

## BLOCK DISTANCE MATRICES\*

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**Abstract.** In this paper, block distance matrices are introduced. Suppose  $F$  is a square block matrix in which each block is a symmetric matrix of some given order. If  $F$  is positive semidefinite, the block distance matrix  $D$  is defined as a matrix whose  $(i, j)$ -block is given by  $D_{ij} = F_{ii} + F_{jj} - 2F_{ij}$ . When each block in  $F$  is  $1 \times 1$  (i.e., a real number),  $D$  is a usual Euclidean distance matrix. Many interesting properties of Euclidean distance matrices to block distance matrices are extended in this paper. Finally, distance matrices of trees with matrix weights are investigated.

**Key words.** Distance matrices, Laplacian matrices, Trees.

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**1. Introduction.** In this paper, we introduce and investigate the properties of block distance matrices. This study is motivated by Euclidean distance matrices (EDM) which are a special class of nonnegative matrices with interesting properties and applications in molecular conformation problems in chemistry [3], electrical network problems [8] and multidimensional scaling in statistics [4].

An  $n \times n$  matrix  $D = [d_{ij}]$  is called a Euclidean distance matrix if there exists a set of  $n$  vectors, say  $\{x_1, \dots, x_n\}$ , in a finite dimensional inner product space such that  $d_{ij} = \|x_i - x_j\|^2$ . A symmetric matrix  $A = [a_{ij}]$  is called a *Gram* matrix if  $a_{ij} = \langle y_i, y_j \rangle$ , for some  $n$  vectors  $y_1, \dots, y_n$  in a finite dimensional real inner product space. It is well-known that a symmetric matrix is a Gram matrix if and only if it is positive semidefinite. Using this fact and the parallelogram law, it is easy to see that every entry in a EDM satisfies the equation  $d_{ij} = \|x_i\|^2 + \|x_j\|^2 - 2\langle x_i, x_j \rangle$ . We take this as the starting point and define a block distance matrix.

**DEFINITION 1.1.** We say that  $A = [A_{ij}]$  is a block matrix if each  $A_{ij}$  is a real matrix of some fixed order. Now  $A$  is called an  $n \times n$  *block-symmetric* matrix if it is a block matrix with  $n$  rows and  $n$  columns and for all  $i, j \in \{1, \dots, n\}$ ,  $A_{ij} = A_{ji}$ . We will call each  $A_{ij}$  a block of  $A$ . We define  $\mathcal{B}^{n,s}$  to be the set of all  $n \times n$  block-symmetric matrices in which all the blocks are symmetric matrices of order  $s$ .

Clearly, a  $n \times n$  block-symmetric matrix has  $n^2$  blocks. Suppose  $B \in \mathcal{B}^{n,s}$ . Then it is a symmetric matrix of order  $ns$  with real entries. To explain these notions, we consider the following example.

**EXAMPLE 1.2.** Let  $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12} & A_{22} \end{bmatrix}$ , where  $A_{11} = \begin{pmatrix} 1 & -2 \\ -2 & 4 \end{pmatrix}$ ,  $A_{12} = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ , and  $A_{22} = \begin{pmatrix} 0 & -3 \\ -3 & 5 \end{pmatrix}$ . Now  $A_{11}$ ,  $A_{12}$  and  $A_{22}$  are blocks of  $A$ ,  $A$  is a  $2 \times 2$  block matrix and  $A \in \mathcal{B}^{2,2}$ . Furthermore  $A$  is a  $4 \times 4$  symmetric matrix.

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We now define a block distance matrix.

DEFINITION 1.3. A matrix  $D \in \mathcal{B}^{n,s}$  is called a *block distance matrix* if there exists a positive semidefinite matrix  $F \in \mathcal{B}^{n,s}$  such that for all  $i, j \in \{1, \dots, n\}$ ,  $D_{ij} = F_{ii} + F_{jj} - 2F_{ij}$ . To illustrate, we give an example.

