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Moore-Penrose inverse of a hollow symmetric matrix and a predistance matrix

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Abstract: By a hollow symmetric matrix we mean a symmetric matrix with zero diagonal elements. The notion contains those of predistance matrix and Euclidean distance matrix as its special cases. By a centered symmetric matrix we mean a symmetric matrix with zero row (and hence column) sums. There is a one-to-one correspondence between the classes of hollow symmetric matrices and centered symmetric matrices, and thus with any hollow symmetric matrix $\boldsymbol{D}$ we may associate a centered symmetric matrix $\boldsymbol{B}$, and vice versa. This correspondence extends a similar correspondence between Euclidean distance matrices and positive semidefinite matrices with zero row and column sums. We show that if $\boldsymbol{B}$ has rank r, then the corresponding $\boldsymbol{D}$ must have rank r, $r+1$ or $r+2$. We give a complete characterization of the three cases. We obtain formulas for the Moore-Penrose inverse $\boldsymbol{D}^+$ in terms of $\boldsymbol{B}^+$, extending formulas obtained in Kurata and Bapat (Linear Algebra and Its Applications, 2015). If $\boldsymbol{D}$ is the distance matrix of a weighted tree with the sum of the weights being zero, then $\boldsymbol{B}^+$ turns out to be the Laplacian of the tree, and the formula for $\boldsymbol{D}^+$ extends a well-known formula due to Graham and Lovász for the inverse of the distance matrix of a tree.

Keywords: Euclidean distance matrix, Predistance matrix, Positive semidefinite matrix, hollow matrix, Moore-Penrose inverse, Laplacian matrix, Tree

MSC: 15B48, 05C05

1 Introduction

A *hollow symmetric* matrix is a symmetric matrix with zero diagonal elements. If a hollow symmetric matrix is nonnegative (that is, all its elements are nonnegative), then it is called a *predistance* matrix. Let $\mathcal{S}_n$ be the set of all $n \times n$ symmetric matrices, which is a linear space of dimension $n(n+1)/2$. Let $\mathcal{S}_H(n)$ and $\mathcal{S}_H^+(n)$ be the set of hollow symmetric matrices and predistance matrices, respectively. That is,

$$\begin{aligned} \mathcal{S}_H(n) &= \{\boldsymbol{D} = (d_{ij}) \in \mathcal{S}_n \mid d_{11} = \ldots = d_{nn} = 0\}, \\ \mathcal{S}_H^+(n) &= \{\boldsymbol{D} = (d_{ij}) \in \mathcal{S}_H(n) \mid d_{ij} \geq 0 \; (i, j = 1, \ldots, n)\}. \end{aligned} \tag{1}$$

Needless to say, while $\mathcal{S}_H(n)$ is a linear subspace of $\mathcal{S}_n$ (with dimension $n(n-2)/2$) , the set $\mathcal{S}_H^+(n)$ is a convex cone in $\mathcal{S}_n$. The most important subset of $\mathcal{S}_H^+(n)$ may be the set of $n \times n$ *Euclidean distance matrices (EDMs)*. Here, an $n \times n$ predistance matrix $\boldsymbol{D} = (d_{ij})$ is said to be an $n \times n$ EDM, if there exist n points $\boldsymbol{p}_1, \cdots, \boldsymbol{p}_n$ in some Euclidean space $\mathbb{R}^r$ such that

$$d_{ij} = \|\boldsymbol{p}_i - \boldsymbol{p}_j\|^2 \;\; (i, j = 1, 2, \cdots, n), \tag{2}$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^r$. The minimum of such r is called the *embedding dimension* of $\boldsymbol{D}$.

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Recall that a symmetric matrix is said to be *positive semidefinite* (psd) if its eigenvalues are all nonnegative. We write $A \succeq 0$ to denote that A is psd. By a *centered symmetric matrix* we mean a symmetric matrix with zero row (and hence column) sums. As is well known, a necessary and sufficient condition for a predistance matrix $\boldsymbol{D}$ to be an EDM is that

$$-\frac{1}{2}\boldsymbol{PDP} \succeq \boldsymbol{0} \text{ with } \boldsymbol{P} = \boldsymbol{I}_n - \frac{1}{n}\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}} \tag{3}$$

(see, for example, Gower [6], pp. 82), where $\boldsymbol{e}$ denotes the vector of all ones of appropriate dimension. This characterization is based on a one-to-one correspondence between the set of EDMs and a set of positive semidefinite (psd) matrices. To state this more precisely, let Λ_n be the set of $n \times n$ EDMs and let

$$\Omega_n(\boldsymbol{e}) = \{\boldsymbol{B} \in \mathcal{S}_n \mid \boldsymbol{B} \succeq \boldsymbol{0},\ \boldsymbol{Be} = \boldsymbol{0}\}$$

be the set of $n \times n$ centered symmetric psd matrices, both of which form convex cones in $\mathcal{S}_n$. Then the following two mappings τ and κ are mutually inverse:

$$\begin{aligned} \tau &\ :\ \Lambda_n \longrightarrow \Omega_n(\boldsymbol{e}) : \boldsymbol{D} \longrightarrow -\frac{1}{2}\boldsymbol{PDP}^{\mathrm{T}}, \\ \kappa &\ :\ \Omega_n(\boldsymbol{e}) \longrightarrow \Lambda_n : \boldsymbol{B} = (b_{ij}) \longrightarrow (b_{ii} + b_{jj} - 2b_{ij}) = \boldsymbol{e}\boldsymbol{b}^{\mathrm{T}} + \boldsymbol{b}\boldsymbol{e}^{\mathrm{T}} - 2\boldsymbol{B}, \end{aligned} \tag{4}$$

where $\boldsymbol{b} = (b_{11}, b_{22}, \cdots, b_{nn})^{\mathrm{T}}$ is the vector consisting of the diagonal elements of $\boldsymbol{B}$ (see for instance [9], pp.380). The matrix B is often referred to as the *Gram matrix* associated with the EDM D.

EDMs can be classified into two types: spherical EDMs and nonspherical EDMs. An EDM $\boldsymbol{D}$ is called *spherical* if the points $\boldsymbol{p}_1, \cdots, \boldsymbol{p}_n$ satisfying (2) are on a hypersphere in $\mathbb{R}^r$. Otherwise it is called *nonspherical*. This paper is based on the following two results due to Tarazaga, Hayden and Wells [12] and Kurata and Bapat [10]. The former is on characterizations of spherical EDM, and the latter discusses generalized inverse matrices of spherical and nonspherical EDMs.

Proposition 1. (Theorems 2.1, 3.1 and 3.2 of Tarazaga, Hayden and Wells [12]) *Let $\boldsymbol{D} \in \Lambda_n$ be an EDM and $\boldsymbol{B} = \tau(\boldsymbol{D})$ be the corresponding psd matrix. Then $\boldsymbol{D}$ admits the following expression:*

$$-\frac{1}{2}\boldsymbol{D} = \boldsymbol{B} + \boldsymbol{z}\boldsymbol{e}^{\mathrm{T}} + \boldsymbol{e}\boldsymbol{z}^{\mathrm{T}} + \lambda\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}, \tag{5}$$

where the quantities $\boldsymbol{z} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$ are given by

$$\boldsymbol{z} = -(1/2)\boldsymbol{Pb} \ \ and \ \ \lambda = -\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n \ \ with \ \ \boldsymbol{b} = (b_{11}, \dots, b_{nn})^{\mathrm{T}}.$$

Furthermore,

(i) $\boldsymbol{D}$ is spherical if and only if

$$\boldsymbol{z} \in R(\boldsymbol{B}), \tag{6}$$

where $R(\cdot)$ denotes the range (column space) of a matrix.

(ii) Let $r = \operatorname{rank} \boldsymbol{B}$. Then

$$\operatorname{rank} \boldsymbol{D} = \begin{cases} r+1 & \textit{if and only if } \boldsymbol{D} \textit{ is spherical}, \\ r+2 & \textit{if and only if } \boldsymbol{D} \textit{ is nonspherical}. \end{cases} \tag{7}$$

By definition, we have $\boldsymbol{z}^{\mathrm{T}}\boldsymbol{e} = 0$ and $\lambda < 0$ as long as $\boldsymbol{D} \neq \boldsymbol{0}$. It is well known that the rank of $\boldsymbol{B}$ coincides with the embedding dimension ([11], Theorem 1).

