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ON DISTANCE LAPLACIAN MATRICES OF WEIGHTED TREES

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Abstract. Let T be a weighted tree on n vertices and $D(T) := [[d_{ij}]]$ be the distance matrix of T. The distance Laplacian matrix of T is defined as

$$L_D(T) := \mathrm{Diag}(\sum_{j=1}^{n} d_{1j}, \ldots, \sum_{j=1}^{n} d_{nj}) - D(T).$$

We aim to show that all off-diagonal entries in the Moore-Penrose inverse of $L_D(T)$ are non-positive. Specifically, this result implies that the Moore-Penrose inverse of $L_D(T)$ is an $\mathbf{M}$-matrix.

1. Introduction

A tree is a *connected* acyclic graph. Let T be a tree on n vertices with vertex set $V(T)$ and edge set $E(T)$. Assume that $V(T) := \{1, \ldots, n\}$ and to each edge (p,q) of T, a positive number w_{pq} is assigned. We say that w_{pq} is the *weight* of (p,q). The distance between any two vertices i and j of T, denoted by β_{ij}, is the sum of all the weights in the path that connects i and j. Define

$$d_{ij} := \begin{cases} \beta_{ij} & i \neq j \\ 0 & \text{else.} \end{cases}$$

The distance matrix and the distance Laplacian matrix of T are now, respectively,

$$D(T) := [[d_{ij}]] \quad \text{and} \quad L_D(T) := \mathrm{Diag}(\sum_{j=1}^{n} d_{1j}, \ldots, \sum_{j=1}^{n} d_{nj}) - D(T).$$

As the graph/network is connected, the distance Laplacian matrix is the combinatorial/classical Laplacian of a complete network with weights given by the distances. If i and j are any two vertices of T, define

$$\gamma_{ij} := \begin{cases} \frac{1}{w_{ij}} & (i,j) \in E(T) \\ 0 & \text{else.} \end{cases}$$

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The Laplacian matrix of T, denoted by $L(T)$, is the $n \times n$ matrix

$$L(T) := \mathrm{Diag}(\sum_{j=1}^{n} \gamma_{1j}, \ldots, \sum_{j=1}^{n} \gamma_{nj}) - [[\gamma_{ij}]].$$

The values γ_{ij} are the conductances in the context of electrical network resistances. Following the Kirchhoff laws on series resistances, the distance between any pair of vertices in a weighted tree coincide with the effective resistance between them, and hence the distance and Laplacian matrices $L(T)$ and $D(T)$ are connected by the relation

$$d_{ij} = \alpha_{ii} + \alpha_{jj} - 2\alpha_{ij}, \tag{1}$$

where α_{ij} is the $(i,j)^{\text{th}}$ entry in the Moore-Penrose inverse of $L(T)$: see Klein and Randić [12]. Matrices $L(T)$ and $L_D(T)$ have some common features.

(i) Both are positive semidefinite.

(ii) All row/column sums are equal to *zero*.

(iii) Rank is $n-1$.

(iv) All off-diagonal entries are non-positive.

Items (i) and (iv) imply that $L_D(T)$ and $L(T)$ are $\mathbf{M}$-matrices. The objective of this paper is to deduce a new property of $L_D(T)$: The Moore-Penrose inverse of $L_D(T)$ is an $\mathbf{M}$-matrix. As usual, we use the notation $A^{\dagger}$ to denote the Moore-Penrose inverse of A. In general, $L(T)^{\dagger}$ is not an $\mathbf{M}$-matrix. A significant result from [10] states that $L(T)^{\dagger}$ is an $\mathbf{M}$-matrix if and only if T is a star. A similar characterization of weighted trees can be found in [11]. It can be noted that resistive electrical networks represented by connected graphs exhibit desirable properties if the Moore-Penrose inverse of their Laplacian matrices are $\mathbf{M}$-matrices: see [13].

Based on the previous discussion, we investigate the existence of a matrix associated with a given connected graph that possesses the fundamental characteristics of a classical Laplacian matrix, while also having the property that its Moore-Penrose inverse is an $\mathbf{M}$-matrix. Our result in this paper asserts that if T is any weighted tree, then $L_D(T)$ is such a special matrix. To provide a concise and precise statement, we can approach it from a combinatorial perspective. Consider the complete graph K_n with n vertices, where each edge is assigned a weight d_{ij} representing the distance between the vertex i and vertex j in a weighted tree with n vertices. In this context, our investigation reveals that the Moore-Penrose inverse of the classical Laplacian exhibits the remarkable characteristic of being an $\mathbf{M}$-matrix.

Consider the more general problem described as follows: Let G be a complete graph with assigned weights on its edges. The question is under what conditions the Moore-Penrose inverse of the Laplacian matrix of G is an $\mathbf{M}$-matrix. In the case, where all the weights are equal to one, it is proven in [6] that the Moore-Penrose inverse of the Laplacian matrix is an $\mathbf{M}$-matrix. The question extends for a general connected graph. In [6], the authors present a remarkable result: For connected graphs that are distance regular, if the Moore-Penrose inverse of their combinatorial Laplacian matrices are $\mathbf{M}$-matrices, then the diameter of those graphs must be at most *three*.

Another related question in matrix theory is when the Moore-Penrose inverse of an $\mathbf{M}$-matrix is again an $\mathbf{M}$-matrix. In [5], this question is addressed specifically for singular Jacobi $\mathbf{M}$-matrices that are tridiagonal. Under certain conditions, it is shown that the Moore-Penrose inverse of these matrices are $\mathbf{M}$-matrices. Additionally, [5] demonstrates that for any integer n, there exists a singular, symmetric and tridiagonal $n \times n$ $\mathbf{M}$-matrix whose Moore-Penrose inverse is also an $\mathbf{M}$-matrix. For any path with arbitrary weights, its combinatorial Laplacian matrix is always a Jacobi $\mathbf{M}$-matrix. Using the results on Jacobi $\mathbf{M}$-matrices in [5], we can observe that if P is a weighted path with more than four vertices, then the Moore-Penrose inverse of the combinatorial Laplacian of P is not an $\mathbf{M}$-matrix, as noted in [11].