EXAMPLE 1.4. Let

$$F = \begin{bmatrix} A & -A & 0 \\ -A & A+B & -B \\ 0 & -B & B \end{bmatrix}$$

where  $A = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}$  and  $B$  is the  $2 \times 2$  identity matrix. It may be verified that  $F$  is a  $6 \times 6$  positive semidefinite matrix. Now according to Definition 1.3,

$$D = \begin{bmatrix} 0 & 4A+B & A+B \\ 4A+B & 0 & A+4B \\ A+B & A+4B & 0 \end{bmatrix}$$

is a block distance matrix. It is clear that every EDM is a block distance matrix. Unlike EDMs, however block distance matrices can have negative entries. In this article, we extend many interesting properties of EDMs to block distance matrices. In particular, we show that if  $D$  is a block distance matrix in  $\mathcal{B}^{n,s}$  with at least one block positive definite then  $D$  has exactly  $s$  positive eigenvalues. We then extend the well-known theorem of Schoenberg [7] for Euclidean distance matrices to block distance matrices and characterize a block distance matrix by the eigenvalues of its bordered matrix. Finally, we obtain a result for the null space of a block distance matrix. Using this result we extend some useful properties of EDMs proved in [4] to block distance matrices.

In Section 3, we consider distance matrices which arise from trees. A graph  $G = (V, E)$  consists of a finite set of vertices  $V$  and a set of edges  $E$ . A tree is a connected acyclic graph. For fundamental results on graph theory, we refer to [6]. Let  $T$  be a tree with  $n$  vertices. To each edge of  $T$ , we assign a *weight* which is a positive definite matrix. We assume that all the weights are of fixed order  $s$ . The distance between two vertices  $i$  and  $j$  is the sum of all the weights in the path connecting  $i$  and  $j$ . Suppose  $d_{ij}$  is the distance between  $i$  and  $j$ . Now the distance matrix is the matrix with  $d_{ij}$  in the  $(i, j)$  position.

We show that distance matrices of trees are block distance matrices. When all the weights are positive scalars, many significant results are known for distance matrices. Suppose  $D$  is the distance matrix of a tree with  $n$  vertices having unit weights. In this case, Graham and Lovász [5] established an interesting formula for the inverse of the distance matrix. We extend this formula to distance matrices of trees with matrix weights.

We mention a few notations and definitions. Denote by  $I_s$  the identity matrix of order  $s$ . Let  $J = (e \otimes I_s)(e \otimes I_s)^T$  where  $e = (1, \dots, 1)^T$  is the  $n$ -vector of all ones. Thus  $J$  is a matrix in  $\mathcal{B}^{n,s}$  with every block equal to  $I_s$ . The null space of  $J$  is denoted by  $N(J)$ . Let  $U = e \otimes I_s$ . For  $A \in \mathcal{B}^{n,s}$ , let  $\text{diag } A$  be the  $n \times n$  block matrix with

$A_{ii}$  along its diagonal, the other blocks being zero. The projection matrix  $I - \frac{1}{n}J$  is denoted by  $P$ . The inertia of a symmetric matrix  $A$  is denoted by  $\text{In } A$ . Thus  $\text{In } A$  is a three-tuple indicating the number of positive, negative and zero eigenvalues of  $A$ . Let  $e_i$  be the  $n$ -vector with one in the position  $i$  and zeros elsewhere and  $E_i = e_i \otimes I_s$ .

We now recall the definition of Moore-Penrose inverse of a symmetric matrix. For details we refer to [2].

DEFINITION 1.5. Let  $A$  be a symmetric matrix with real entries. Then  $H$  is called a  $g$ -inverse of  $A$  if the equation  $AHA = A$  is satisfied. If  $H$  satisfies  $HAH = H$ , then we say that  $H$  is an outer-inverse of  $A$ . The Moore-Penrose inverse of  $A$  is the symmetric matrix  $A^\dagger$  satisfying the following conditions: (i)  $A^\dagger$  is a  $g$ -inverse of  $A$ , (ii)  $A^\dagger$  is an outer-inverse of  $A$ , and (iii)  $A^\dagger A$  is symmetric.