The next result is concerned with the Moore-Penrose inverse of $\boldsymbol{D}$, where for a matrix $\boldsymbol{A}$, the *Moore-Penrose inverse* of $\boldsymbol{A}$ is defined as a matrix $\boldsymbol{A}^+$ satisfying the following four conditions:

$$\text{(i) } \boldsymbol{AA}^+\boldsymbol{A} = \boldsymbol{A},\ \text{(ii) } \boldsymbol{A}^+\boldsymbol{AA}^+ = \boldsymbol{A}^+,\ \text{(iii) } (\boldsymbol{AA}^+)^{\mathrm{T}} = \boldsymbol{AA}^+,\ \text{(iv) } (\boldsymbol{A}^+\boldsymbol{A})^{\mathrm{T}} = \boldsymbol{A}^+\boldsymbol{A}. \tag{8}$$

As is well-known, the Moore-Penrose inverse always exists and is unique. (See, for example, page 9 of [2].) For an exposition of the theory of generalized inverse we refer to [4]. Note that when A is nonsingular, $A^+ = A^{-1}$. Thus in the following result, when D is nonsingular, we have a formula for D^{-1}.

Proposition 2. (Theorems 3 and 4 of Kurata and Bapat [10]) *Let $\boldsymbol{D} \in \Lambda_n$ be an EDM. The Moore-Penrose inverse $\boldsymbol{D}^+$ is expressed as follows:*

(i) When $\boldsymbol{D}$ is spherical,

$$-2\boldsymbol{D}^+ = \boldsymbol{B}^+ - \frac{1}{n\gamma}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}, \tag{9}$$

with $\boldsymbol{x} = \bar{\boldsymbol{e}} + (\sqrt{n}/2)\boldsymbol{B}^+\boldsymbol{b}$ and $\gamma = \boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^+\boldsymbol{b}/4$, where $\bar{\boldsymbol{e}} = \boldsymbol{e}/\sqrt{n}$.

(ii) When $\boldsymbol{D}$ is nonspherical,

$$-2\boldsymbol{D}^+ = \boldsymbol{B}^+ - \frac{1}{n\gamma}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} + n\gamma\left(\boldsymbol{y} + \frac{1}{n\gamma}\boldsymbol{x}\right)\left(\boldsymbol{y} + \frac{1}{n\gamma}\boldsymbol{x}\right)^{\mathrm{T}},$$

with $\boldsymbol{y} = -2\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b}/(\sqrt{n}\boldsymbol{b}^{\mathrm{T}}\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b})$, where $\bar{\boldsymbol{Z}}$ is an $n \times (n - r - 1)$ matrix such that

$$\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{B} = \boldsymbol{0},\ \bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{e} = \boldsymbol{0} \ \text{and}\ \bar{\boldsymbol{Z}}^{\mathrm{T}}\bar{\boldsymbol{Z}} = \boldsymbol{I}_{n-r-1}.$$

The above result is obtained in a different form by Balaji and Bapat [1], Theorems 3.1 and 3.4, which derived a formula for $\boldsymbol{D}^+$ for the first time.

In this paper, we extend the above two propositions on EDMs to the space $\mathcal{S}_H(n)$ of hollow symmetric matrices and then derive some new results on the distance matrix of a tree. In Section 2, we discuss the rank of $\boldsymbol{D} \in \mathcal{S}_H(n)$ and clarify how it relates to the rank of $\boldsymbol{B}$. The result gives not only an extension of (ii) of Proposition 1, but also an insight into the Laplacian matrix of a weighted tree. In Section 3, Proposition 2 is extended to a hollow symmetric matrix $\boldsymbol{D}$. Section 4 is devoted to establishing some formulas on the distance matrix of a tree with possibly negative weights. Throughout this paper, we exclude the case $\boldsymbol{D} = \boldsymbol{0}$, since it is trivial.

Let $\mathcal{S}_C(n)$ be the set of all $n \times n$ centered symmetric matrices:

$$\mathcal{S}_C(n) = \{\boldsymbol{B} \in \mathcal{S}_n \mid \boldsymbol{B}\boldsymbol{e} = \boldsymbol{0}\}, \tag{10}$$

which is a linear subspace of $\mathcal{S}_n$ and contains $\Omega_n(\boldsymbol{e})$ as its subset. As shown by Critchley [5], Theorem 2.2, and Johnson and Tarazaga [9], pp.380, there is a one-to-one correspondence between $\mathcal{S}_H(n)$ and $\mathcal{S}_C(n)$. Indeed, the mapping τ and κ defined on Λ_n and $\Omega_n(\boldsymbol{e})$ in (4) can be viewed as mappings between $\mathcal{S}_H(n)$ and $\mathcal{S}_C(n)$. Furthermore they are linear and still mutually inverse. This extension is the one that we consider from now on.

Consider a connected graph $G = (V, E)$ with vertex set $V = \{1, \ldots, n\}$ and edge set $E = \{e, \ldots, e_m\}$. The *Laplacian matrix* of G is defined as the $n \times n$ symmetric matrix $\boldsymbol{L} = (\ell_{ij})$ indexed by the vertices such that, for $i \neq j$, $\ell_{ij} = -1$ if the vertices i and j are adjacent, $\ell_{ij} = 0$ if i and j are not adjacent, and for each i, $\ell_{ii} = \delta_i$, where δ_i is the degree of the vertex i. It is well-known that the Laplacian matrix $\boldsymbol{L}$ is a centered psd matrix:

$$\boldsymbol{L} \succeq \boldsymbol{0} \ \text{and}\ \boldsymbol{L}\boldsymbol{e} = \boldsymbol{0}, \tag{11}$$

in other words, $\boldsymbol{L} \in \Omega_n(\boldsymbol{e})$. The rank of the Laplacian matrix of a connected graph equals always to $n - 1$. Moreover a connected graph is a tree if and only if $m = n - 1$, where m stands for the number of its edges.

Let the *distance matrix* $\boldsymbol{D} = (d_{ij})$ *of a tree* T be a nonnegative symmetric matrix such that $d_{ii} = 0$ ($i = 1, \ldots, n$) and d_{ij} is equal to the length (the number of edges) of the unique path between vertices i and j. Then, interestingly, $\boldsymbol{D}$ is a nonsingular spherical EDM and its inverse is expressed as

$$\boldsymbol{D}^{-1} = -\frac{1}{2}\boldsymbol{L} + \frac{1}{2(n-1)}\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}} \ \text{with}\ \boldsymbol{\tau} = (2 - \delta_1, \ldots, 2 - \delta_n)^{\mathrm{T}}, \tag{12}$$

which is a classical result due to Graham and Lovász [7], pp.66. (For a more detailed explanation on this topic, see, for example, Chapter 9 of Bapat [2].) As can be seen, for example, from (i) of Proposition 2, in the expression (9) of $\boldsymbol{D}^+$, the matrix $\boldsymbol{B}^+$ plays a role similar to the one played by the Laplacian matrix $\boldsymbol{L}$ in (12) in the sense that $\boldsymbol{B}^+$ is also a centered psd matrix: $\boldsymbol{B} \succeq \boldsymbol{0}$ and $\boldsymbol{B}^+\boldsymbol{e} = \boldsymbol{0}$.

2 Ranks of D and B = τ(D)

In this section, we clarify the relation between the ranks of a hollow symmetric matrix $\boldsymbol{D}$ and its corresponding matrix $\boldsymbol{B} = \tau(\boldsymbol{D})$.

Fix a hollow symmetric matrix $\boldsymbol{D} = (d_{ij}) \in \mathcal{S}_H(n)$. Then there exists a centered symmetric matrix $\boldsymbol{B} = (b_{ij}) \in \mathcal{S}_C(n)$ satisfying $\boldsymbol{D} = \kappa(\boldsymbol{B})$:

$$\boldsymbol{D} = \boldsymbol{e}\boldsymbol{b}^{\mathrm{T}} + \boldsymbol{b}\boldsymbol{e}^{\mathrm{T}} - 2\boldsymbol{B}, \tag{13}$$

where $\boldsymbol{b} = (b_{11}, \ldots, b_{nn})^{\mathrm{T}}$. Although the vector $\boldsymbol{b}$ is nonnegative when $\boldsymbol{D}$ is an EDM, it is not necessarily nonnegative in our case.