Now, we consider a weighted tree T. The problem under consideration is to show that the Moore-Penrose inverse of the distance Laplacian of T is an $\mathbf{M}$-matrix. This problem can also be posed for the combinatorial Laplacian of T. The works in [11] provide characterizations for all weighted trees whose Moore-Penrose inverse of the combinatorial Laplacian is an $\mathbf{M}$-matrix. Furthermore, [3] presents a relevant result concerning distance-biregular graphs. Specifically, it characterizes all distance-biregular graphs whose group inverse of the combinatorial Laplacian is an $\mathbf{M}$-matrix. We recall that the group inverse of a symmetric matrix coincides with its Moore-Penrose inverse.

Distance matrices of connected graphs, particularly trees, have been extensively studied due to their interesting properties and applications. For instance, there exists a well-known formula to compute the determinant of the distance matrix of a tree, which depends soley on the weights. Additionally, Graham and Lovász [8] established a combinatorial interpretation for all the coefficients in the characteristic polynomial of the distance matrix of a tree. The monograph [4] provides a compilation of well-known results on distance matrices. Distance Laplacian matrices of connected graphs were introduced in [1], where their relationship to algebraic connectivity was investigated. The techniques employed in our paper are novel and rely on crucial observations derived from numerical experiments.

2. Preliminaries

We consider only real matrices.

2.1. Notation

(N1) If $A = [[a_{ij}]]$ is an $n \times n$ matrix, then the submatrix obtained by deleting the i^{th} row and the j^{th} column will be denoted by $A(i|j)$. Let

$$1 \leqslant s_1 < s_2 < \cdots < s_k \leqslant n \text{ and } 1 \leqslant t_1 < t_2 \cdots < t_m \leqslant n.$$

Define $\Omega_1 := (s_1, \ldots, s_k)$ and $\Omega_2 := (t_1, \ldots, t_m)$. Then, $A[\Omega_1, \Omega_2]$ will denote the $k \times m$ matrix with $(i, j)^{\text{th}}$ entry equal to $a_{s_i t_j}$.

(N2) The column vector of all ones in $\mathbb{R}^n$ will be denoted by $\mathbf{1}$. If $m < n$, then $\mathbf{1}_m$ will denote the column vector of all ones in $\mathbb{R}^m$. The notation J will be the $n \times n$ matrix with all entries equal to 1. Zero matrices with more than one row/column will be denoted by O and a column vector with all entries equal to 0 by $\mathbf{0}$.

(N3) The transpose of a matrix A is denoted by A'. If B is a square matrix, then the Moore-Penrose inverse of B is the unique $n \times n$ matrix $B^\dagger$ satisfying

$$BB^\dagger B = B,\ B^\dagger BB^\dagger = B^\dagger,\ (B^\dagger B)' = B^\dagger B \text{ and } (BB^\dagger)' = BB^\dagger.$$

(N4) A $\mathbf{Z}$-matrix is an $n \times n$ matrix where all the off diagonal entries are non-positive. If all the principal minors of a $\mathbf{Z}$-matrix are non-negative, then it is called a $\mathbf{M}$-matrix. Therefore, a symmetric $\mathbf{Z}$-matrix is an $\mathbf{M}$-matrix if and only if it is positive semidefinite. $\mathbf{M}$-matrices have several interesting properties. The topic of Chapter 5 in Fiedler [7] is on $\mathbf{M}$-matrices.

(N5) To denote the subgraph induced by a set of vertices $W \subseteq V(T)$, we use the notation $\langle W \rangle$. If u and v are any two vertices, then $\mathbf{P}_{uv}$ will denote the path connecting u and v in T. The set of all vertices of a subgraph H is denoted by $V(H)$.

2.2. Basic results and techniques

(P1) *Matrix determinant lemma* (page 66, [9]): Let A be a $m \times m$ matrix and x, y be $m \times 1$ vectors. Then

$$\det(A + xy') = \det(A) + y' \operatorname{adj}(A) x.$$

If A is invertible, then

$$\det(A + xy') = \det(A)(1 + y' A^{-1} x).$$

(P2) Triangle inequality (page 95, [4]): If $i, j, k \in \{1, \dots, n\}$, then

$$d_{ik} \leqslant d_{ij} + d_{jk},$$

and equality happens if and only if $j \in \mathbf{P}_{ik}$.

(P3) The following observation will be useful in the proof. Let ν be a positive integer and the sets $L_1, \dots, L_N$ partition $\{1, \dots, \nu\}$. Let $A = [a_{uv}]$ be a $\nu \times \nu$ matrix such that $A[L_i, L_j] = O$ for all $i < j$. Then there exists a permutation matrix P such that

$$P'AP = \begin{bmatrix} A[L_1,L_1] & O & \dots & O \\ A[L_2,L_1] & A[L_2,L_2] & \dots & O \\ \dots & \dots & \ddots & \vdots \\ A[L_N,L_1] & A[L_N,L_2] & \dots & A[L_N,L_N] \end{bmatrix}.$$

As a consequence, we note the following.

(a) If $a_{xy} = 0$ for all $x \in L_i$, $y \in L_j$ and $i < j$, then A is similar to a block lower triangular matrix with i^{th} diagonal block equal to $A[L_i, L_i]$.

(b) If $a_{xy} = 0$ for all $x \in L_i$, $y \in L_j$ and $i > j$, then A is similar to a block upper triangular matrix with i^{th} diagonal block equal to $A[L_i, L_i]$.

(c) If $a_{xy} = 0$ for all $x \in L_i$, $y \in L_j$ and $i \neq j$, then A is similar to a block diagonal matrix with i^{th} diagonal block equal to $A[L_i, L_i]$.

3. Main result

We now prove our result.

THEOREM 1. *Let T be a weighted tree on n vertices. Let $D = [[d_{ij}]]$ be the distance matrix of T. Then, the Moore-Penrose inverse of*

$$\mathrm{Diag}\Big(\sum_{j=1}^{n} d_{1j}, \ldots, \sum_{j=1}^{n} d_{nj}\Big) - D$$

is an $\mathbf{M}$-matrix.