**2. Basic properties.** In this section, we prove some fundamental properties of block distance matrices. Throughout this section, we assume that  $D \in \mathcal{B}^{n,s}$  and  $D$  is a block distance matrix.

**2.1. Eigenvalues of block distance matrices.** We begin with the following lemma.

LEMMA 2.1. *Every off-diagonal block of  $D$  is positive semidefinite.*

*Proof.* Since  $D$  is a block distance matrix, there exists a positive semidefinite block matrix  $F$  such that  $D_{ij} = F_{ii} + F_{jj} - 2F_{ij}$ . Let  $i \neq j$  and  $V = [I_s, -I_s]^T$ . Then  $D_{ij} = V^T G V$  where  $G = \begin{bmatrix} F_{ii} & F_{ij} \\ F_{ij} & F_{jj} \end{bmatrix}$ . Clearly  $G$  is positive semidefinite and so is  $D_{ij}$ .  $\square$

In the next theorem we show that a block distance matrix has exactly  $s$  positive eigenvalues if at least one block is positive definite.

THEOREM 2.2. *Suppose that at least one block of  $D$  is positive definite. Then  $D$  has exactly  $s$  positive eigenvalues.*

*Proof.* Let  $D_{ij} = F_{ii} + F_{jj} - 2F_{ij}$ , where  $F \in \mathcal{B}^{n,s}$  is positive semidefinite. Then  $D$  satisfies the equation  $D = (\text{diag } F)J + J(\text{diag } F) - 2F$ . Now, if  $x \in N(J)$  then  $x^T D x \leq 0$ , which implies that  $D$  is negative semidefinite on  $N(J)$ . Since the dimension of  $N(J)$  is  $ns - s$ ,  $D$  has at least  $ns - s$  nonpositive eigenvalues.

By our assumption  $D$  has at least one off-diagonal block which is positive definite. Thus  $U^T D U$  is positive definite. Let  $x$  be a vector in the column space of  $J$ . Then  $Jy = x$  for some  $y \in \mathbb{R}^{ns}$  and hence  $x^T D x = y^T U E U^T y$  where  $E = U^T D U$ . Thus,  $D$  is positive definite on the column space of  $J$ . Now  $\text{rank } J = s$  and therefore  $D$  has at least  $s$  positive eigenvalues. This completes the proof.  $\square$

**2.2. Schoenberg's theorem for block distance matrices.** It is well-known that an  $n \times n$  matrix  $E$  is an EDM if and only if  $E$  has zero diagonal and  $E$  is negative semidefinite on the hyperplane  $\{e\}^\perp$ . We now obtain a similar result for block distance matrices.

THEOREM 2.3. *Let  $D \in \mathcal{B}^{n,s}$ . Then  $D$  is a block distance matrix if and only if it is negative semidefinite on  $N(J)$  and the diagonal blocks are zero.*

*Proof.* If  $D$  is a block distance matrix, then there exists a positive semidefinite block matrix  $F$  such that  $D = (\text{diag } F)J + J(\text{diag } F) - 2F$ . Clearly the diagonal blocks of  $D$  must be zero. It is easy to see that if  $x \in N(J)$ , then  $x^T D x \leq 0$ .