Let

$$r = \operatorname{rank} \boldsymbol{B}. \tag{14}$$

To calculate the rank of $\boldsymbol{D}$, we begin with confirming that the equality (5) in Proposition 1 remains true even when $\boldsymbol{D}$ is a hollow symmetric matrix. By using the identity $\boldsymbol{I}_n = \boldsymbol{P} + (1/n)\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}$, we have

$$\boldsymbol{b} = \boldsymbol{P}\boldsymbol{b} + \frac{\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}}{n}\boldsymbol{e}.$$

Substituting it into (13) yields

$$\begin{aligned} -\frac{1}{2}\boldsymbol{D} &= \boldsymbol{B} - (1/2)\boldsymbol{b}\boldsymbol{e}^{\mathrm{T}} - (1/2)\boldsymbol{e}\boldsymbol{b}^{\mathrm{T}} \\ &= \boldsymbol{B} - (1/2)\boldsymbol{P}\boldsymbol{b}\boldsymbol{e}^{\mathrm{T}} - (1/2)\boldsymbol{e}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{P} - \frac{\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}}{n}\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}} \\ &= \boldsymbol{B} + \boldsymbol{z}\boldsymbol{e}^{\mathrm{T}} + \boldsymbol{e}\boldsymbol{z}^{\mathrm{T}} + \lambda\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}, \end{aligned} \tag{15}$$

where $\boldsymbol{z} = -(1/2)\boldsymbol{P}\boldsymbol{b}$ and $\lambda = -(\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b})/n$. Thus we have extended (5) to the case in which $\boldsymbol{D} \in \mathcal{S}_H(n)$.

We use (15) to calculate the rank of $\boldsymbol{D}$. By the Spectral Theorem, there exists a matrix $\bar{\boldsymbol{C}}$ of order $n \times r$ matrix such that

$$\boldsymbol{B} = \bar{\boldsymbol{C}}\boldsymbol{\Theta}\bar{\boldsymbol{C}}^{\mathrm{T}}, \ \boldsymbol{\Theta} = \operatorname{diag}(\theta_1, \ldots, \theta_r) : r \times r, \ \bar{\boldsymbol{C}}^{\mathrm{T}}\bar{\boldsymbol{C}} = \boldsymbol{I}_r, \tag{16}$$

where $\operatorname{diag}(\theta_1, \ldots, \theta_r)$ denotes the diagonal matrix with diagonal elements $\theta_1, \ldots, \theta_r$, which are the nonnull eigenvalues of B. Since θ_i's are nonnull, $\boldsymbol{\Theta}$ is a nonsingular matrix. Let $\bar{\boldsymbol{e}} = \boldsymbol{e}/\sqrt{n}$ so that $\bar{\boldsymbol{e}}^{\mathrm{T}}\bar{\boldsymbol{e}} = 1$. Then there exists an $n \times (n - r - 1)$ matrix $\bar{\boldsymbol{Z}}$ such that

$$\boldsymbol{\Gamma} = (\bar{\boldsymbol{e}}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}}) : n \times n$$

is an orthogonal matrix. Since $\boldsymbol{z}^{\mathrm{T}}\boldsymbol{e} = 0$, we can write $\boldsymbol{z}$ in (15) as

$$\boldsymbol{z} = \bar{\boldsymbol{C}}\boldsymbol{p} + \bar{\boldsymbol{Z}}\boldsymbol{u} \ \text{ for some } \boldsymbol{p} \in \mathbb{R}^r \text{ and } \boldsymbol{u} \in \mathbb{R}^{n-r-1}. \tag{17}$$

Substituting (16) and (17) into (15) yields

$$\begin{aligned} -\frac{1}{2}\boldsymbol{D} &= \bar{\boldsymbol{C}}\boldsymbol{\Theta}\bar{\boldsymbol{C}}^{\mathrm{T}} + \sqrt{n}(\bar{\boldsymbol{C}}\boldsymbol{p} + \bar{\boldsymbol{Z}}\boldsymbol{u})\bar{\boldsymbol{e}}^{\mathrm{T}} + \sqrt{n}\bar{\boldsymbol{e}}(\bar{\boldsymbol{C}}\boldsymbol{p} + \bar{\boldsymbol{Z}}\boldsymbol{u})^{\mathrm{T}} + n\lambda\bar{\boldsymbol{e}}\bar{\boldsymbol{e}}^{\mathrm{T}} \\ &= (\bar{\boldsymbol{e}}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}}) \begin{pmatrix} n\lambda & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta} & \boldsymbol{0} \\ \sqrt{n}\boldsymbol{u} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \bar{\boldsymbol{e}}^{\mathrm{T}} \\ \bar{\boldsymbol{C}}^{\mathrm{T}} \\ \bar{\boldsymbol{Z}}^{\mathrm{T}} \end{pmatrix} \\ &= \boldsymbol{\Gamma}\boldsymbol{U}\boldsymbol{\Gamma}^{\mathrm{T}} \end{aligned} \tag{18}$$

with

$$\boldsymbol{U} = \begin{pmatrix} n\lambda & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta} & \boldsymbol{0} \\ \sqrt{n}\boldsymbol{u} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}.$$

Let

$$\boldsymbol{T} = \begin{pmatrix} 1 & \sqrt{n}\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{I}_{n-r-1} \end{pmatrix}.$$

Then the matrix $\boldsymbol{U}$ is further decomposed as

$$\boldsymbol{U} = \boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}} \text{ with } \tilde{\boldsymbol{U}} = \begin{pmatrix} n(\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p}) & \boldsymbol{0} & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \boldsymbol{0} & \boldsymbol{\Theta} & \boldsymbol{0} \\ \sqrt{n}\boldsymbol{u} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}. \tag{19}$$

Since $\boldsymbol{\Gamma}$ and $\boldsymbol{T}$ are nonsingular, it holds that

$$\operatorname{rank} \boldsymbol{D} = \operatorname{rank} \boldsymbol{U} = \operatorname{rank} \tilde{\boldsymbol{U}}.$$

By noting the location of zero matrices in $\tilde{\boldsymbol{U}}$, we can calculate its rank as

$$\begin{aligned} \operatorname{rank} \tilde{\boldsymbol{U}} &= \operatorname{rank}(\boldsymbol{0}, \boldsymbol{\Theta}, \boldsymbol{0}) + \operatorname{rank} \begin{pmatrix} n(\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p}) & \boldsymbol{0} & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{u} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \\ &= r + \operatorname{rank} \begin{pmatrix} n(\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p}) & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{u} & \boldsymbol{0} \end{pmatrix} \quad (\text{since } \operatorname{rank} \boldsymbol{\Theta} = r). \end{aligned}$$

Thus, when $\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} \neq 0$, the rank is determined as

$$\operatorname{rank} \boldsymbol{D} = \begin{cases} r+2 & \text{if } \boldsymbol{u} \neq \boldsymbol{0} \\ r+1 & \text{if } \boldsymbol{u} = \boldsymbol{0}. \end{cases} \tag{20}$$

On the other hand, when $\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} = 0$, we have

$$\operatorname{rank} \boldsymbol{D} = \begin{cases} r+2 & \text{if } \boldsymbol{u} \neq \boldsymbol{0} \\ r & \text{if } \boldsymbol{u} = \boldsymbol{0}. \end{cases} \tag{21}$$

By summarizing the above results in terms of the original notation, we obtain

Theorem 3. *Let $\boldsymbol{D}$ be a hollow symmetric matrix and $\boldsymbol{B} = (b_{ij})$ the corresponding centered symmetric matrix. Let $r = \operatorname{rank} \boldsymbol{B}$ and $\gamma = \boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4$. Then the rank of $\boldsymbol{D}$ is determined as*

$$\operatorname{rank} \boldsymbol{D} = \begin{cases} r & \text{if } \boldsymbol{z} \in R(\boldsymbol{B}) \text{ and } \gamma = 0 \\ r+1 & \text{if } \boldsymbol{z} \in R(\boldsymbol{B}) \text{ and } \gamma \neq 0 \\ r+2 & \text{if } \boldsymbol{z} \notin R(\boldsymbol{B}) \end{cases} \tag{22}$$