Proof. We define

$$S := \mathrm{Diag}\Big(\sum_{j=1}^{n} d_{1j}, \ldots, \sum_{j=1}^{n} d_{nj}\Big) - D.$$

In view of Gershgorin circle theorem, we conclude that S is positive semidefinite and so is $S^{\dagger}$. Hence, we need to show only that all off-diagonal entries in $S^{\dagger}$ are non-positive. Let $s^{\dagger}_{ij}$ be the $(i,j)^{\text{th}}$ entry of $S^{\dagger}$. By a permutation similarity argument, it suffices to show that $s^{\dagger}_{12}$ is non-positive. Let $C := S(1|2)$. Since $S\mathbf{1} = 0$, all cofactors of S will be equal. Let γ be the common cofactor of S. In particular, $\gamma = -\det(C)$. As $S(1|1)$ is strictly diagonally dominant, $S(1|1)$ is non-singular and therefore, $\gamma > 0$. Thus, $\mathrm{rank}(S) = n-1$. We now have the following claim.

CLAIM 1. $s^{\dagger}_{12} = \frac{\mathbf{1}'_{n-1} C^{-1} \mathbf{1}_{n-1}}{n^2}$.

Proof of the claim. Let ξ be the $(1,2)^{\text{th}}$-entry of $(S+J)^{-1}$. Then, $\xi = -\frac{\det(C+J(1|2))}{\det(S+J)}$. As $\det(S) = 0$ and $\mathrm{adj}(S) = \gamma J$, by the matrix determinant lemma (P1),

$$\det(S+J) = n^2\gamma \ \text{ and } \ \det(C+J(1|2)) = \det(C)(1+\mathbf{1}'_{n-1}C^{-1}\mathbf{1}_{n-1}).$$

Since $\det(C) = -\gamma$,

$$\xi = \frac{1+\mathbf{1}'_{n-1}C^{-1}\mathbf{1}_{n-1}}{n^2}. \tag{2}$$

As the null-space of S is spanned by $\mathbf{1}$, $SS^{\dagger} = I - \frac{J}{n}$, and hence $(S+J)^{-1} = S^{\dagger} + \frac{J}{n^2}$. Therefore, $s^{\dagger}_{12} = \xi - \frac{1}{n^2}$. The claim now follows by substituting for ξ obtained in equation (2). $\square$

For any $i,j \in \{3,\dots,n\}$, define

$$R_{ij} := \begin{cases} -d_{21}+d_{i1}+d_{2j}-d_{ij} & i \neq j \\ -d_{21}+d_{i1}+d_{2i}+\sum_{k=1}^{n} d_{ik} & i = j. \end{cases}$$

Let R denote the $(n-2)\times(n-2)$ matrix

$$\begin{bmatrix} R_{33} & R_{34} & \dots & R_{3n} \\ \vdots & \ddots & \vdots & \vdots \\ R_{n3} & R_{n4} & \dots & R_{nn} \end{bmatrix}.$$

CLAIM 2. $s^{\dagger}_{12} \leqslant 0$ if and only if $\det(R) \geqslant 0$.

Proof of the claim. Define

$$Q := \begin{bmatrix} 1 & \mathbf{1}'_{n-2} \\ \mathbf{0} & I_{n-2} \end{bmatrix}.$$

Then, $Q^{-1} = \begin{bmatrix} 1 & -\mathbf{1}'_{n-2} \\ \mathbf{0} & I_{n-2} \end{bmatrix}$. By a direct computation,

$$Q'^{-1}CQ^{-1} = \begin{bmatrix} s_{21} & -s_{21}+s_{23} & \dots & -s_{21}+s_{2n} \\ -s_{21}+s_{31} & s_{21}-s_{31}-s_{23}+s_{33} & \dots & s_{21}-s_{31}-s_{2n}+s_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ -s_{21}+s_{n1} & s_{21}-s_{n1}-s_{23}+s_{n3} & \dots & s_{21}-s_{n1}-s_{2n}+s_{nn} \end{bmatrix}.$$

The entries of S can be written as

$$s_{ij} = \begin{cases} -d_{ij} & i \neq j \\ \sum_{k=1}^{n} d_{ik} & i = j. \end{cases}$$

Hence,

$$(Q'^{-1}CQ^{-1})(1|1) = R. \tag{3}$$

As

$$\det(C) = -\gamma < 0 \quad\text{and}\quad \det(Q) = 1,$$

we get

$$\det(Q'^{-1}CQ^{-1}) = -\gamma < 0.$$

By a simple computation,

$$(QC^{-1}Q')_{11} = \mathbf{1}'_{n-1}C^{-1}\mathbf{1}_{n-1}. \tag{4}$$

Using (3),

$$(QC^{-1}Q')_{11} = \frac{1}{\det(Q'^{-1}CQ^{-1})}\det((Q'^{-1}CQ^{-1})(1|1)) = -\frac{1}{\gamma}\det(R). \tag{5}$$

By (4) and (5),

$$\mathbf{1}'_{n-1}C^{-1}\mathbf{1}_{n-1} = -\frac{1}{\gamma}\det(R).$$

By claim 1, it follows that $s^{\dagger}_{12} \leqslant 0$ if and only if $\det(R) \geqslant 0$. Claim 2 is now complete. □

Our aim is now to demonstrate that $\det(R) \geqslant 0$. We first observe that the diagonal entries of R are non-negative.

CLAIM 3. $R_{ii} > 0 \quad i = 3,\dots,n$.

Proof of the claim. By the triangle inequality,

$$-d_{21} + d_{i1} + d_{2i} \geqslant 0 \quad i = 3,\dots,n.$$

Hence

$$R_{ii} = -d_{21} + d_{i1} + d_{2i} + \sum_{k=1}^{n} d_{ik} > 0 \quad i = 3,\dots,n. \quad \square$$

CLAIM 4. Let $\alpha \in V(\mathbf{P}_{12})$. Suppose there exists a connected component $\widetilde{X}$ of $T \smallsetminus (\alpha)$ not containing 1 and 2. Let $u \in V(\widetilde{X})$ be the vertex adjacent to α. Consider a connected subgraph X of $\widetilde{X}$ containing u. Put $E := V(X)$. Then, $R[E,E]$ is a positive semidefinite matrix.