We now prove the converse. Assume that  $D \in \mathcal{B}^{n,s}$ ,  $D_{ii} = 0$  and for all  $x \in N(J)$ ,  $x^T D x \leq 0$ . Let  $Y = -\frac{1}{2} P D P$ , where  $P := I - \frac{J}{n}$ . Clearly,  $Y \in \mathcal{B}^{n,s}$ . We claim that  $Y$  is positive semidefinite. Suppose that  $z \in \mathbb{R}^{ns}$ . Then  $z = z_1 + z_2$  where  $z_1$  and  $z_2$  are vectors in the column space and null space of  $J$  respectively. Since  $P z_1 = 0$ ,  $z^T Y z = z_2^T Y z_2$ . As  $P z_2 = z_2$  and  $D$  is negative semidefinite on  $N(J)$ ,  $z_2^T Y z_2 \geq 0$ . Therefore  $Y$  is positive semidefinite. Recall that  $E_i := e_i \otimes I_s$ . In other words,  $E_i = [0, \dots, 0, I_s, 0, \dots, 0]^T$  where  $I_s$  is in the  $i$ th position. Therefore  $J E_i = U$ . Note that the  $(i, j)$ -block of  $Y$  is  $E_i^T Y E_j$ . Hence

$$(2.1) \quad -2Y_{ij} = D_{ij} - \frac{1}{n} E_i^T D U - \frac{1}{n} U^T D E_j + \frac{1}{n^2} U^T D U.$$

Since  $D_{ii} = 0$ ,

$$Y_{ii} = \frac{1}{2n} E_i^T D U + \frac{1}{2n} U^T D E_i - \frac{1}{2n^2} U^T D U.$$

It is easy to see that

$$\frac{1}{2n} E_i^T D U = \frac{1}{2n} U^T D E_i.$$

Therefore from (2.1),

$$(2.2) \quad Y_{ii} = \frac{1}{n} E_i^T D U - \frac{1}{2n^2} U^T D U.$$

Similarly,

$$(2.3) \quad Y_{jj} = \frac{1}{n} U^T D E_j - \frac{1}{2n^2} U^T D U.$$

Now (2.1), (2.2), (2.3) imply that

$$D_{ij} = Y_{ii} + Y_{jj} - 2Y_{ij}.$$

This completes the proof.  $\square$

**2.3. Bordered matrix of a block distance matrix.** In the next two results, we characterize block distance matrices using bordered matrices. Let  $E \in \mathcal{B}^{n,s}$ . Then the bordered matrix of  $E$  is defined to be the following matrix:

$$\tilde{E} := \begin{bmatrix} E & U \\ U^T & 0 \end{bmatrix}.$$

**THEOREM 2.4.** *Suppose  $D$  is a block distance matrix with at least one block positive definite. Then the bordered matrix of  $D$  has exactly  $s$  positive eigenvalues.*

*Proof.* Since  $D$  has exactly  $s$  positive eigenvalues by Theorem 2.2,  $\tilde{D}$  has at least  $s$  positive eigenvalues by the interlacing property of eigenvalues. Let

$$N = \{(x^T, y^T)^T : x \in N(J) \text{ and } y \in \mathbb{R}^s\}.$$

Then  $N$  is an  $ns$  dimensional subspace of  $\mathbb{R}^{ns+s}$ . If  $z \in N$ , it is easy to see that  $z^T \tilde{D}z = x^T Dx$ . By Theorem 2.3,  $z^T \tilde{D}z \leq 0$  and therefore  $\tilde{D}$  has at least  $ns$  nonpositive eigenvalues. This implies that  $\tilde{D}$  has exactly  $s$  positive eigenvalues.  $\square$

**THEOREM 2.5.** *Assume that a bordered matrix  $\tilde{E}$  has exactly  $s$  positive eigenvalues. Further assume that  $\text{diag } E = 0$ . Then  $E$  is a block distance matrix.*

*Proof.* If for some nonzero vector  $x \in N(J)$ , it happens that  $x^T Ex > 0$ , then  $\tilde{E}$  will be positive definite on the subspace

$$W = \{(\alpha x^T, y^T)^T : \alpha \in \mathbb{R} \text{ and } y \in \mathbb{R}^s\}.$$

Since the dimension of  $W$  is  $s+1$ ,  $\tilde{E}$  will have at least  $s+1$  positive eigenvalues. This will be a contradiction and now the result follows from Theorem 2.3.  $\square$

**2.4. Null space of a block distance matrix.** In this section, we assume that  $D \in \mathcal{B}^{n,s}$  is a block distance matrix with the property that at least one block is positive definite.