Proof. We only need to show that

$$\boldsymbol{u} = \boldsymbol{0} \iff \boldsymbol{z} \in R(\boldsymbol{B}) \tag{23}$$

and

$$\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} = 0 \iff \boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4 = 0. \tag{24}$$

It follows from (17) that $\boldsymbol{u} = \boldsymbol{0}$ is equivalent to $\boldsymbol{z} \in R(\bar{\boldsymbol{C}})$. Since $R(\bar{\boldsymbol{C}}) = R(\boldsymbol{B})$ (see (16)), the condition is further equivalent to

$$\boldsymbol{z} \in R(\boldsymbol{B}).$$

Thus (23) is proved. Next we check (24). By the definition of λ, it holds that $\lambda = -\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n$. By using (17), we see that

$$\boldsymbol{p} = \bar{\boldsymbol{C}}^{\mathrm{T}}\boldsymbol{z}.$$

Since $\boldsymbol{z} = -(1/2)\boldsymbol{P}\boldsymbol{b}$ (by definition) and $\boldsymbol{P}\bar{\boldsymbol{C}} = \bar{\boldsymbol{C}}$ (since $\bar{\boldsymbol{C}}^{\mathrm{T}}\boldsymbol{e} = \boldsymbol{0}$), we have

$$\boldsymbol{p} = -\frac{1}{2}\bar{\boldsymbol{C}}^{\mathrm{T}}\boldsymbol{b}.$$

Furthermore, as is easily seen,

$$\boldsymbol{B}^{+} = \bar{\boldsymbol{C}}\boldsymbol{\Theta}^{-1}\bar{\boldsymbol{C}}^{\mathrm{T}}$$

holds and hence

$$\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} = \frac{1}{4}\boldsymbol{b}^{\mathrm{T}}\bar{\boldsymbol{C}}\boldsymbol{\Theta}^{-1}\bar{\boldsymbol{C}}\boldsymbol{b} = \frac{1}{4}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}.$$

Thus (24) is obtained. The proof is complete. □

As in (ii) of Proposition 1, when $\boldsymbol{D}$ is an EDM, the case where rank $\boldsymbol{D}$ = rank $\boldsymbol{B}$ does not happen. That is, no EDM (except $\boldsymbol{D} = \boldsymbol{0}$) satisfies the condition $-\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4$. Indeed, if $\boldsymbol{D}$ is an EDM, the corresponding $\boldsymbol{B}$ is psd and hence $\boldsymbol{B}^{+}$ is also psd and $\boldsymbol{b}$ is nonnegative nonnull vector, which implies $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4 \geq 0$ and $-\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n < 0$, and thus the equality does not hold.

On the other hand, the above theorem suggests that when $\boldsymbol{D}$ is extended to a hollow symmetric matrix, its rank may be equal to rank $\boldsymbol{B}$. Hence it is of interest to ask whether there exists a hollow symmetric matrix $\boldsymbol{D}$ that satisfies the condition $-\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4$. The answer is affirmative. But since, to explain an example of such matrices, we need the notion of weighted tree, we postpone it to Section 4. See Theorem 12, in which it is shown that a "distance matrix" of a weighted tree with arbitrary weights satisfies the condition if the total sum of the weights is zero. In this case, the distance between vertices i, j is defined as the sum of the weights of the edges in the unique path between i and j, if $i \neq j$, and 0 if $i = j$. Hence the resulting distance matrix is a hollow symmetric matrix that may have some negative elements.

3 Moore-Penrose Inverse of a Hollow Symmetric Matrix

In this section, we derive the Moore-Penrose inverse of a hollow symmetric matrix, which can be viewed as an extension of Proposition 2.

As is stated in (18) and (19), $\boldsymbol{D}$ is of the form

$$-(1/2)\boldsymbol{D} = \boldsymbol{\Gamma}\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{\Gamma}^{\mathrm{T}},$$

where the two matrices $\boldsymbol{\Gamma}$ and $\boldsymbol{T}$ are nonsingular. We will see below that the Moore-Penrose inverse can be expressed as

$$-2\boldsymbol{D}^{+} = \boldsymbol{\Gamma}(\boldsymbol{T}^{-1})^{\mathrm{T}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\boldsymbol{\Gamma}^{\mathrm{T}}, \tag{25}$$

where $\boldsymbol{T}^{-1}$ is given by

$$\boldsymbol{T}^{-1} = \begin{pmatrix} 1 & -\sqrt{n}\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{I}_{n-r-1} \end{pmatrix}.$$

To see this, recall that, in general, for any orthogonal matrix $\boldsymbol{H}$ and any symmetric matrix $\boldsymbol{S}$, the equality $(\boldsymbol{H}\boldsymbol{S}\boldsymbol{H}^{\mathrm{T}})^{+} = \boldsymbol{H}\boldsymbol{S}^{+}\boldsymbol{H}^{\mathrm{T}}$ holds. Applying this fact, we have

$$-2\boldsymbol{D}^{+} = \boldsymbol{\Gamma}(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})^{+}\boldsymbol{\Gamma}^{\mathrm{T}}.$$

Thus it suffices to show that

$$(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})^{+} = (\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}. \tag{26}$$

Here, we should note that for any nonsingular matrix $\boldsymbol{G}$ and any symmetric matrix $\boldsymbol{S}$, the equality $(\boldsymbol{G}\boldsymbol{S}\boldsymbol{G}^{\mathrm{T}})^{+} = (\boldsymbol{G}^{\mathrm{T}})^{-1}\boldsymbol{S}^{+}\boldsymbol{G}^{-1}$ does not necessarily hold. (More precisely, while the matrix in the right hand side always satisfies the conditions (i) and (ii) in (8), it does not always satisfy (iii) and (iv). In other words, the matrix is just a {1,2}-inverse of $\boldsymbol{G}\boldsymbol{S}\boldsymbol{G}^{\mathrm{T}}$.) However, as will be seen below, both $\boldsymbol{T}$ and $\tilde{\boldsymbol{U}}^{+}$ are of quite simple structure, due to which the equality (26) happens to be valid. That is, the matrix in the right hand side of (26) will turn out to meet the conditions (iii) and (iv).

The Moore-Penrose inverse of $\boldsymbol{D}$ takes different forms according to whether $\boldsymbol{z} \in R(\boldsymbol{B})$ holds or not.

Theorem 4. *Let $\boldsymbol{D}$ be a hollow symmetric matrix such that $\boldsymbol{z} \in R(\boldsymbol{B})$ and $\gamma \neq 0$, where $\gamma = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b}/4 + \boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}/n$. Then the Moore-Penrose inverse $\boldsymbol{D}^{+}$ is expressed as*

$$-2\boldsymbol{D}^{+} = \boldsymbol{B}^{+} - \frac{1}{n\gamma}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}, \tag{27}$$

where $\boldsymbol{x} = \bar{\boldsymbol{e}} - (\sqrt{n}/2)\boldsymbol{B}^{+}\boldsymbol{b}$.