Proof of the claim. If $E = \{u\}$, then $R[E,E] = [[R_{uu}]]$. By claim 3, $R_{uu} > 0$ and hence the lemma is true in this case. Suppose E has at least two elements. We now show that $R[E,E]$ is symmetric. Let $r,s \in E$. Recall that

$$R_{rs} = -d_{21} + d_{r1} + d_{2s} - d_{rs}. \tag{6}$$

Since r and s belong to a component of $T \smallsetminus \alpha$ which does not contain 1 and 2, we have

$$d_{r1} = d_{r\alpha} + d_{\alpha 1} \text{ and } d_{s2} = d_{s\alpha} + d_{\alpha 2}. \tag{7}$$

By (6) and (7),

$$R_{rs} = -d_{21} + d_{r\alpha} + d_{\alpha 1} + d_{s\alpha} + d_{\alpha 2} - d_{rs}. \tag{8}$$

Again by a similar reasoning in (7),

$$d_{r2} = d_{r\alpha} + d_{\alpha 2} \text{ and } d_{s1} = d_{s\alpha} + d_{\alpha 1}. \tag{9}$$

By (8) and (9),

$$R_{rs} = -d_{21} + d_{s1} + d_{r2} - d_{rs},$$

which is R_{sr}. Thus, $R[E,E]$ is symmetric. We know that $u \in E$ and also adjacent to α. Let Ω be the set of all non-pendant vertices in T. Since X is connected, and has at least two vertices, u is adjacent to a vertex in E. Hence $u \in E \cap \Omega$, so $E \cap \Omega \neq \emptyset$. Let $\delta \in E$ be such that

$$d_{\delta\alpha} = \max\{d_{x\alpha} : x \in E \cap \Omega\}.$$

Since X is a tree, there exists a pendant vertex adjacent to δ. Without loss of generality, let $E = \{x_1, \dots, x_{t-1}, x_t\}$, where $x_1 = u$, $x_{t-1} = \delta$ and x_t is a pendant vertex adjacent to x_{t-1}. By the definition of R,

$$\begin{aligned} R_{ix_{t-1}} - R_{ix_t} &= -d_{21} + d_{i1} + d_{2x_{t-1}} - d_{ix_{t-1}} - (-d_{21} + d_{i1} + d_{2x_t} - d_{ix_t}) \\ &= (d_{2x_{t-1}} - d_{2x_t}) - (d_{ix_{t-1}} - d_{ix_t}). \end{aligned} \tag{10}$$

Since x_t is a pendant vertex and is adjacent to x_{t-1}, we have

$$d_{2x_{t-1}} - d_{2x_t} = -d_{x_t x_{t-1}}.$$

If $i \in \{x_1, \dots, x_{t-2}\}$ then,

$$d_{ix_{t-1}} - d_{ix_t} = -d_{x_t x_{t-1}}.$$

From (10), we now get

$$R_{ix_{t-1}} = R_{ix_t} \text{ for all } i \in \{x_1, x_2, \dots, x_{t-2}\}. \tag{11}$$

By the definition of R_{ij},

$$R_{x_{t-1}x_t} = -d_{21} + d_{x_{t-1}1} + d_{2x_t} - d_{x_{t-1}x_t}. \tag{12}$$

Vertices 2 and x_t belong to different components of $T \smallsetminus (\alpha)$. Also, x_t and x_{t-1} are adjacent and x_t is pendant in X. Hence,

$$d_{2x_t} = d_{2\alpha} + d_{\alpha x_t} = d_{2\alpha} + d_{\alpha x_{t-1}} + d_{x_{t-1}x_t}. \tag{13}$$

By (12) and (13),

$$R_{x_{t-1}x_t} = -d_{21} + d_{x_{t-1}1} + d_{2\alpha} + d_{\alpha x_{t-1}}.$$

As $\alpha \in V(\mathbf{P}_{12})$, $d_{21} = d_{2\alpha} + d_{\alpha 1}$. Hence

$$R_{x_{t-1}x_t} = -d_{\alpha 1} + d_{x_{t-1}1} + d_{\alpha x_{t-1}}. \tag{14}$$

As $1 \notin V(\tilde{X})$, $d_{x_{t-1}1} = d_{x_{t-1}\alpha} + d_{\alpha 1}$. Hence by (14),

$$R_{x_{t-1}x_t} = 2d_{\alpha x_{t-1}}. \tag{15}$$

Since $x_{t-1} = \delta$,

$$R_{x_{t-1}x_t} = 2d_{\alpha\delta}. \tag{16}$$

We now show that all diagonal entries of $R[E,E]$ are at least $2d_{\delta\alpha}$. Let $r \in E$. By definition,

$$R_{rr} = -d_{21} + d_{r1} + d_{2r} + \sum_{k=1}^{n} d_{rk}. \tag{17}$$

Since $r \in E$, $1 \notin E$ and $2 \notin E$,

$$d_{r1} = d_{r\alpha} + d_{1\alpha} \text{ and } d_{r2} = d_{r\alpha} + d_{2\alpha}. \tag{18}$$

By (17) and (18),

$$R_{rr} = -d_{21} + d_{r\alpha} + d_{1\alpha} + d_{r\alpha} + d_{2\alpha} + \sum_{k=1}^{n} d_{rk}. \tag{19}$$

As $d_{21} = d_{2\alpha} + d_{\alpha 1}$, (19) simplifies to

$$R_{rr} = 2d_{r\alpha} + \sum_{k=1}^{n} d_{rk}. \tag{20}$$

Case 1: Suppose $r \notin \{\delta, x_t\}$.
Then

$$R_{rr} = 2d_{r\alpha} + \sum_{k=1}^{n} d_{rk} \geqslant 2d_{r\alpha} + d_{r\delta} + d_{rx_t}. \tag{21}$$

By the triangle inequality,

$$d_{r\alpha} + d_{r\delta} \geqslant d_{\delta\alpha} \text{ and } d_{r\alpha} + d_{rx_t} \geqslant d_{x_t\alpha}.$$

In view of (21),

$$R_{rr} \geqslant d_{x_t\alpha} + d_{\delta\alpha}.$$

As δ is the only vertex adjacent to the pendant vertex x_t,

$$R_{rr} \geqslant d_{x_t\alpha} + d_{\delta\alpha} = d_{\delta\alpha} + d_{\delta x_t} + d_{\delta\alpha} \geqslant 2d_{\delta\alpha}.$$

Case 2: If $r = \delta$, then it is immediate from (20).