**THEOREM 2.6.** *The null space of  $D$  is contained in  $N(J)$ .*

*Proof.* Assume that there exists a vector  $x \notin N(J)$  such that  $Dx = 0$ . Let  $x = y + z$ , where  $z$  is in the column space of  $J$  and  $y$  is in the null space of  $J$ . Since  $x^T Dy = 0$ , we must have  $y^T Dy + z^T Dy = 0$ . We know that  $D$  is negative semidefinite on  $N(J)$  and therefore  $z^T Dy$  must be nonnegative. Now  $x^T Dz = 0$ . Hence  $y^T Dz + z^T Dz = 0$ . Since  $z$  is in the column space of  $J$ ,  $z^T Dz > 0$ . This shows that  $y^T Dz < 0$  which is a contradiction. Thus  $x \in N(J)$ .  $\square$

If  $E$  is a EDM, then for any  $g$ -inverse  $E^-$ , it is known from [4] that  $EE^-e = e$  and  $e^T E^-e \geq 0$ . We now extend these results to block distance matrices.

**COROLLARY 2.7.** *If  $D^-$  is a  $g$ -inverse of  $D$ , then  $DD^-U = U$ .*

*Proof.* By Theorem 2.6 the column space of  $U$  is in the column space of  $D$  and so  $DD^-U = U$ .  $\square$

**COROLLARY 2.8.** *Let  $D$  be a block distance matrix with at least one block positive definite. If  $D^-$  is a  $g$ -inverse of  $D$ , then  $U^T D^-U$  is positive semidefinite.*

*Proof.* Let  $\tilde{D}$  be the bordered matrix of  $D$ . By Corollary 2.7,  $DD^-U = U$  and hence the following identity is easily verified:

$$(2.4) \quad \begin{bmatrix} I & 0 \\ -U^T D^- & I \end{bmatrix} \begin{bmatrix} D & U \\ U^T & 0 \end{bmatrix} \begin{bmatrix} I & -D^-U \\ 0 & I \end{bmatrix} = \begin{bmatrix} D & 0 \\ 0 & -U^T D^-U \end{bmatrix}.$$

It is well-known that if  $X$  is an  $n \times n$  symmetric matrix, then for any  $n \times n$  nonsingular matrix  $Y$ ,  $\text{In}(X) = \text{In}(Y^T X Y)$ . Therefore it follows from (2.4) that  $\text{In}(-U^T D^-U) = \text{In } \tilde{D} - \text{In } D$ . Thus by Theorem 2.4, all the eigenvalues of  $U^T D^-U$  are nonnegative and therefore it is positive semidefinite.  $\square$

**3. Distance matrices of trees with matrix weights.** In this section, we consider distance matrices of trees with weights being positive definite matrices. We show that such matrices are block distance matrices and prove a formula for their inverses. Assume that  $T$  is a tree with vertices  $\{v_1, \dots, v_n\}$  and edges  $\{e_1, \dots, e_{n-1}\}$ . To each edge of  $T$ , we assign a  $s \times s$  positive definite matrix  $W_i$ , which we call the weight of the edge  $e_i$ . The *distance* between the vertices  $v_i$  and  $v_j$  is the sum of the

weights of all edges in the path connecting  $v_i$  and  $v_j$ . The distance matrix of  $T$  is the matrix in  $\mathcal{B}^{n,s}$  whose  $(i, j)$  block is the distance between  $v_i$  and  $v_j$ .

