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Squared distance matrix of a tree: Inverse and inertia

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A B S T R A C T

Let T be a tree with vertices $V(T) = \{1, \ldots, n\}$. The distance between vertices $i, j \in V(T)$, denoted d_{ij}, is defined to be the length (the number of edges) of the path from i to j. We set $d_{ii} = 0, i = 1, \ldots, n$. The squared distance matrix Δ of T is the $n \times n$ matrix with (i, j)-element equal to 0 if $i = j$, and d_{ij}^2 if $i \neq j$. It is known that Δ is nonsingular if and only if the tree has at most one vertex of degree 2. We obtain a formula for Δ^{-1}, if it exists. When the tree has no vertex of degree 2, the formula is particularly simple and depends on a certain "two-step" Laplacian of the tree. We determine the inertia of Δ. The inverse and the inertia of the edge orientation matrix are also described.

1. Introduction and preliminary results

Let G be a connected graph with vertex set $V(G) = \{1, \ldots, n\}$ and edge set $E(G)$. The distance between vertices $i, j \in V(G)$, denoted d_{ij}, is defined to be the minimum length

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(the number of edges) of a path from i to j (or an (i,j)-path). We set $d_{ii} = 0, i = 1, \dots, n$. The distance matrix $D(G)$, or simply D, is the $n \times n$ matrix with (i,j)-element equal to 0 if $i = j$ and d_{ij} if $i \neq j$.

According to a well-known result due to Graham and Pollak [8], if T is a tree with n vertices, then the determinant of the distance matrix D of T is $(-1)^{n-1}(n-1)2^{n-2}$. Thus the determinant depends only on the number of vertices in the tree and not on the tree itself. A formula for the inverse of the distance matrix of a tree was given by Graham and Lovász [7]. These two results have generated considerable interest and a plethora of extensions and generalizations have been proved (see, for example, [1–3,5,10] and the references contained therein).

Let T be a tree with vertex set $\{1, \dots, n\}$ and let D be the distance matrix of T. The squared distance matrix Δ is defined to be the Hadamard product $D \circ D$, and thus has the (i,j)-element d_{ij}^2. A formula for the determinant of Δ was proved in [6]. It turns out that the determinant of Δ depends only on the degree sequence of T. Furthermore, Δ is nonsingular if and only if the tree has at most one vertex of degree 2. In this paper we obtain a formula for Δ^{-1} when it exists. We also determine the inertia of Δ.

We introduce more notation. Let G be a connected graph with vertex set $V(G) = \{1, \dots, n\}$ and edge set $E(G)$. We denote the degree of vertex i by δ_i, $i = 1, \dots, n$; and we let δ be the vector $(\delta_1, \dots, \delta_n)'$. We use the notation $i \sim j$ to indicate that vertices i and j are adjacent. Recall that the Laplacian matrix $L(G)$, or simply L, is the $n \times n$ matrix with its (i,j)-element, $i \neq j$, equal to -1, if $i \sim j$, and zero otherwise. The diagonal elements of L are $\delta_1, \dots, \delta_n$. We set $\tau_i = 2 - \delta_i$, $i = 1, \dots, n$; and let $\tau = (\tau_1, \dots, \tau_n)'$. We let $\mathbf{1}$ be the column vector of all ones, of appropriate size. The square matrix of appropriate size with all elements equal to 1 will be denoted by J.

We will also consider the vertex-edge incidence matrix of an oriented graph. Let G be a connected graph with vertex set $V(G) = \{1, \dots, n\}$ and edge set $E(G) = \{e_1, \dots, e_m\}$. We assign an orientation to each edge of G. The incidence matrix Q of G is the matrix with its rows indexed by $V(G)$ and the columns indexed by $E(G)$. The entry corresponding to row i and column e_j is 1 if e_j originates at i, -1 if e_j terminates at i, and zero if e_j and i are not incident. Note that $L = QQ'$. We refer to [1] for basic properties of the incidence and the Laplacian matrices.

Some known results are summarized next.

Theorem 1. *Let T be a tree with vertex set $\{1, \dots, n\}$, and let D and L, respectively, be the distance matrix and the Laplacian of T. Then the following assertions hold.*

(i) $\det D = (-1)^{n-1}(n-1)2^{n-2}$.
(ii) $Q'DQ = -2I$.
(iii) $LDL = -2L$.
(iv) $D\tau = (n-1)\mathbf{1}$.
(v) $D^{-1} = -\frac{1}{2}L + \frac{1}{2(n-1)}\tau\tau'$.
(vi) $-\frac{1}{2}DL = I - \frac{1}{2}\mathbf{1}\tau'$.