Case 3: Suppose $r = x_t$. Since x_t is pendant and adjacent only to δ, by (20),

$$R_{x_t x_t} \geqslant 2d_{x_t\alpha} = 2(d_{\delta\alpha} + d_{x_t\delta}) \geqslant 2d_{\delta\alpha}.$$

Thus, all the diagonal entries in $R[E,E]$ are at least $2d_{\delta\alpha}$.

Define a $t \times t$ matrix

$$P := \begin{bmatrix} 2d_{\delta\alpha} & R_{x_1x_2} & \dots & R_{x_1x_t} \\ R_{x_2x_1} & 2d_{\delta\alpha} & \dots & R_{x_2x_t} \\ \dots & \dots & \ddots & \dots \\ R_{x_tx_1} & R_{x_tx_2} & \dots & 2d_{\delta\alpha} \end{bmatrix}.$$

As $R[E,E]$ is a symmetric matrix, P is symmetric.

We now show that P is positive semidefinite. We will prove this by using induction on $|E|$. Suppose $|E|=2$. Write $E=\{x_1,x_2\}$, where $u=x_1$. Now,

$$P=\begin{bmatrix} 2d_{\alpha u} & 2d_{\alpha u} \\ 2d_{\alpha u} & 2d_{\alpha u} \end{bmatrix}.$$

Clearly, P is positive semidefinite. Suppose the result is true if $|E|<t$. Define a $t\times t$ matrix by

$$Q_1 := \begin{bmatrix} I_{t-2} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}' & 1 & -1 \\ \mathbf{0}' & 0 & 1 \end{bmatrix}.$$

We show that $Q_1'PQ_1$ is positive semidefinite. Equations (11) and (16) imply that the last two columns of P are equal. Hence, by a direct computation,

$$Q_1'PQ_1 = \begin{bmatrix} P(x_t|x_t) & \mathbf{0} \\ & \mathbf{0}' \; 0 \end{bmatrix}. \tag{22}$$

Define

$$X' := X \smallsetminus (x_t).$$

Because x_t is pendant, it follows that X' is a connected subgraph of X and $u\in V(X')$. Set

$$E' := V(X') = \{x_1,\dots,x_{t-1}\}, \text{ where } x_1 = u.$$

Define

$$d_{\mu\alpha} := \max\{d_{x\alpha} : x\in\Omega\cap E'\}.$$

By the induction hypothesis,

$$P_1 := \begin{bmatrix} 2d_{\mu\alpha} & R_{x_1x_2} & \dots & R_{x_1x_{t-1}} \\ R_{x_2x_1} & 2d_{\mu\alpha} & \dots & R_{x_2x_{t-1}} \\ \dots & \dots & \ddots & \dots \\ R_{x_{t-1}x_1} & R_{x_{t-1}x_2} & \dots & 2d_{\mu\alpha} \end{bmatrix}$$

is positive semidefinite. Put

$$P_2 := \begin{bmatrix} 2d_{\delta\alpha}-2d_{\mu\alpha} & 0 & \dots & 0 \\ 0 & 2d_{\delta\alpha}-2d_{\mu\alpha} & \dots & 0 \\ \vdots & \dots & \ddots & \vdots \\ 0 & 0 & \dots & 2d_{\delta\alpha}-2d_{\mu\alpha} \end{bmatrix}.$$

Then,

$$P(x_t|x_t) = P_1 + P_2.$$

Since $d_{\delta\alpha}-d_{\mu\alpha}\geqslant 0$, $P(x_t|x_t)$ is positive semidefinite and so is P. Define

$$\Lambda := \mathrm{Diag}(R_{x_1x_1}-2d_{\delta\alpha},\dots,R_{x_tx_t}-2d_{\delta\alpha}).$$

Then,

$$R[E,E] = P + \Lambda.$$

Since, all diagonal entries are at least $2d_{\delta\alpha}$ and P is positive semidefinite, $R[E,E]$ is positive semidefinite. The proof of the claim is complete.

Let the degree of vertex 1 be m. Then $T \setminus (1)$ has m components. We denote the vertex sets of these components by by $V_1', V_2, \ldots, V_m$. Additionally, let us assume that $2 \in V_1'$. Define

$$V_1 := V_1' \setminus \{2\}.$$

We now have the following claim. □

CLAIM 5. R is similar to a block lower triangular matrix with diagonal blocks equal to $R[V_1,V_1], R[V_2,V_2], \ldots, R[V_m,V_m]$.

Proof of the claim. We know that $V_1 \cup \cdots \cup V_m = \{3,\ldots,n\}$ and $V_i \cap V_j = \emptyset$. We recall that

$$R = [R_{\alpha\beta}] \quad 3 \leqslant \alpha, \beta \leqslant n.$$

By item (a) in (P3), it suffices to show that if $i < j$, $x \in V_i$ and $y \in V_j$, then $R_{xy} = 0$. By definition,

$$R_{xy} = -d_{21} + d_{x1} + d_{2y} - d_{xy}. \tag{23}$$

Since x and y belong to different components of $T \setminus (1)$,

$$d_{xy} = d_{x1} + d_{y1}. \tag{24}$$

Using (24) in (23),

$$R_{xy} = -d_{21} + d_{2y} - d_{y1}. \tag{25}$$

We recall that $2 \in V_1'$ and $y \in V_j$. Since $1 \leqslant i < j$, we see that $1 < j$. Hence, 2 and y belong to different components of $T \setminus (1)$. Thus, $d_{2y} = d_{21} + d_{y1}$. By (25), $R_{xy} = 0$. The proof of the claim is complete. Thus, it follows that

$$\det(R) = \prod_{i=1}^{m} \det(R[V_i,V_i]). \tag{26}$$

Let $j \in \{2,\ldots,m\}$. Substituting $\widetilde{X} = X = \langle V_j \rangle$, $E = V_j$ and $\alpha = 1$ in claim 4, we see that $R[V_j,V_j]$ is positive semidefinite for all $j = 2,\ldots,m$. In particular, we have

$$\det(R[V_j,V_j]) \geqslant 0 \qquad j = 2,\ldots,m. \tag{27}$$

We now partition V_1. Define

$$V_A := \{y \in V_1 : 2 \notin V(\mathbf{P}_{1y})\} \text{ and } V_B := \{y \in V_1 : 2 \in V(\mathbf{P}_{1y})\}.$$

Then,

$$V_1 = V_A \cup V_B \text{ and } V_A \cap V_B = \emptyset. \quad \square$$

CLAIM 6. If $x \in V_B$ and $y \in V_A$, then $2 \in V(\mathbf{P}_{xy})$.