We associate another matrix with  $T$ . Let  $B_k = W_k^{-1}$ . Suppose the vertices  $v_i$  and  $v_j$  are adjacent and  $e_k$  is the edge connecting them. We set  $L_{ij} = -B_k$ . If the vertices are not adjacent, we put  $L_{ij} = 0$ . Let the diagonal block  $L_{ii}$  be chosen so that the sum of all the blocks in the  $i$ th row is zero. The  $n \times n$  block matrix  $L = [L_{ij}]$  thus obtained is called the *Laplacian* matrix of  $T$ . It can be easily shown that the column space of  $L$  is  $N(J)$  and therefore its rank is  $ns - s$ . Further it can be noted that the Laplacian matrix is positive semidefinite.

We give an example to illustrate the above definitions.

EXAMPLE 3.1. Let  $T$  be the tree with vertices  $\{v_1, v_2, v_3\}$  and edges  $\{e_1, e_2\}$  where  $e_1$  is the edge connecting  $v_1$  and  $v_2$ , and  $e_2$  is the edge connecting  $v_2$  and  $v_3$ . Suppose  $W_1 = \begin{pmatrix} 1 & -6 \\ -6 & 37 \end{pmatrix}$  and  $W_2 = \begin{pmatrix} 5 & -1 \\ -1 & 3 \end{pmatrix}$ . Let  $B_1 = W_1^{-1}$  and  $B_2 = W_2^{-1}$ .

Let  $W_1$  be the weight of  $e_1$  and  $W_2$  be the weight of  $e_2$ . Then the distance matrix of  $T$  is

$$D = \begin{bmatrix} 0 & W_1 & W_1 + W_2 \\ W_1 & 0 & W_2 \\ W_1 + W_2 & W_2 & 0 \end{bmatrix}.$$

The Laplacian of  $T$  is

$$L = \begin{bmatrix} B_1 & -B_1 & 0 \\ -B_1 & B_1 + B_2 & -B_2 \\ 0 & -B_2 & B_2 \end{bmatrix}.$$

We first prove the following identity.

LEMMA 3.2. Let  $T$  be a tree with vertex set  $\{v_1, \dots, v_n\}$  and edge set  $\{e_1, \dots, e_{n-1}\}$ . For  $i \in \{1, \dots, n-1\}$ , let  $W_i$  denote a positive definite matrix of order  $s$ . Let the weight of the edge  $e_i$  be  $W_i$ ,  $i = 1, 2, \dots, n$ . Suppose that  $D$  is the distance matrix and  $L$  is the Laplacian of  $T$ . Then

$$L = -\frac{1}{2}LDL.$$

*Proof.* We prove the result by induction. It is easy to verify the result if the tree has only two vertices. Suppose that the result is true for trees with  $n - 1$  vertices.

Without any loss of generality, assume that  $v_n$  is a pendant vertex and is adjacent to  $v_{n-1}$ . Let the distance between  $v_n$  and  $v_{n-1}$  be  $W$ . Let  $K = -\frac{1}{2}LDL$ .

Let  $A_i$  be the  $i$ th column of blocks of  $L$ . Then  $-2K_{ij} = A_i^T D A_j = A_j^T D A_i$ .

Let  $S$  be the subtree obtained by deleting  $v_n$  from  $T$ . Suppose that  $M$  is the Laplacian matrix and  $E$  is the distance matrix of  $S$ . Then  $D$  can be written as

$$D = \begin{bmatrix} E & V \\ V^T & 0 \end{bmatrix},$$

where  $V = [E_{1n-1} + W, \dots, E_{n-1n-2} + W, W]^T$ . Suppose that the  $i$ th column of blocks of  $M$  is given by  $M_i$ .

Let  $i, j \in \{1, \dots, n-2\}$ . In this case  $L_{ij} = M_{ij}$  and  $A_i = \begin{bmatrix} M_i \\ 0 \end{bmatrix}$ . Therefore  $A_i^T D A_j = M_i^T E M_j$ . It follows by the induction assumption that  $A_i^T D A_j = -2M_{ij}$  and so  $K_{ij} = M_{ij}$ .