Proof. Since $\boldsymbol{z} \in R(\boldsymbol{B})$ is equivalent to $\boldsymbol{u} = \boldsymbol{0}$ in (17), the matrix $\tilde{\boldsymbol{U}}$ reduces to

$$\tilde{\boldsymbol{U}} = \begin{pmatrix} n(\lambda - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p}) & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Theta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} = \begin{pmatrix} -n\gamma & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Theta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix},$$

whose inverse is easily obtained as

$$\tilde{\boldsymbol{U}}^{+} = \begin{pmatrix} -(1/n\gamma) & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Theta}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}.$$

We need to prove that (26) is valid. To do so, it suffices to show that the two matrices

$$(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})\left\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\right\} \text{ and } \left\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\right\}(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})$$

are symmetric. As is stated above, since $\tilde{\boldsymbol{U}}^{+}$ and $\boldsymbol{T}$ have quite simple forms, both of them happens to be symmetric. Indeed, by a direct calculation, we have

$$(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})\left\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\right\} = \boldsymbol{T}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1} = \begin{pmatrix} 1 & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \text{ (symmetric)}$$

and

$$\left\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\right\}(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}}) = \boldsymbol{T}^{-1}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T} = \begin{pmatrix} 1 & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \text{ (symmetric).}$$

Thus we have

$$-2\boldsymbol{D}^{+} = \boldsymbol{\Gamma}(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\boldsymbol{\Gamma}^{\mathrm{T}}.$$

Since $\boldsymbol{\Gamma}(\boldsymbol{T}^{-1})^{\mathrm{T}} = (\boldsymbol{x}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}})$ holds, the Moore-Penrose inverse of $-(1/2)\boldsymbol{D}$ is derived as

$$\begin{aligned} -2\boldsymbol{D}^{+} &= (\boldsymbol{x}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}}) \begin{pmatrix} -(1/n\gamma) & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Theta}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{x}^{\mathrm{T}} \\ \bar{\boldsymbol{C}}^{\mathrm{T}} \\ \bar{\boldsymbol{Z}}^{\mathrm{T}} \end{pmatrix} \\ &= -\frac{1}{n\gamma}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} + \bar{\boldsymbol{C}}\boldsymbol{\Theta}^{-1}\bar{\boldsymbol{C}}^{\mathrm{T}}. \end{aligned}$$

The proof is complete. □

Next we consider the case of $\boldsymbol{z} \notin R(\boldsymbol{B})$, in which the approach taken above also works.

Theorem 5. *Let $\boldsymbol{D}$ be a hollow symmetric matrix such that $\boldsymbol{z} \notin R(\boldsymbol{B})$. Then the Moore-Penrose inverse $\boldsymbol{D}^{+}$ is expressed as*

$$-2\boldsymbol{D}^{+} = \boldsymbol{B}^{+} + \boldsymbol{x}\boldsymbol{y}^{\mathrm{T}} + \boldsymbol{y}\boldsymbol{x}^{\mathrm{T}} + n\gamma\boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$$

and hence if $\gamma \neq 0$,

$$-2\boldsymbol{D}^{+} = \boldsymbol{B}^{+} - \frac{1}{n\gamma}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} + n\gamma\left(\boldsymbol{y} + \frac{1}{n\gamma}\boldsymbol{x}\right)\left(\boldsymbol{y} + \frac{1}{n\gamma}\boldsymbol{x}\right)^{\mathrm{T}}$$

where $\boldsymbol{y} = -2\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b}/(\sqrt{n}\boldsymbol{b}^{\mathrm{T}}\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b})$.

Proof. It is straightforward to see that the Moore-Penrose inverse of $\tilde{\boldsymbol{U}}$ in (19) is given by

$$\tilde{\boldsymbol{U}}^{+}=\begin{pmatrix} 0 & \mathbf{0} & \boldsymbol{u}^{\mathrm{T}}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}) \\ \mathbf{0} & \boldsymbol{\Theta}^{-1} & \mathbf{0} \\ \boldsymbol{u}^{\mathrm{T}}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}) & \mathbf{0} & \gamma\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}/(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u})^{2} \end{pmatrix}.$$

As in the proof of Theorem 4, we need to prove that (26) is valid. That is, it is necessary to show that the two matrices $(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}})\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\} = \boldsymbol{T}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}$ and $\{(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\}(\boldsymbol{T}\tilde{\boldsymbol{U}}\boldsymbol{T}^{\mathrm{T}}) = \boldsymbol{T}^{-1}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}$ are symmetric. By a direct but simple calculation again, we have

$$\boldsymbol{T}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}=\begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}}\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}} \end{pmatrix} \text{ (symmetric)}$$

and

$$\boldsymbol{T}^{-1}\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}=\begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}}\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}} \end{pmatrix} \text{ (symmetric).}$$

Thus we have $-2\boldsymbol{D}^{+} = \boldsymbol{\Gamma}(\boldsymbol{T}^{\mathrm{T}})^{-1}\tilde{\boldsymbol{U}}^{+}\boldsymbol{T}^{-1}\boldsymbol{\Gamma}^{\mathrm{T}}$. Since $\boldsymbol{\Gamma}(\boldsymbol{T}^{-1})^{\mathrm{T}} = (\boldsymbol{x}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}})$ holds, the Moore-Penrose inverse of $\boldsymbol{D}$ is derived as

$$\begin{aligned} -2\boldsymbol{D}^{+} &= (\boldsymbol{x}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}})\begin{pmatrix} 0 & \mathbf{0} & \boldsymbol{u}^{\mathrm{T}}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}) \\ \mathbf{0} & \boldsymbol{\Theta}^{-1} & \mathbf{0} \\ \boldsymbol{u}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}) & \mathbf{0} & \gamma\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}/(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u})^{2} \end{pmatrix}\begin{pmatrix} \boldsymbol{x}^{\mathrm{T}} \\ \bar{\boldsymbol{C}}^{\mathrm{T}} \\ \bar{\boldsymbol{Z}}^{\mathrm{T}} \end{pmatrix} \\ &= \boldsymbol{B}^{+} + \boldsymbol{x}\boldsymbol{a}^{\mathrm{T}} + \boldsymbol{a}\boldsymbol{x}^{\mathrm{T}} + n\gamma\boldsymbol{a}\boldsymbol{a}^{\mathrm{T}} \text{ with } \boldsymbol{a} = \bar{\boldsymbol{Z}}\boldsymbol{u}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}), \end{aligned}$$

where the equalities $\boldsymbol{B}^{+} = \bar{\boldsymbol{C}}\boldsymbol{\Theta}^{-1}\bar{\boldsymbol{C}}^{\mathrm{T}}$ is used.

Finally we show that $\boldsymbol{a}$ is equal to $\boldsymbol{y}$ that is defined in the statement of the theorem. To do so, use $\boldsymbol{u} = \bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{z} = -(1/2)\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b}$. Then we have

$$\boldsymbol{a} = \bar{\boldsymbol{Z}}\boldsymbol{u}/(\sqrt{n}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}) = \bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{z}/(\sqrt{n}\boldsymbol{z}^{\mathrm{T}}\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{z}) = -2\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b}/(\sqrt{n}\boldsymbol{b}^{\mathrm{T}}\bar{\boldsymbol{Z}}\bar{\boldsymbol{Z}}^{\mathrm{T}}\boldsymbol{b}) = \boldsymbol{y}.$$

Thus we have

$$-2\boldsymbol{D}^{+} = \boldsymbol{B}^{+} + \boldsymbol{x}\boldsymbol{y}^{\mathrm{T}} + \boldsymbol{y}\boldsymbol{x}^{\mathrm{T}} + n\gamma\boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}.$$

This completes the proof. □

Finally we consider the case in which $\boldsymbol{z} \in R(\boldsymbol{B})$ and $\gamma = 0$. In this case, (25) is not true. But the matrix $\boldsymbol{U}$ in (18) is simple enough to calculate the Moore-Penrose inverse directly. Indeed, $\boldsymbol{U}$ is of the form

$$\boldsymbol{U}=\begin{pmatrix} n\lambda & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} & \sqrt{n}\boldsymbol{u}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta} & \mathbf{0} \\ \sqrt{n}\boldsymbol{u} & \mathbf{0} & \mathbf{0} \end{pmatrix}=\begin{pmatrix} n\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} & \mathbf{0} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix},$$

since $\gamma = 0 \iff \lambda = \boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p}$ and $\boldsymbol{z} \in R(\boldsymbol{B}) \iff \boldsymbol{u} = \mathbf{0}$. By letting $\boldsymbol{\Theta}_1$ and $\boldsymbol{\Theta}_2$ be any diagonal matrices such that $\boldsymbol{\Theta} = \boldsymbol{\Theta}_1\boldsymbol{\Theta}_2$, we have the following maximal rank decomposition:

$$\begin{aligned} \begin{pmatrix} n\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}^{-1}\boldsymbol{p} & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta} \end{pmatrix} &= \begin{pmatrix} n\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}_2^{-1}\boldsymbol{\Theta}_1^{-1}\boldsymbol{p} & \sqrt{n}\boldsymbol{p}^{\mathrm{T}} \\ \sqrt{n}\boldsymbol{p} & \boldsymbol{\Theta}_1\boldsymbol{\Theta}_2 \end{pmatrix} \\ &= \begin{pmatrix} \sqrt{n}\boldsymbol{p}^{\mathrm{T}}\boldsymbol{\Theta}_2^{-1} \\ \boldsymbol{\Theta}_1 \end{pmatrix}\left(\sqrt{n}\boldsymbol{\Theta}_1^{-1}\boldsymbol{p},\ \boldsymbol{\Theta}_2\right) \\ &= \boldsymbol{X}\boldsymbol{Y}^{\mathrm{T}} \text{ (say),} \end{aligned}$$