Proof of the claim. Suppose $2 \notin V(\mathbf{P}_{xy})$. Since $y \in V_A$, we see that $2 \notin V(\mathbf{P}_{1y})$. Therefore, $2 \notin V(\mathbf{P}_{1x})$. This contradicts $x \in V_B$. Hence the claim is true. □

CLAIM 7. $R[V_1,V_1]$ is similar to a block upper triangular matrix with diagonal blocks equal to $R[V_A,V_A]$ and $R[V_B,V_B]$.

Proof of the claim. Let $x \in V_B$ and $y \in V_A$. In view of item (b) in (P3), it suffices to show that $R_{xy} = 0$. In view of the previous claim,

$$d_{2y} + d_{2x} = d_{xy}. \tag{28}$$

By definition,

$$R_{xy} = -d_{21} + d_{x1} + d_{2y} - d_{xy}. \tag{29}$$

As $x \in V_B$,

$$d_{1x} - d_{21} = d_{2x}. \tag{30}$$

By (29) and (30),

$$R_{xy} = d_{2x} + d_{2y} - d_{xy}.$$

Equation (28) now gives $R_{xy} = 0$. The proof of the claim is complete. □

The following is now immediate:

$$\det(R[V_1,V_1]) = \det(R[V_A,V_A])\det(R[V_B,V_B]). \tag{31}$$

We now partition V_A. Let the path $\mathbf{P}_{12}$ have the vertex set $\{1,u_1,\ldots,u_q,2\}$ and edge set $\{(1,u_1),(u_1,u_2),\ldots,(u_q,2)\}$. For $i = 1,\ldots,q$, define

$$U_i := \{y \in V_A : d_{u_i y} \leqslant d_{u_j y} \quad \text{for all} \;\; i \neq j\}.$$

Clearly $u_i \in U_i$. We shall prove the following claim now.

CLAIM 8. The following items hold.

(i) If $y \in U_i$, then $u_i \in V(\mathbf{P}_{y2}) \cap V(\mathbf{P}_{y1})$.

(ii) If $y \in U_i$, then $u_i \in V(\mathbf{P}_{yu_j})$ for $j \neq i$.

(iii) $U_1,\ldots,U_q$ partition V_A.

(iv) Let $y \in U_i$ and $z \in U_j$. If $i \neq j$, then

$$\mathbf{P}_{yz} = \mathbf{P}_{yu_i} \cup \mathbf{P}_{u_i u_j} \cup \mathbf{P}_{u_j z}.$$

(v) Each $\langle U_i \rangle$ is a tree.

Proof of the claim. Assume that $u_i \notin V(\mathbf{P}_{1y})$. Because u_1 is the only vertex in V_1 adjacent to 1, we deduce that $i \neq 1$ and hence $u_i \notin V(\mathbf{P}_{u_1 y})$ implying $\mathbf{P}_{u_1 y} \cup \mathbf{P}_{u_1 u_i}$ contains $\mathbf{P}_{y u_i}$. Now, $u_{i-1} \in V(\mathbf{P}_{y u_i})$. This implies $d_{u_{i-1} y} < d_{u_i y}$. But this cannot happen as $y \in U_i$, so $u_i \in V(\mathbf{P}_{1y})$ and by a similar argument, $u_i \in V(\mathbf{P}_{2y})$. This proves (i).

Let $j > i$. By (i) and from the definition of u_i and u_j,

$$u_i \in V(\mathbf{P}_{2y}) \text{ and } u_j \in V(\mathbf{P}_{2u_i}).$$

Thus,

$$\mathbf{P}_{2y} = \mathbf{P}_{2u_j} \cup \mathbf{P}_{u_j u_i} \cup \mathbf{P}_{u_i y}.$$

The above equation implies

$$u_i \in V(\mathbf{P}_{y u_j}) \text{ for all } j > i.$$

A similar argument leads to

$$u_i \in V(\mathbf{P}_{y u_j}) \text{ for all } j < i.$$

This proves (ii).

If possible, let $y \in U_i \cap U_j$, where $j \neq i$. By (ii), it follows that

$$u_i \in V(\mathbf{P}_{u_j y}) \text{ and } u_j \in V(\mathbf{P}_{u_i y}).$$

But these two cannot happen simultaneously. Hence, $y \notin U_i \cap U_j$. Thus, $U_i \cap U_j = \emptyset$. From the definition of $U_1, \ldots, U_q$, we have

$$U_1 \cup \cdots \cup U_q \subseteq V_A.$$

Let $x \in V_A$. Choose $k \in \{1, \ldots, q\}$ such that

$$d_{x u_k} := \min(d_{x u_1}, \ldots, d_{x u_q}).$$

Then, $x \in U_k$. Hence $V_A \subseteq U_1 \cup \cdots \cup U_q$. This proves (iii).

(iv) follows from (ii).

We now claim that $\langle U_i \rangle$ is a tree. Let $y \in U_i$. Since $y, u_i \in V_1'$ and $\langle V_1' \rangle$ is a tree, we have

$$V(\mathbf{P}_{y u_i}) \subseteq V_1'. \tag{32}$$

To show that $\langle U_i \rangle$ is a tree, it now suffices to show that $V(\mathbf{P}_{y u_i}) \subseteq U_i$. Let $x \in V(\mathbf{P}_{y u_i})$. Assuming $x \notin U_i$, we shall get a contradiction. By (32), we now have only three cases:

$$\text{(a) } x \in U_j \text{ when } j \neq i \quad \text{(b) } x = 2 \quad \text{(c) } x \in V_B.$$

Assume (a). In view of item (iv) above, we see that $u_i \in V(\mathbf{P}_{xy})$. But, we know that $x \in V(\mathbf{P}_{y u_i})$. This is a contradiction. So, (a) is not true. If (b) is true, then $2 \in V(\mathbf{P}_{y u_i})$. However, (i) implies $u_i \in V(\mathbf{P}_{y2})$. This is a contradiction. Hence, $x \neq 2$. If we assume (c), then $x \in V(\mathbf{P}_{y u_i})$. By claim 6, $2 \in V(\mathbf{P}_{yx})$ and therefore $2 \in V(\mathbf{P}_{y u_i})$ implying case (b) is true which is a contradiction. Hence, $V(\mathbf{P}_{y u_i}) \subseteq U_i$ and thus $\langle U_i \rangle$ is a tree. This proves (v). The proof of the claim is complete. $\square$

We now consider $R[V_A, V_A]$.