Now let  $i = n$  and  $j = n$ . In this case  $L_{ij} = W^{-1}$ . As  $v_n$  is a pendant vertex,  $A_n = [0, \dots, 0, -W^{-1}, W^{-1}]^T$ . It is easy to see that  $D A_n = [I_s, \dots, I_s, I_s, -I_s]^T$  and hence  $A_n^T D A_j = -2W^{-1}$ . Therefore  $K_{ij} = W^{-1}$ .

We now consider the case when  $i \in \{1, \dots, n-2\}$  and  $j = n$ . In this case  $L_{ij} = 0$ . As already noted,  $D A_n = [I_s, \dots, I_s, I_s, -I_s]^T$  and  $A_i = [M_{i1}, \dots, M_{in-1}, 0]^T$ . Therefore  $A_i^T D A_j = \sum_{k=1}^{n-1} M_{ik} = 0$ , as  $M$  is a Laplacian matrix. Thus  $K_{ij} = 0$ .

We have proved that  $K_{ij} = L_{ij}$  when  $i \in \{1, \dots, n-2\}$  and  $j \in \{1, \dots, n-2, n\}$ . Since  $K$  and  $L$  are symmetric matrices,  $K_{ji} = K_{ij} = L_{ij} = L_{ji}$ . Now the proof is complete by noting that  $U^T K = 0 = U^T L$ .  $\square$

LEMMA 3.3. *If  $L$  is the Laplacian matrix of a weighted tree, then  $LL^\dagger = I - \frac{1}{n}J$ .*

*Proof.* Let  $P := I - \frac{1}{n}J$ . If  $x$  is in the column space of  $J$ , then  $x = Jy$  for some  $y$ . Then  $LL^\dagger x = LL^\dagger Jy = L^\dagger L Jy = 0$ , since  $LJ = 0$ . Also,  $Px = 0$ , since  $J^2 = nJ$ . Thus  $LL^\dagger x = Px$ .

Now suppose  $x \in N(J)$  and let  $LL^\dagger x = y$ . Then  $J(x - y) = 0$  since  $JL = 0$  and hence  $x - y \in N(J)$ . Also,  $LLL^\dagger x = Ly$ . Thus,  $Lx = Ly$  and hence  $x - y$  is in the column space of  $J$ . Therefore  $x = y$  and hence  $LL^\dagger x = x$ . Clearly,  $Px = x$  and thus  $LL^\dagger x = Px$  in this case as well. Combining the two parts it follows that  $LL^\dagger x = Px$  for all  $x$  and therefore  $LL^\dagger = P$ .  $\square$

THEOREM 3.4. *Distance matrices of trees with matrix weights are block distance matrices.*

*Proof.* By Lemma 3.2 and Lemma 3.3,

$$(3.1) \quad -\frac{1}{2}PDP = L^\dagger,$$

where  $P = I - \frac{1}{n}J$ . Since  $L$  is a positive semidefinite matrix,  $L^\dagger$  is also positive semidefinite and it is easy to see from (3.1) (as in Theorem 2.3) that  $D_{ij} = L_{ii}^\dagger + L_{jj}^\dagger - 2L_{ij}^\dagger$ . Therefore  $D$  is a block distance matrix.  $\square$

We now prove the Graham and Lovász formula for distance matrices of trees with matrix weights. The proof is based on the following lemma.

LEMMA 3.5. *Let  $A \in \mathcal{B}^{n,s}$ . Suppose  $AA^\dagger U = U$  and  $\det U^T A^\dagger U \neq 0$ . Then,*

$$(3.2) \quad (PAP)^\dagger = A^\dagger - A^\dagger U F^{-1} U^T A^\dagger,$$

where  $F = U^T A^\dagger U$ .

