM if and only if D is negative semidefinite on

$$M := \{e\}^{\perp} = \{x \in \Re^n : e^T x = 0\}.$$

Let V be the $n \times (n-1)$ matrix whose columns form an orthonormal basis of M; that is, V satisfies:

$$V^T e = 0 \; , \quad V^T V = I_{n-1} \; . \tag{2}$$

The orthogonal projection on M, denoted by J, is then given by $J := VV^T = I - ee^T/n$. Hence, it follows that D with zero diagonal is EDM if and only if

$$B := -\frac{1}{2} \, JDJ \succeq 0. \tag{3}$$

Furthermore, the embedding dimension of D is equal to the rank of B. Let $\text{rank}\, B = r$. Then, the points $p^1, p^2, \ldots, p^n$ that generate D are given by the rows of the $n \times r$ matrix P where $B := PP^T$. Note that since $Be = 0$, it follows that the centroid of the points p^i, $i = 1, \ldots, n$ coincides with the origin.

Let $p^1, p^2, \ldots, p^n$ be points in $\Re^r$ whose centroid coincides with the origin. Assume that the points $p^1, p^2, \ldots, p^n$ are not contained in a proper hyperplane. Then

$$P := \begin{bmatrix} {p^1}^T \\ {p^2}^T \\ \vdots \\ {p^n}^T \end{bmatrix}$$

is of rank r. Let $B = PP^T$. Then it easily follows that the EDM matrix D generated by p^i, $i = 1, \ldots, n$ is given by

$$D = \text{diag}\, B e^T + e \, (\text{diag}\, B)^T - 2B. \tag{4}$$

Let Z be an $n \times \bar{r}$ matrix, $\bar{r} = n - 1 - r$, whose columns form a basis for the null space of the $(r+1) \times n$ matrix $\begin{bmatrix} P^T \\ e^T \end{bmatrix}$. i.e.,

$$P^T Z = 0, \quad e^T Z = 0, \quad \text{and } Z \text{ is full column rank.} \tag{5}$$

Let ${z^i}^T$ denote the i-th row of Z. i.e.,

$$Z := \begin{bmatrix} {z^1}^T \\ {z^2}^T \\ \vdots \\ {z^n}^T \end{bmatrix}.$$

Then z^i is called the Gale transform of p^i; and Z is called a *Gale matrix* corresponding to D. Three remarks are in order here. First, clearly the Gale matrix Z as defined in (5) is not unique. Different Gale matrices are obtained by multiplying Z on the right by a nonsingular $\bar{r} \times \bar{r}$ matrix Q. Second, the entries of Z are rational whenever the entries of P are rational. Third, the columns of Z represent the affine dependence relations among the points $p^1, p^2, \ldots, p^n$, i.e., among the rows of P.

3 Main Results

Next we give the two main results of the paper. The proofs are given in Section 4.

Theorem 3.1 *Let D be a Euclidean distance matrix and let Z be a Gale matrix corresponding to D. Then, the columns of DZ are proportional to e.*

From the definition of Z, another equivalent statement of Theorem 3.1 is

Theorem 3.2 *Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be coefficients, not all zero, of the affine dependence equation of the points $p^1, p^2, \ldots, p^n$, in $\Re^r$, i.e.,*

$$\sum_{j=1}^{n} \lambda_j p^j = 0, \quad \sum_{j=1}^{n} \lambda_j = 0.$$

Then

$$\sum_{j=1}^{n} \lambda_j \, \|p^i - p^j\|^2 = \alpha \text{ for all } i = 1, \ldots, n,$$

for some scalar α independent of i.

Theorem 3.3 *Let D be a Euclidean distance matrix and let Z be a Gale matrix corresponding to D. Then* **the following are equivalent***:*

1.

$$D = \lambda(E - C), \tag{6}$$

for some nonnegative scalar λ and some correlation matrix C;

2.

$$DZ = 0. \tag{7}$$

4 Proof of the Main Results

We start by proving the following technical lemma.

Lemma 4.1 *Let D be a Euclidean distance matrix and let B be the matrix defined in (3). Then:*

1.

$$-\frac{1}{2}V^T DV = V^T BV;$$

2.

$$\mathcal{N}(V^T DV) = \mathcal{N}(P^T V).$$

Proof. The first part follows directly from (4) and the definition of V. This yields the second part since $B = PP^T$ and $\mathcal{N}(V^T BV) = \mathcal{N}(V^T PP^T V) = \mathcal{N}(P^T V)$. ■

The following lemma was first proved in [2], where Euclidean distance matrices and Gale transforms were used to study the problems of realizability and rigidity of weighted graphs. We include the proof here for completeness.