CLAIM 9. $R[V_A, V_A]$ is similar to a block upper triangular matrix with the diagonal block in the $(i,i)^{\text{th}}$-position equal to $R[U_i, U_i]$.

Proof of the claim. Let $i > j$. Pick any two elements $r \in U_i$ and $s \in U_j$. By item (c) in (P3), it suffices to show that

$$R_{rs} = 0.$$

We recall that

$$R_{rs} = -d_{21} + d_{r1} + d_{2s} - d_{rs}. \tag{33}$$

By item (i) and (iv) of claim 8,

$$d_{r1} = d_{ru_i} + d_{u_i1}, \;\; d_{2s} = d_{2u_j} + d_{u_js} \;\text{ and }\; d_{rs} = d_{ru_i} + d_{u_ju_i} + d_{su_j}. \tag{34}$$

Thus (33) and (34) give

$$\begin{aligned} R_{rs} &= -d_{21} + d_{ru_i} + d_{u_i1} + d_{2u_j} + d_{u_js} - (d_{ru_i} + d_{u_ju_i} + d_{su_j}) \\ &= -d_{21} + d_{u_i1} + d_{2u_j} - d_{u_ju_i}. \end{aligned}$$

Since $i > j$ and $\mathbf{P}_{12}$ has edges $\{(1,u_1),(u_1,u_2),\ldots,(u_{q-1},u_q),(u_q,2)\}$, we get

$$-d_{21} + d_{u_i1} = -d_{u_i2} \;\text{ and }\; d_{2u_j} - d_{u_ju_i} = d_{2u_i}.$$

Thus, $R_{rs} = 0$. This completes the proof of the claim. $\square$

Thus, we have

$$\det(R[V_A, V_A]) = \prod_{i=1}^{q} \det(R[U_i, U_i]). \tag{35}$$

We further partition U_i into disjoint sets. Fix $i \in \{1,\ldots,q\}$. Let u_i be adjacent to p_i vertices in $\langle U_i \rangle$. Then, $\langle U_i \rangle \smallsetminus (u_i)$ has p_i components. Let these components be denoted by $G_{i1},\ldots,G_{ip_i}$. Define $Q_{ik} := V(G_{ik})$.

CLAIM 10. The following items hold.

(i) $\det(R[U_i, U_i]) = R_{u_iu_i}(\prod_{k=1}^{p_i} \det(R[Q_{ik}, Q_{ik}]))$.

(ii) $G_{i1},\ldots,G_{ip_i}$ are the connected components of $T \smallsetminus (u_i)$.

(iii) $\det(R[U_i, U_i]) \geqslant 0$.

Proof of the claim. Let $a \in Q_{ir}$, $b \in Q_{is}$ and $r \neq s$. By definition,

$$R_{ab} = -d_{21} + d_{a1} + d_{2b} - d_{ab}.$$

Since $u_i \in V(\mathbf{P}_{12})$,

$$R_{ab} = -d_{2u_i} - d_{u_i1} + d_{a1} + d_{2b} - d_{ab}. \tag{36}$$

As $a \in U_i$, it follows from item (i) of claim 8 that

$$d_{au_i} = d_{a1} - d_{1u_i}. \tag{37}$$

Substituting (37) in (36),

$$R_{ab} = -d_{2u_i} + d_{u_i a} + d_{2b} - d_{ab}. \tag{38}$$

As $b \in U_i$, it follows from item (i) of claim 8 that

$$d_{bu_i} = d_{2b} - d_{2u_i}. \tag{39}$$

Using (39) in (38),

$$R_{ab} = d_{bu_i} + d_{u_i a} - d_{ab}. \tag{40}$$

Finally, since a and b belong to different components of $\langle U_i \rangle \smallsetminus (u_i)$,

$$d_{bu_i} + d_{u_i a} = d_{ab}. \tag{41}$$

Using (41) in (40)

$$R_{ab} = 0.$$

We now show that $R_{u_i x} = 0$ for any $x \in Q_{is}$. By definition,

$$R_{u_i x} = -d_{21} + d_{u_i 1} + d_{2x} - d_{u_i x}.$$

Since u_i lies on $\mathbf{P}_{12}$,

$$R_{u_i x} = -d_{u_i 2} + d_{2x} - d_{u_i x}. \tag{42}$$

As $x \in Q_{is} \subset U_i$, by item (i) of claim 8,

$$d_{xu_i} + d_{2u_i} = d_{2x}. \tag{43}$$

By (42) and (43), $R_{u_i x} = 0$. Similarly, $R_{xu_i} = 0$.

By item (c) in (P3), we now conclude that $R[U_i, U_i]$ is similar to a block diagonal matrix with diagonal blocks

$$R_{u_i u_i}, \quad R[Q_{ik}, Q_{ik}] \qquad k = 1, \ldots, p_i.$$

Hence

$$\det(R[U_i, U_i]) = R_{u_i u_i}\Big(\prod_{k=1}^{p_i} \det(R[Q_{ik}, Q_{ik}])\Big).$$

This completes the proof of (i).

By definition $G_{i1}, \ldots, G_{ip_i}$ are the connected components of $\langle U_i \rangle \smallsetminus (u_i)$. So, each G_{ik} is connected. Suppose G_{ik} is not a connected component of $T \smallsetminus (u_i)$. Then, there exists $v \in V(T) \smallsetminus \{u_i\}$ but not in Q_{ik} such that v is adjacent to a vertex $g \in Q_{ik}$. Suppose $v \in Q_{ij}$ for some $j \neq k$. But Q_{ik} and Q_{ij} are components of $\langle U_i \rangle \smallsetminus (u_i)$ and hence $u_i \in V(\mathbf{P}_{gv})$. This is not possible. Suppose $v \in U_j$ where $j \neq i$. Then, item (iv) in claim 8 implies $u_i \in V(\mathbf{P}_{gv})$. This is not possible. Suppose $v \in V_B$. Then, in view of claim 6, we get $2 \in V(\mathbf{P}_{vg})$. Again, this is not possible. Let $v \in V_2 \cup \cdots \cup V_m$. Since $g \in V_1$, $1 \in \mathbf{P}_{gv}$. This is a contradiction. Thus, G_{ik} is a connected component of $T \smallsetminus (u_i)$. The proof of (ii) is complete.