where $\boldsymbol{X}$ and $\boldsymbol{Y}$ are $(r+1)\times r$ full rank matrices. Thus the Moore-Penrose inverse of $\boldsymbol{XY}^{\mathrm{T}}$ is given by

$$\begin{aligned}(\boldsymbol{XY}^{\mathrm{T}})^{+} &= \boldsymbol{Y}(\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y})^{-1}(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}} \\ &= \begin{pmatrix} \sqrt{n}\boldsymbol{p}^{\mathrm{T}} \\ \boldsymbol{\Theta} \end{pmatrix} \boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}(\sqrt{n}\boldsymbol{p}, \boldsymbol{\Theta}) \text{ with } \boldsymbol{G} = n\boldsymbol{pp}^{\mathrm{T}} + \boldsymbol{\Theta}^2,\end{aligned}$$

from which we have

$$\boldsymbol{U}^{+} = \begin{pmatrix} n\boldsymbol{p}^{\mathrm{T}}\boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{p} & \sqrt{n}\boldsymbol{p}^{\mathrm{T}}\boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{\Theta} & \boldsymbol{0} \\ \sqrt{n}\boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{p} & \boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}\boldsymbol{\Theta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix},$$

and hence

$$\begin{aligned}-2\boldsymbol{D}^{+} &= \boldsymbol{\Gamma}\boldsymbol{U}^{+}\boldsymbol{\Gamma}^{\mathrm{T}} = (\bar{\boldsymbol{e}}, \bar{\boldsymbol{C}}, \bar{\boldsymbol{Z}})\boldsymbol{U}^{+}\begin{pmatrix} \bar{\boldsymbol{e}}^{\mathrm{T}} \\ \bar{\boldsymbol{C}}^{\mathrm{T}} \\ \bar{\boldsymbol{Z}}^{\mathrm{T}} \end{pmatrix} \\ &= (\sqrt{n}\bar{\boldsymbol{e}}\boldsymbol{p}^{\mathrm{T}} + \bar{\boldsymbol{C}}\boldsymbol{\Theta})\boldsymbol{G}^{-1}\boldsymbol{\Theta}\boldsymbol{G}^{-1}(\sqrt{n}\boldsymbol{p}\bar{\boldsymbol{e}}^{\mathrm{T}} + \boldsymbol{\Theta}\bar{\boldsymbol{C}}^{\mathrm{T}}). \qquad (28)\end{aligned}$$

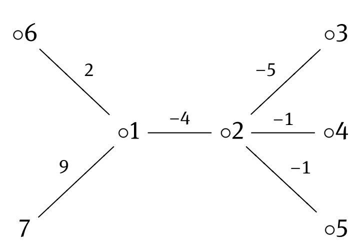
Theorem 6. *Let $\boldsymbol{D}$ be a hollow symmetric matrix such that $\boldsymbol{z} \in R(\boldsymbol{B})$ with $\gamma = 0$. Then the Moore-Penrose inverse $-2\boldsymbol{D}^{+}$ is expressed as (28).*

4 Distance Matrix of a Tree with Arbitrary Weights

Let T be a weighted tree with vertex set $V(T) = \{1, \ldots, n\}$ and edge set $E(T) = \{e_1, \ldots, e_{n-1}\}$, where the edge e_j is assigned the weight w_j, which we assume to be a real number (possibly negative). The *distance* d_{ij} between vertices i and j is defined to be the sum of the weights of the edges on the (unique) ij-path. We set $d_{ii} = 0, i = 1, \ldots, n$. The *distance matrix* $\boldsymbol{D}$ of T is the $n \times n$ matrix $\boldsymbol{D}$ with its (i, j)-element equal to d_{ij}. Needless to say, $\boldsymbol{D} = (d_{ij})$ is a hollow symmetric matrix: $\boldsymbol{D} \in \mathcal{S}_H(n)$.

If the weights are all nonzero, then the Laplacian matrix $\boldsymbol{L} = (\ell_{ij})$ of T is defined as follows. The rows and the columns of $\boldsymbol{L}$ are indexed by $V(T)$. For $i \neq j$, the (i, j)-element of $\boldsymbol{L}$ is zero if i and j are not adjacent and it is $-1/w(\{i, j\})$ if i and j are adjacent, where $\{i, j\}$ is the edge joining i and j and $w(\{i, j\})$ denotes the weight assigned on $\{i, j\}$. For $i = 1, \ldots, n$, the element ℓ_{ii} is set equal to $-\sum_{j\neq i} \ell_{ij}$. It is obvious that $\boldsymbol{L} \in \mathcal{S}_C(n)$, and as will be seen soon, the Laplacian matrix thus defined is also the Laplacian matrix of $\boldsymbol{D}$ in our sense. That is, $\boldsymbol{L}$ is the Moore-Penrose inverse of $\boldsymbol{B} = \tau(\boldsymbol{D})$. (See Lemma 10 below.)

Example Consider the weighted tree



Its distance matrix is

$$\boldsymbol{D} = \begin{bmatrix} 0 & -4 & -9 & -5 & -5 & 2 & 9 \\ -4 & 0 & -5 & -1 & -1 & -2 & 5 \\ -9 & -5 & 0 & -6 & -6 & -7 & 0 \\ -5 & -1 & -6 & 0 & -2 & -3 & 4 \\ -5 & -1 & -6 & -2 & 0 & -3 & 4 \\ 2 & -2 & -7 & -3 & -3 & 0 & 11 \\ 9 & 5 & 0 & 4 & 4 & 11 & 0 \end{bmatrix}$$

and its Laplacian matrix is

$$\boldsymbol{L} = \begin{bmatrix} 13/36 & 1/4 & 0 & 0 & 0 & -1/2 & -1/9 \\ 1/4 & -49/20 & 1/5 & 1 & 1 & 0 & 0 \\ 0 & 1/5 & -1/5 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ -1/2 & 0 & 0 & 0 & 0 & 1/2 & 0 \\ -1/9 & 0 & 0 & 0 & 0 & 0 & 1/9 \end{bmatrix}.$$

If T is an unweighted tree (that is, $w_j = 1, j = 1, \dots, n-1$) with n vertices, then according to a classical result of Graham and Pollak [8], pp.2511, the determinant of $\boldsymbol{D}$ is given by $\det \boldsymbol{D} = (-1)^{n-1}(n-1)2^{n-2}$. Thus the determinant of the distance matrix depends only on the number of vertices. A formula for $\boldsymbol{D}^{-1}$ was given by Graham and Lovász [7], pp.66. Extensions of these results for weighted trees have been obtained, for example, by Bapat, Kirkland and Neumann [3], Theorem 2.1. We state the results next. It may be remarked that the trees in which some of the edge-weights are negative have not been considered in the literature. Thus the results in [3] were proved assuming that all the weights are positive. However the proof reveals that the results hold even when the weights are more general. To state them, we denote the degree of the vertex i by $\delta_i, i = 1, \dots, n$. We set $\tau_i = 2 - \delta_i, i = 1, \dots, n$ and let $\boldsymbol{\tau}$ be the $n \times 1$ vector with components $\tau_1, \dots, \tau_n$.

Theorem 7. (Bapat, Kirkland and Neumann [3]), Theorem 2.1 and Corollary 2.5 *Let T be a weighted tree with vertex set $V(T) = \{1, \dots, n\}$, let $\boldsymbol{D}$ and $\boldsymbol{L}$ be the distance matrix and the Laplacian of T, respectively. Then the following assertions hold:*

(i) $\det \boldsymbol{D} = (-1)^{n-1}2^{n-2}(\sum_j w_j)(\prod_j w_j)$

(ii) Let the weights be all nonzero and suppose $\sum_{j=1}^{n-1} w_j \neq 0$. Then $\boldsymbol{D}$ is nonsingular and

$$\boldsymbol{D}^{-1} = -\frac{1}{2}\boldsymbol{L} + \frac{1}{2\sum_{j=1}^{n-1} w_j}\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}.$$

In this section we obtain a formula for $\boldsymbol{D}^{+}$, when $\sum_j w_j = 0$, thereby extending (ii) of Theorem 7 to the case when $\boldsymbol{D}$ is singular. The following result is known for an unweighted tree (see [2],Lemma 9.7). We include a proof which is different from the one given in [2] for the unweighted case. Recall that we denote by $\boldsymbol{e}$ the vector of all ones of the appropriate size.