Assertion (i) is due to Graham and Pollak [8], while (v) is proved in Graham and Lovász [7] and (vi) is a consequence of (iv), (v). Assertions (ii)–(iv) can be found in [1,2]. We begin by providing an elementary, new proof of (iv). The proof technique will be used again. We continue to use the notation introduced earlier.

Lemma 2. *Let T be a tree with vertex set $\{1, \ldots, n\}$, and let D be the distance matrix of T. Then*

$$D\tau = (n-1)\mathbf{1}. \tag{1}$$

Proof. Let $i \in \{1, \ldots, n\}$ be fixed. We need to show $\sum_{j=1}^n d_{ij}\tau_j = n-1$, or equivalently,

$$2\sum_{j=1}^n d_{ij} = \sum_{j=1}^n d_{ij}\delta_j + n - 1. \tag{2}$$

For $j \in \{1, \ldots, n\}, j \neq i$, let $\gamma(j)$ denote the immediate predecessor of j on the (i,j)-path in T. Note that $d_{ij} = d_{i\gamma(j)} + 1$. We have

$$\begin{aligned} 2\sum_{j=1}^n d_{ij} &= 2\sum_{j\neq i} d_{ij} \\ &= \sum_{j\neq i}(d_{i\gamma(j)} + 1) + \sum_{j\neq i} d_{ij} \\ &= \sum_{j\neq i} d_{ij}(\delta_j - 1) + \sum_{j\neq i} d_{ij} + n - 1, \end{aligned} \tag{3}$$

where (3) follows in view of the fact that j occurs as a predecessor in $\delta_j - 1$ paths from i. Clearly, (2) follows from (3) and the proof is complete. $\square$

We let $\tilde{\tau}$ be the diagonal matrix with diagonal elements $\tau_1, \ldots, \tau_n$.

Lemma 3. *Let T be a tree with vertex set $\{1, \ldots, n\}$, and let D, Δ and L be the distance matrix, the squared distance matrix and the Laplacian of T, respectively. Then*

$$\Delta L = (2D + J)\tilde{\tau} - 2J. \tag{4}$$

Proof. Let $i \in \{1, \ldots, n\}$. Then

$$\begin{aligned} (\Delta L)_{ii} &= \sum_{s=1}^n d_{is}^2 \ell_{si} \\ &= \sum_{s\sim i} d_{is}^2 \ell_{si} \end{aligned}$$

$$= -\sum_{s\sim i} d_{is}^2$$
$$= -\delta_i. \tag{5}$$

The (i,i)-element of $(2D + J)\tilde{\tau} - 2J$ is $\tau_{ii} - 2$, which equals $-\delta_i$. It follows from this observation and (5) that the (i,i)-element of ΔL equals the (i,i)-element of $(2D + J)\tilde{\tau} - 2J$.

Now let $i, j \in \{1, \dots, n\}, i \neq j$. We have

$$\begin{aligned}
(\Delta L)_{ij} &= \sum_{s=1}^{n} d_{is}^2 \ell_{sj} \\
&= \delta_j d_{ij}^2 - \sum_{s\sim j} d_{is}^2 \\
&= \delta_j d_{ij}^2 - (d_{ij} - 1)^2 - (\delta_j - 1)(d_{ij} + 1)^2 \\
&= -\delta_j + 2d_{ij}(2 - \delta_j) \\
&= -\delta_j + 2d_{ij}\tau_j. \qquad (6)
\end{aligned}$$

The (i,j)-element of $(2D + J)\tilde{\tau} - 2J$ is $(2d_{ij} + 1)\tau_j - 2 = 2d_{ij}\tau_j + \tau_j - 2 = -\delta_j + 2d_{ij}\tau_j$. It follows from this observation and (6) that the (i,j)-elements of ΔL and $(2D + J)\tilde{\tau} - 2J$ are equal. This completes the proof. □

Lemma 4. *Let T be a tree with vertex set $\{1, \dots, n\}$, and let D and Δ be the distance matrix and the squared distance matrix of T, respectively. Then $D\delta = \Delta\tau$.*