*Proof.* Let  $T$  be the right hand side of (3.2) and  $K = PAP$ . Then by a direct verification, we see that  $TAT = T$ . Since  $P$  is the orthogonal projection onto the subspace  $N(J)$ ,  $TP = T$ . As  $T$  is symmetric,  $PT = T$ . Thus,  $TKT = T$ . We now claim that  $TK = KT$ , that is,  $TK$  is symmetric. Consider  $PAA^\dagger$ . Since  $AA^\dagger U = U$ ,  $JAA^\dagger = J$ . Thus,  $JAA^\dagger$  is symmetric and so is  $PAA^\dagger$ . As  $PU = 0$ ,  $PAT = PAA^\dagger$ .

Since  $PT = T$ ,  $PAPT = PAT$ . Now  $PAP = K$  and therefore  $KT$  is symmetric. It remains to show that  $GTK = T$ . From the definition of  $K$  and  $TP = PT = T$ , it follows that  $GTK = KTAP = PATAP$ . But  $PAT = PAA^\dagger$  and hence  $PATAP = K$ . This completes the proof.  $\square$

Applying the above result for block distance matrices, we get the following result using Corollary 2.7.

**THEOREM 3.6.** *Let  $D$  be a block distance matrix. Suppose  $F = U^T D^\dagger U$  is positive definite and  $L = (-\frac{1}{2}PDP)^\dagger$ . Then*

$$D^\dagger = -\frac{1}{2}L + D^\dagger U F^{-1} U^T D^\dagger.$$

We now prove the Graham and Lovász formula for the distance matrix of a weighted tree.

**THEOREM 3.7.** *Let  $T$  be a weighted tree with  $n$  vertices. Suppose  $D$  and  $L$  are respectively the distance and Laplacian matrices of  $T$ . Let  $\delta_i$  denote the degree of the  $i$ th vertex of  $T$  and  $\tau = (2 - \delta_1, \dots, 2 - \delta_n)^T$ . If  $\Delta = \tau \otimes I_s$  and  $R$  is the sum of all the weights of  $T$ , then*

$$D^{-1} = -\frac{1}{2}L + \frac{1}{2}\Delta R^{-1}\Delta^T.$$

*Proof.* We claim that  $D$  is nonsingular. We have shown in Lemma 3.2 that

$$(3.3) \quad \frac{LDL}{2} = -L.$$

Further from Lemma 3.3,  $LL^\dagger = I - \frac{J}{n}$ . By Theorem 2.6, if  $x$  is a vector in the null space of  $D$ , then  $x$  must be a vector in the null space of  $J$ . Equation (3.3) and  $LL^\dagger = I - \frac{J}{n}$  now imply that  $x^T D x = 0 = x^T L^\dagger x$ . As null space of  $L$  is the column space of  $J$ , it follows that  $x = 0$ . Therefore  $D$  is nonsingular.

By Lemmas 3.2 and 3.3,  $PDP = -2L^\dagger$ . By Lemma 1 in [1],  $D\Delta = UR$ . Thus  $D^{-1}U = \Delta R^{-1}$ . Since  $U^T \Delta = 2I_s$ ,  $U^T D^{-1}U = 2R^{-1}$ . Let  $F = 2R^{-1}$ .

Therefore by Theorem 3.6,

$$D^{-1} = -\frac{1}{2}L + (D^{-1}U)F^{-1}U^T D^{-1},$$

and thus,

$$D^{-1} = -\frac{1}{2}L + \frac{1}{2}\Delta R^{-1}\Delta^T. \square$$

When the weights are scalars and equal to one, we get the formula given in [5]:

**THEOREM 3.8** (Graham and Lovász [5]). *If  $T$  is a tree on  $n$  vertices with Laplacian  $L$  and distance matrix  $E$ , then*

$$E^{-1} = -\frac{1}{2}L + \frac{1}{2(n-1)}\tau\tau^T,$$



where  $\tau$  is defined as in Theorem 3.7.

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