Lemma 8. *Let T be a weighted tree with vertex set $V(T) = \{1, \dots, n\}$. Let $\boldsymbol{D}$ be the distance matrix of T. Then*

$$\boldsymbol{D}\boldsymbol{\tau} = \left(\sum_{j=1}^{n-1} w_j\right)\boldsymbol{e}.$$

Proof. Let $i \in V(T)$ be fixed. For $j \in V(T), j \neq i$, let $j(i)$ be the predecessor of j on the $i - j$ path. Then $d_{ij} = d_{ij(i)} + w(\{j(i), j\})$. Since $d_{ii} = 0$, we have

$$\sum_{j=1}^{n} d_{ij} = \sum_{j \neq i} d_{ij(i)} + \sum_{j \neq i} w(\{j(i), j\}). \tag{29}$$

Note that any vertex k adjacent to j appears as a predecessor of a path to j precisely $\delta_k - 1$ times. We have

$$\begin{aligned}2\sum_{j=1}^{n} d_{ij} &= \sum_{j=1}^{n} d_{ij} + \sum_{j=1}^{n} d_{ij}\\ &= \sum_{j\neq i} d_{ij} + \sum_{j\neq i} d_{ij(i)} + \sum_{j\neq i} w(\{j(i), j\})\\ &= \sum_{j\neq i} d_{ij} + \sum_{k\neq i}(\delta_k - 1)d_{ik} + \sum_{\ell=1}^{n-1} w_\ell\\ &= \sum_{k\neq i} \delta_k d_{ik} + \sum_{\ell=1}^{n-1} w_\ell\end{aligned}$$

It follows that

$$\begin{aligned}\sum_{j=1}^{n} d_{ij}\tau_j &= \sum_{j=1}^{n} d_{ij}(2-\delta_j)\\ &= 2\sum_{j=1}^{n} d_{ij} - \sum_{j=1}^{n} \delta_j d_{ij}\\ &= \sum_{\ell=1}^{n-1} w_\ell\end{aligned}$$

and the proof is complete. □

The next result is known for the case of an unweighted tree (see [2], Lemma 9.8). The proof for the weighted case is similar and is omitted.

Lemma 9. *Let T be a weighted tree with vertex set $V(T) = \{1, \dots, n\}$ with all the weights being nonzero. Let $\boldsymbol{D}$ be the distance matrix of T and let $\boldsymbol{L}$ be the Laplacian of T. Then*

$$\boldsymbol{LD} + 2\boldsymbol{I}_n = \boldsymbol{\tau e}^{\mathrm{T}},\ \ \boldsymbol{DL} + 2\boldsymbol{I}_n = \boldsymbol{e\tau}^{\mathrm{T}},\ \ \boldsymbol{LDL} = -2\boldsymbol{L}.$$

By using the lemma, let us confirm

Lemma 10. *$\boldsymbol{L}$ is the Moore-Penrose inverse of $\boldsymbol{B}$:*

$$\boldsymbol{L} = \boldsymbol{B}^{+}.$$

Proof. Since $\boldsymbol{LP} = \boldsymbol{PL} = \boldsymbol{L}$ holds, the last equality in Lemma 9 can be expressed as

$$\boldsymbol{LPDPL} = -2\boldsymbol{L}, \tag{30}$$

which is equivalent to $\boldsymbol{LBL} = \boldsymbol{L}$. Thus $\boldsymbol{L}$ satisfies the condition (ii) in (8). Similarly, by postmultiplying the first equality in Lemma 9 by $\boldsymbol{P}$ and using $\boldsymbol{L} = \boldsymbol{LP}$, we have $\boldsymbol{LPDP} + 2\boldsymbol{P} = \boldsymbol{\tau e}^{\mathrm{T}}\boldsymbol{P}$, which is further expressed as $\boldsymbol{LB} - \boldsymbol{P} = \boldsymbol{0}$ since $\boldsymbol{Pe} = \boldsymbol{0}$. This shows that $\boldsymbol{LB}$ is symmetric. By arguing in the same way, we can prove that $\boldsymbol{BL}$ is also symmetric. Finally, premultiplying $\boldsymbol{LB} - \boldsymbol{P} = \boldsymbol{0}$ by $\boldsymbol{B}$ and using $\boldsymbol{BP} = \boldsymbol{B}$ entails $\boldsymbol{BLB} = \boldsymbol{B}$. Thus $\boldsymbol{L}$ satisfies the four conditions in (8), or equivalently, $\boldsymbol{L} = \boldsymbol{B}^{+}$. □

The following is the main result of this section.

Theorem 11. *Let T be a weighted tree with vertex set $V(T) = \{1, \dots, n\}$, with all the weights being nonzero, and suppose $\sum_{\ell=1}^{n-1} w_\ell = 0$. Let $\boldsymbol{D}$ be the distance matrix of T and let $\boldsymbol{L}$ be the Laplacian of T. Then $\boldsymbol{D}$ is singular and*

$$\boldsymbol{D}^{+} = -\frac{1}{2}\boldsymbol{L} + \boldsymbol{u\tau}^{\mathrm{T}} + \boldsymbol{\tau u}^{\mathrm{T}},$$

where

$$\boldsymbol{u} = \frac{1}{2}\left(\boldsymbol{D}^{+}\boldsymbol{e} - \frac{\boldsymbol{e}^{\mathrm{T}}\boldsymbol{D}^{+}\boldsymbol{e}}{4}\boldsymbol{\tau}\right).$$

Proof. First note that by Theorem 7, $\det \boldsymbol{D} = (-1)^{n-1}2^{n-2}\sum_{\ell} w_\ell = 0$ and hence $\boldsymbol{D}$ is singular. Let i be a pendant vertex of T and let $\boldsymbol{D}(i,i)$ be the submatrix obtained by deleting row i and column i of $\boldsymbol{D}$. Then $\boldsymbol{D}(i,i)$ is the distance matrix of $T\setminus\{i\}$, and by Theorem 7, $\det \boldsymbol{D} \neq 0$. Thus $\boldsymbol{D}$ has rank $n-1$. Since $\sum_{\ell=1}^{n-1} w_\ell = 0$, then by Lemma 8, $\boldsymbol{D}\boldsymbol{\tau} = \boldsymbol{0}$. Thus $\boldsymbol{\tau}$ spans the null space of $\boldsymbol{D}$ and hence

$$\boldsymbol{D}\boldsymbol{D}^{+} = \boldsymbol{D}^{+}\boldsymbol{D} = \boldsymbol{I}_n - \frac{\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}}{\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}}, \tag{31}$$

which is the projection on the orthogonal complement of the null space of $\boldsymbol{D}$. Let

$$\boldsymbol{H} = -\frac{1}{2}\boldsymbol{L} + \boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}},$$

where $\boldsymbol{u}$ is as given in the hypothesis. Since $\boldsymbol{D}\boldsymbol{\tau} = \boldsymbol{0}$, then $\boldsymbol{D}\boldsymbol{H} = -\frac{1}{2}\boldsymbol{D}\boldsymbol{L} + \boldsymbol{D}\boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}}$. By Lemma 9 and (31) it follows that $\boldsymbol{D}\boldsymbol{H} = \boldsymbol{I}_n - \frac{\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}}{\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}}$. It can be shown similarly that $\boldsymbol{H}\boldsymbol{D} = \boldsymbol{I}_n - \frac{\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}}{\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}}$. Thus both $\boldsymbol{D}\boldsymbol{H}$ and $\boldsymbol{H}\boldsymbol{D}$ are symmetric. Also $\boldsymbol{D}\boldsymbol{H}\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{I}_n - \frac{\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}}{\boldsymbol{\tau}^{\mathrm{T}}\boldsymbol{\tau}}) = \boldsymbol{D}$. It remains to verify $\boldsymbol{H}\boldsymbol{D}\boldsymbol{H} = \boldsymbol{H}$. A simple computation shows that

$$\boldsymbol{u}^{\mathrm{T}}\boldsymbol{D}\boldsymbol{u} = \boldsymbol{e}^{\mathrm{T}}\boldsymbol{u}. \tag{32}$$