Proof. Let $i \in \{1, \dots, n\}$ be fixed. We must show that $\sum_{j=1}^{n} d_{ij}\delta_j = \sum_{j=1}^{n} d_{ij}^2(2 - \delta_j)$, or equivalently,

$$2\sum_{j\neq i} d_{ij}^2 = \sum_{j\neq i} d_{ij}\delta_j + \sum_{j\neq i} d_{ij}^2\delta_j. \tag{7}$$

For $j \in \{1, \dots, n\}, j \neq i$, let $\gamma(j)$ denote the immediate predecessor of j on the (i,j)-path in T. Note that $d_{ij} = d_{i\gamma(j)} + 1$. We have

$$\begin{aligned}
2\sum_{j\neq i} d_{ij}^2 &= \sum_{j\neq i} d_{ij}^2 + \sum_{j\neq i} (d_{i\gamma(j)} + 1)^2 \\
&= \sum_{j\neq i} d_{ij}^2 + \sum_{j\neq i} d_{i\gamma(j)}^2 + 2\sum_{j\neq i} d_{i\gamma(j)} + n - 1 \\
&= \sum_{j\neq i} d_{ij}^2 + \sum_{j\neq i} (\delta_j - 1)d_{ij}^2 + 2\sum_{j\neq i} (\delta_j - 1)d_{ij} + n - 1. \qquad (8)
\end{aligned}$$

By Lemma 2, $D\tau = (n - 1)\mathbf{1}$, and hence $\sum_{j\neq i} d_{ij}(2 - \delta_j)d_{ij} = \sum_{j=1}^{n} d_{ij}(2 - \delta_j) = n - 1$. Therefore

$$2\sum_{j\neq i}(\delta_j-1)d_{ij}=\sum_{j\neq i}\delta_j d_{ij}-\sum_{j\neq i}(2-\delta_j)d_{ij}=\sum_{j\neq i}\delta_j d_{ij}-(n-1). \tag{9}$$

Using (8) and (9) we get (7) and the proof is complete. □

2. Inverse of the squared distance matrix

In this section we first consider trees with no vertex of degree 2 and obtain a formula for the inverse of its squared distance matrix. Let cof A denote the sum of the cofactors of the matrix A. The following result will be used.

Theorem 5. *(See [5].) Let T be a tree with vertex set $\{1,\dots,n\}$, with no vertex of degree 2, and let Δ be the squared distance matrix of T. Then*

(i) $\det\Delta=(-1)^n4^{n-2}\prod_{i=1}^n\tau_i\left(2n-1-2\sum_{i=1}^n\frac{1}{\tau_i}\right)$.
(ii) $cof\,\Delta=(-1)^{n-1}2\cdot4^{n-2}\prod_{i=1}^n\tau_i$.

We introduce some further notation in addition to the notation introduced earlier. Let T be a tree with vertex set $\{1,\dots,n\}$, and let the degree of each vertex be different from 2. Then $\tau_i\neq0$, $i=1,\dots,n$. We set $\hat{\tau}$ to be the diagonal matrix with diagonal elements $\frac{1}{\tau_1},\dots,\frac{1}{\tau_n}$. Thus $\hat{\tau}=\tilde{\tau}^{-1}$. We define

$$\nu=\tilde{\tau}\mathbf{1}-L\hat{\tau}\mathbf{1}\text{ and }\beta=\left(2n-1-2\sum_{i=1}^n\frac{1}{\tau_i}\right)^{-1}.$$

Note that for $i=1,\dots,n$;

$$\nu_i=\tau_i+\sum_{s\sim i}\frac{1}{\tau_s}+1-\frac{2}{\tau_i}.$$

Lemma 6. *Let T be a tree with vertex set $\{1,\dots,n\}$ with no vertex of degree 2, and let Δ and L be the squared distance matrix and the Laplacian of T, respectively. Then*

$$\Delta\nu=-\frac{1}{\beta}\mathbf{1}.$$

Proof. We have

$$\begin{aligned}\Delta\nu&=\Delta\tilde{\tau}\mathbf{1}-\Delta L\hat{\tau}\mathbf{1}\\&=\Delta\tilde{\tau}\mathbf{1}-(2D+J)\tilde{\tau}\hat{\tau}\mathbf{1}+2J\hat{\tau}\mathbf{1}\quad\text{by Lemma 3}\\&=\Delta\tilde{\tau}\mathbf{1}-(2D+J)\mathbf{1}+2J\hat{\tau}\mathbf{1}\\&=\Delta\tau-(2D+J)\mathbf{1}+2J\hat{\tau}\mathbf{1}\end{aligned}$$