Fix $k \in \{1, \dots, p_i\}$. Set $\tilde{X} = X = G_{ik}$, $E = Q_{ik}$ and $\alpha = u_i$. By (ii), $\langle X \rangle$ is a connected component of $T \smallsetminus (u_i)$. Hence, by claim 4, $\det(R[Q_{ik}, Q_{ik}]) \geqslant 0$. In view of item (i), we conclude that $\det(R[U_i, U_i]) \geqslant 0$. The proof of (iii) is complete. □

From equation (35) and claim 10, we have

$$\det(R[V_A, V_A]) \geqslant 0. \tag{44}$$

Let $\langle V_B \rangle$ have s components and let the vertex sets of these components be $W_1, \dots, W_s$.

CLAIM 11. If $i \neq j$, $z_i \in W_i$ and $z_j \in W_j$, then $2 \in V(\mathbf{P}_{z_i z_j})$.

Proof of the claim. Since z_i and z_j belong to different components of $\langle V_B \rangle$, there exists a vertex x such that

$$x \in V_1', \;\; x \notin V_B, \;\; \text{and} \;\; x \in V(\mathbf{P}_{z_i z_j}).$$

If $x = 2$, then we are done. Now, assume $x \neq 2$. Then, $x \in V_A$. Since $z_i \in V_B$, claim 6 implies that $2 \in V(\mathbf{P}_{z_i x})$ and hence $2 \in V(\mathbf{P}_{z_i z_j})$. The proof of the claim is complete. □

CLAIM 12. $\langle W_1 \rangle, \dots, \langle W_s \rangle$ are connected components of $T \smallsetminus (2)$.

Proof of the claim. Each $\langle W_j \rangle$ is connected. Suppose $\langle W_j \rangle$ is not a component in $T \smallsetminus (2)$. Then there exists a vertex $g \in W_j$ adjacent to $v \in V(T \smallsetminus (2)) \smallsetminus W_j$. Let $v \in W_k$, where $k \neq j$. Then, by claim 11, $2 \in V(\mathbf{P}_{vg})$. This is not possible. Suppose $v \in V_A$. Then, by claim 6, $2 \in V(\mathbf{P}_{vg})$. This is a contradiction. If $v \notin V_1'$, then $v \in V_2 \cup \cdots \cup V_m$ implying that $1 \in V(\mathbf{P}_{vg})$. This is a contradiction. Thus, $\langle W_j \rangle$ is a component in $T \smallsetminus (2)$. This completes the proof of the claim. □

Finally, we now show that $\det(R[V_B, V_B]) \geqslant 0$.

CLAIM 13. The following items hold.

(i) $\det(R[V_B, V_B]) = \prod_{\nu=1}^{s} \det(R[W_\nu, W_\nu])$.

(ii) $\det(R[W_i, W_i]) \geqslant 0 \quad i = 1, \dots, s$.

(iii) $\det(R[V_B, V_B]) \geqslant 0$.

Proof of the claim. The sets $W_1, \dots, W_s$ partition V_B. Let $a \in W_i$ and $b \in W_j$. We claim that if $i \neq j$, then $R_{ab} = 0$. By definition

$$R_{ab} = -d_{21} + d_{a1} + d_{2b} - d_{ab}. \tag{45}$$

By claim 11, $2 \in V(\mathbf{P}_{ab})$. Hence

$$d_{ab} = d_{a2} + d_{2b}. \tag{46}$$

By (45) and (46),

$$R_{ab} = -d_{21} + d_{a1} + d_{2b} - d_{a2} - d_{2b} = -d_{21} + d_{a1} - d_{a2}. \tag{47}$$

Since $a \in V_B$, $2 \in V(\mathbf{P}_{a1})$,

$$d_{a1} = d_{a2} + d_{21}. \tag{48}$$

By (47) and (48),

$$R_{ab} = 0.$$

By (P3), $R[V_B, V_B]$ is similar to a block diagonal matrix with diagonal blocks

$$R[W_1, W_1], \ldots, R[W_s, W_s].$$

Therefore,

$$\det(R[V_B, V_B]) = \prod_{i=1}^{s} \det(R[W_i, W_i]).$$

This completes the proof of (i).

The proof of (ii) follows by substituting $\widetilde{X} = X = \langle W_i \rangle$, $E = W_i$ and $\alpha = 2$ in Claim 4.

(iii) is immediate from (i) and (ii). □

We now proceed to finalize the proof. By utilizing (26), (31), (44), and item (iii) in claim 13, we conclude that $\det(R) \geqslant 0$. Consequently, by claim 2, we deduce that $s^{\dagger}_{12} \leqslant 0$. The proof is complete. □

3.1. Illustration

The following example illustrates our result for a tree T with 5 vertices.

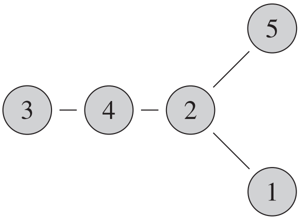

Figure 1: T

The distance Laplacian matrix of T is

$$\begin{bmatrix} 8 & -1 & -3 & -2 & -2 \\ -1 & 5 & -2 & -1 & -1 \\ -3 & -2 & 9 & -1 & -3 \\ -2 & -1 & -1 & 6 & -2 \\ -2 & -1 & -3 & -2 & 8 \end{bmatrix}$$

and its Moore-Penrose inverse is

$$\frac{1}{570}\begin{bmatrix} 47 & -20 & -6 & -11 & -10 \\ -20 & 74 & -12 & -22 & -20 \\ -6 & -12 & 42 & -18 & -6 \\ -11 & -22 & -18 & 62 & -11 \\ -10 & -20 & -6 & -11 & 47 \end{bmatrix}.$$

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