Using Lemma 9 and (32) we have

$$\begin{aligned}
\boldsymbol{H}\boldsymbol{D}\boldsymbol{H} &= (-\frac{1}{2}\boldsymbol{L} + \boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}})\boldsymbol{D}\boldsymbol{H}\\
&= (-\frac{1}{2}\boldsymbol{L}\boldsymbol{D} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{D})(-\frac{1}{2}\boldsymbol{L} + \boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}})\\
&= \frac{1}{4}\boldsymbol{L}\boldsymbol{D}\boldsymbol{L} - \frac{1}{2}\boldsymbol{L}\boldsymbol{D}\boldsymbol{u}\boldsymbol{\tau} - \frac{1}{2}\tau\boldsymbol{u}^{\mathrm{T}}\boldsymbol{D}\boldsymbol{L} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{D}\boldsymbol{u}\boldsymbol{\tau}\\
&= -\frac{1}{2}\boldsymbol{L} + (\boldsymbol{I}_n - \frac{\boldsymbol{\tau}\boldsymbol{e}^{\mathrm{T}}}{2})\boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}}(\boldsymbol{I}_n - \frac{\boldsymbol{e}^{\mathrm{T}}\boldsymbol{\tau}^{\mathrm{T}}}{2}) + (\boldsymbol{u}^{\mathrm{T}}\boldsymbol{D}\boldsymbol{u})\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}}\\
&= -\frac{1}{2}\boldsymbol{L} + \boldsymbol{u}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{\tau}\boldsymbol{u}^{\mathrm{T}} - (\boldsymbol{e}^{\mathrm{T}}\boldsymbol{u})\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}} + \boldsymbol{u}^{\mathrm{T}}\boldsymbol{D}\boldsymbol{u}(\boldsymbol{\tau}\boldsymbol{\tau}^{\mathrm{T}})\\
&= \boldsymbol{H},
\end{aligned}$$

in view of (32). Hence $\boldsymbol{H} = \boldsymbol{D}^{+}$ and the proof is complete. □

We end this paper with an answer to the question, raised in the end of Section 2, of whether there exists a hollow symmetric matrix $\boldsymbol{D}$ such that $\operatorname{rank} \boldsymbol{D} = \operatorname{rank} \boldsymbol{B}$.

Let T be a weighted tree with vertex set $V(T) = \{1,\dots,n\}$, with all the weights being nonzero, and suppose $\sum_{\ell=1}^{n-1} w_\ell = 0$. Let $\boldsymbol{D}$ be the distance matrix of T, $\boldsymbol{L} = (\ell_{ij})$ the Laplacian matrix of T. It is well-known that $\boldsymbol{L}$ has rank $n-1$ and as observed in the proof of Theorem 11, $\boldsymbol{D}$ has rank $n-1$ as well. Thus $\operatorname{rank} \boldsymbol{D} = \operatorname{rank} \boldsymbol{L} = \operatorname{rank} \boldsymbol{B}$.

In the next result we prove an identity which is of independent interest, thereby providing another verification of fact that $\operatorname{rank} \boldsymbol{D} = \operatorname{rank} \boldsymbol{B}$.

Theorem 12. *Let T be a weighted tree with vertex set $V(T) = \{1,\dots,n\}$, with all the weights being nonzero, and suppose $\sum_{\ell=1}^{n-1} w_\ell = 0$. Let $\boldsymbol{D}$ be the distance matrix of T, $\boldsymbol{L} = (\ell_{ij})$ the Laplacian matrix of T, $\boldsymbol{B} = (b_{ij})$ the Moore-Penrose inverse for $\boldsymbol{L}$, and $\boldsymbol{b} = (b_{11},\dots,b_{nn})^{\mathrm{T}}$. Then the equality*

$$\boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b} + \frac{4}{n}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b} = 0 \tag{33}$$

holds.

Proof. Let $\boldsymbol{X} = (x_{ij}) = (\boldsymbol{L} + (1/n)\boldsymbol{J})^{-1}$, where $\boldsymbol{J}$ is the $n \times n$ matrix of all ones. Since $\boldsymbol{L}\boldsymbol{e} = \boldsymbol{0}$, the matrix $\boldsymbol{X}$ is nonsingular and satisfies $\boldsymbol{X}^{-1}\boldsymbol{e} = \boldsymbol{e}$ and $\boldsymbol{X}\boldsymbol{e} = \boldsymbol{e}$. By using $\boldsymbol{L} = \boldsymbol{X}^{-1} - (1/n)\boldsymbol{J}$, we can easily see that

$$\boldsymbol{L}^{+} = \boldsymbol{X} - (1/n)\boldsymbol{J}.$$

On the other hand, the vector $\boldsymbol{\tau}$ is expressed as (see Lemma 10.8, [2],p.140)

$$\begin{aligned}\boldsymbol{\tau} &= \boldsymbol{L}\tilde{\boldsymbol{X}}\boldsymbol{e} + \frac{2}{n}\boldsymbol{e} \text{ with } \tilde{\boldsymbol{X}} = \text{diag}\{x_{11}, \dots, x_{nn}\} \\ &= \boldsymbol{L}\left(\boldsymbol{b} + \frac{1}{n}\boldsymbol{e}\right) + \frac{2}{n}\boldsymbol{e} \\ &= \boldsymbol{L}\boldsymbol{b} + \frac{2}{n}\boldsymbol{e}. \end{aligned} \tag{34}$$

From (34) we get the equations

$$\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\tau} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{L}\boldsymbol{b} + \frac{2}{n}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{e}. \tag{35}$$

and

$$\boldsymbol{L}^{+}\boldsymbol{\tau} = \boldsymbol{L}^{+}(\boldsymbol{L}\boldsymbol{b} + \frac{2}{n}\boldsymbol{e}) = (\boldsymbol{I} - (1/n)\boldsymbol{J})\boldsymbol{b} = \tag{36}$$

Using $\boldsymbol{D} = \boldsymbol{e}\boldsymbol{b}^{\mathrm{T}} + \boldsymbol{b}\boldsymbol{e}^{\mathrm{T}} - 2\boldsymbol{L}^{+}$ we get

$$\begin{aligned}\boldsymbol{D}\boldsymbol{\tau} &= \boldsymbol{e}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\tau} + 2\boldsymbol{b} - 2\boldsymbol{L}^{+}\boldsymbol{\tau} \\ &= \boldsymbol{e}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{L}\boldsymbol{b} + \frac{2}{n}\boldsymbol{e}\boldsymbol{b}^{\mathrm{T}}\boldsymbol{e} + 2\boldsymbol{b} - 2(\boldsymbol{I} - (1/n)\boldsymbol{J})\boldsymbol{b} \text{ by (35), (36)} \\ &= (\boldsymbol{b}^{\mathrm{T}}\boldsymbol{L}\boldsymbol{b})\boldsymbol{e} + \frac{4}{n}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}\boldsymbol{e} \text{ since } \boldsymbol{e}^{\mathrm{T}}\boldsymbol{\tau} = 2.\end{aligned}$$

Since $\boldsymbol{D}\boldsymbol{\tau} = 0$ by Lemma 8 and since $\boldsymbol{L} = \boldsymbol{B}^{+}$, it follows from the preceding equation that

$$\boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}^{+}\boldsymbol{b} + \frac{4}{n}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b} = 0$$

and the proof is complete. □

Since rank $\boldsymbol{B}$ = rank $\boldsymbol{L} = n - 1$ and since $\boldsymbol{e}^{\mathrm{T}}\boldsymbol{z} = 0$, where $\boldsymbol{z}$ is as in Theorem 3, it follows that $\boldsymbol{z} \in R(\boldsymbol{B})$. Now using (22) and Theorem 12 we get rank $\boldsymbol{D}$ = rank $\boldsymbol{B}$.

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