Lemma 4.2 *Let D be a Euclidean distance matrix and let U be the matrix whose columns form an orthonormal basis of the null space of $V^T DV$. Then VU is a Gale matrix corresponding to D.*

Proof. It follows from Lemma 4.1 that $P^T VU = V^T DVU = 0$ and from the definition of V in (2) that $e^T VU = 0$. Hence, the columns of VU form an orthonormal basis for the null space of $\begin{bmatrix} P^T \\ e^T \end{bmatrix}$. ∎

Proof of Theorem 3.1. Let Z be a Gale matrix corresponding to D. Then It follows from Lemma 4.2 that $VU = ZQ$ for some nonsingular $\bar{r} \times \bar{r}$ matrix Q. Thus $V^T DZ = V^T DVUQ^{-1} = 0$. Hence, the columns of DZ are proportional to e. ∎

Proof of Theorem 3.3. $D = \lambda(E - C)$ for some nonnegative scalar λ and some correlation matrix C if and only if $E - \frac{1}{\lambda}D$ is positive semidefinite. Let $Q = [\frac{e}{\sqrt{n}}\ V]$. Then, $E - D/\lambda \succeq 0$ if and only if $Q^T\ (E - D/\lambda)\ Q \succeq 0$. But

$$Q^T\ (E - D/\lambda)\ Q = \begin{bmatrix} n - \frac{1}{\lambda\, n}\, e^T De & -\frac{1}{\lambda \sqrt{n}}\, e^T DV \\ -\frac{1}{\lambda \sqrt{n}}\, V^T De & -\frac{1}{\lambda}\, V^T DV \end{bmatrix}.$$

Recall that $V^T(-D)V \succeq 0$ follows from Lemma 4.1. Let W and U be the matrices whose columns form an orthonormal basis for the range space and null space of $V^T(-D)V$, respectively. Hence, $V^T(-D)V = W \Lambda W^T$, where Λ is the diagonal matrix of the positive eigenvalues of $V^T(-D)V$. Let $Q' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & W & U \end{bmatrix}$. Then, $E - D/\lambda$ is positive semidefinite if and only if

$$\begin{aligned} R &= Q'^T Q^T (E - D/\lambda) Q Q' \\ &= \begin{bmatrix} n - \frac{1}{\lambda\, n}\, e^T De & -\frac{1}{\lambda \sqrt{n}}\, e^T DVW & -\frac{1}{\lambda \sqrt{n}}\, e^T DVU \\ -\frac{1}{\lambda \sqrt{n}}\, W^T V^T De & \frac{1}{\lambda}\, \Lambda & 0 \\ -\frac{1}{\lambda \sqrt{n}}\, U^T V^T De & 0 & 0 \end{bmatrix} \succeq 0. \end{aligned} \tag{8}$$

Now for sufficiently large λ the submatrix

$$\begin{bmatrix} n - \frac{1}{\lambda\, n}\, e^T De & -\frac{1}{\lambda \sqrt{n}}\, e^T DVW \\ -\frac{1}{\lambda \sqrt{n}}\, W^T V^T De & \frac{1}{\lambda}\, \Lambda \end{bmatrix}$$

is positive definite. Thus $E - D/\lambda$ is positive semidefinite if and only if $e^T DVU = e^T DZ = 0$. But it follows from Theorem 3.1 that $e^T DZ = 0$ if and only if $DZ = 0$ and the result follows. ∎

5 Example

Next we present the following example to illustrate our new characterization. Given the two Euclidean distance matrices

$$D_1 = \begin{bmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{bmatrix}, \qquad D_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

The Gale matrices corresponding to D_1 and D_2 are

$$Z_1 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}, \qquad Z_2 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix},$$

respectively. Now $D_1 Z_1 = 2e$ and $D_2 Z_2 = 0$. It is easy to verify that $D_2 = E - C_2$, where

$$C_2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \succeq 0.$$

However, there exists no $\lambda \geq 0$ such that $D_1 = \lambda(E - C_1)$ for some correlation matrix C_1.

References

[1] S. AL-HOMIDAN. *Hybrid methods for optimization problems with positive semidefinite matrix constraints.* PhD thesis, University of Dundee, 1993.

[2] A.Y. ALFAKIH. On rigidity and realizability of weighted graphs. *Linear Algebra Appl.*, 325(1-3):57–70, 2001.

[3] M.M. DEZA and M. LAURENT. *Geometry of cuts and metrics.* Springer-Verlag, Berlin, 1997.

[4] D. GALE. Neighboring vertices on a convex polyhedron. In *Linear inequalities and related system*, volume 38 of *Annals of Mathematics Studies*, pages 255–263. Princeton University Press, Princeton, NJ, 1956.

[5] J. C. GOWER. Properties of Euclidean and non-Euclidean distance matrices. *Linear Algebra Appl.*, 67:81–97, 1985.

[6] B. GRÜNBAUM. *Convex polytopes.* Interscience Publishers John Wiley & Sons, Inc., New York, 1967. With the cooperation of Victor Klee, M. A. Perles and G. C. Shephard. Pure and Applied Mathematics, Vol. 16.

[7] R.T. ROCKAFELLAR. *Convex Analysis.* Princeton University Press, Princeton, NJ, USA, 1970.

[8] I.J. SCHOENBERG. Remarks to Maurice Frechet's article: Sur la definition axiomatique d'une classe d'espaces vectoriels distancies applicables vectoriellement sur l'espace de Hilbert. *Ann. Math.*, 36:724–732, 1935.