$$
\begin{aligned}
&= D\delta - 2D\mathbf{1} - n\mathbf{1} + 2\left(\sum_{i=1}^{n}\frac{1}{\tau_i}\right)\mathbf{1} \quad \text{by Lemma 4}\\
&= -D(2\mathbf{1}-\delta) - n\mathbf{1} + 2\left(\sum_{i=1}^{n}\frac{1}{\tau_i}\right)\mathbf{1}\\
&= -D\tau - n\mathbf{1} + 2\left(\sum_{i=1}^{n}\frac{1}{\tau_i}\right)\mathbf{1}\\
&= -(n-1)\mathbf{1} - n\mathbf{1} + 2\left(\sum_{i=1}^{n}\frac{1}{\tau_i}\right)\mathbf{1} \quad \text{by Lemma 2}\\
&= -\left(2n-1-2\sum_{i=1}^{n}\frac{1}{\tau_i}\right)\mathbf{1}\\
&= -\frac{1}{\beta}\mathbf{1},
\end{aligned}
$$

and the proof is complete. □

The following is the main result of this section where we prove a formula for the inverse of the squared distance matrix. Recall that the tree is assumed to have no vertex of degree 2.

Theorem 7. *Let T be a tree with vertex set $\{1,\dots,n\}$ with no vertex of degree 2, and let Δ and L be the squared distance matrix and the Laplacian of T, respectively. Then*

$$\Delta^{-1} = -\frac{1}{4}L\hat{\tau}L - \frac{\beta}{2}\nu\nu'.$$

Proof. Let $X = -\frac{1}{4}L\hat{\tau}L - \frac{\beta}{2}\nu\nu'$. By Lemma 3 and Lemma 6,

$$
\begin{aligned}
\Delta X &= -\frac{1}{4}\Delta L\hat{\tau}L - \frac{\beta}{2}\Delta\nu\nu'\\
&= -\frac{1}{4}((2D+J)\tilde{\tau} - 2J)\hat{\tau}L + \frac{\beta}{2}\frac{1}{\beta}\mathbf{1}\nu'\\
&= -\frac{1}{2}D\tilde{\tau}\hat{\tau}L - \frac{1}{4}J\tilde{\tau}\hat{\tau}L + \frac{1}{2}J\hat{\tau}L + \frac{1}{2}\mathbf{1}\nu'\\
&= -\frac{1}{2}DL + \frac{1}{2}J\hat{\tau}L + \frac{1}{2}\mathbf{1}\nu'. \qquad (10)
\end{aligned}
$$

By Theorem 1(vi), and (10) we have

$$\Delta X = I - \frac{1}{2}\mathbf{1}\tau' + \frac{1}{2}J\hat{\tau}L + \frac{1}{2}\mathbf{1}\nu'. \qquad (11)$$

Since $\nu = \tilde{\tau}\mathbf{1} - L\hat{\tau}\mathbf{1}$, we have

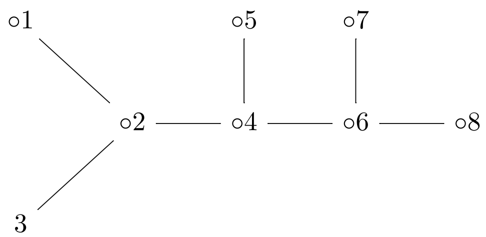
$$\mathbf{1}\nu' = \mathbf{1}\mathbf{1}'\tilde{\tau} - \mathbf{1}\mathbf{1}'\hat{\tau}L = \mathbf{1}\tau' - J\hat{\tau}L. \tag{12}$$

It follows from (11) and (12) that $\Delta X = I$ and the proof is complete. $\square$

The matrix $L\hat{\tau}L$ that appears in Theorem 7 can be described explicitly. The matrix has the form of a "two-step" Laplacian in the sense that its (i, j)-element is nonzero if and only if vertices i and j are at a distance of at most two. The formula is given in the next result. The proof is easy and is omitted.

Lemma 8. *Let T be a tree with vertex set $\{1, \dots, n\}$ with no vertex of degree 2. Let M be the $n \times n$ matrix defined as follows: For $i \neq j$, $m_{ij} = 1 - \frac{1}{\tau_i} - \frac{1}{\tau_j}$ if i and j are adjacent, $m_{ij} = \frac{1}{2\tau_k}$ if i and j are at distance 2 with the common neighbor k, and $m_{ij} = 0$ if $d_{ij} > 2$. Let m_{ii} be defined so that M has row (and column) sums zero, $i = 1, \dots, n$. Then $M = \frac{1}{2}L\hat{\tau}L$.*

Example. Consider the tree



Then it can be verified that

$$M = \begin{pmatrix} 0 & 1 & -1/2 & -1/2 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 3 & -1/2 & -1/2 & 0 & 0 \\ -1/2 & 1 & 0 & -1/2 & 0 & 0 & 0 & 0 \\ -1/2 & 3 & -1/2 & -5 & 1 & 3 & -1/2 & -1/2 \\ 0 & -1/2 & 0 & 1 & 0 & -1/2 & 0 & 0 \\ 0 & -1/2 & 0 & 3 & -1/2 & -4 & 1 & 1 \\ 0 & 0 & 0 & -1/2 & 0 & 1 & 0 & -1/2 \\ 0 & 0 & 0 & -1/2 & 0 & 1 & -1/2 & 0 \end{pmatrix}.$$

In view of Lemma 8, the formula in Theorem 7 takes the form

$$\Delta^{-1} = -\frac{1}{2}M - \frac{\beta}{2}\nu\nu',$$

which is similar to the formula for the inverse of the distance matrix given in Theorem 1.

We now consider trees with precisely one vertex of degree 2. The squared distance matrix of such a tree is nonsingular. We do not have a concise formula, comparable to the one in Theorem 7, for the inverse of the squared distance matrix in this case. However we do obtain an expression for the inverse. Recall the following result about the inverse of a partitioned matrix (see, for example, [1, p. 4]).

Lemma 9. *Let A be an $n \times n$ nonsingular matrix partitioned as*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where A_{11} is square and nonsingular. If $B = A^{-1}$ is compatibly partitioned as

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

then B_{22} is nonsingular and $A_{11}^{-1} = B_{11} - B_{12}B_{22}^{-1}B_{21}$, the Schur complement of B_{22} in B.

Let T be a tree with exactly one vertex degree 2 and let Δ be the squared distance matrix of T. The main idea is to extend T to a tree $\tilde{T}$ with no vertex of degree 2. If $\tilde{\Delta}$ is the squared distance matrix of $\tilde{T}$, then by Lemma 10, Δ^{-1} can be realized as a Schur complement in $\tilde{\Delta}^{-1}$.

We introduce some notation. Let T be a tree with $V(T) = \{1, \dots, n\}$. Let vertex n be the only vertex of T of degree 2, and let $n-1$ and $n-2$ be the neighbors of n. Let $\tilde{T}$ be the tree with $V(\tilde{T}) = \{1, \dots, n+1\}$ obtained by attaching the new vertex $n+1$ to T and making it adjacent to vertex n. Let Δ and $\tilde{\Delta}$ be the squared distance matrices of T and $\tilde{T}$ respectively. We define $\delta, \tau, L, \nu, \beta$ as before, with respect to the tree $\tilde{T}$. Note that

$$\tilde{\Delta} = \begin{pmatrix} \Delta & x \\ x' & 0 \end{pmatrix}$$

for some x. Let $\tilde{\Delta}^{-1}$ be partitioned as

$$\tilde{\Delta}^{-1} = \begin{pmatrix} X & f \\ f' & \alpha \end{pmatrix}.$$

By Lemma 9, $\Delta^{-1} = X - \frac{1}{\alpha} f f'$. Since $\tilde{T}$ has no vertex of degree 2, we have a formula for $\tilde{\Delta}^{-1}$ given by Theorem 7. Thus we have essentially obtained a formula for Δ^{-1}.

We now turn to the edge orientation matrix, defined in [6]. We first recall the definition. Let T be a tree with $V(T) = \{1, \dots, n\}$. We assign an orientation to each edge of T. Let D be the distance matrix of T. Let $e = (ij)$ and $f = (k\ell)$ be edges of T. We say that

e and f are similarly oriented if $d_{ik} = d_{j\ell}$. Otherwise e and f are said to be oppositely oriented.

Definition. The edge orientation matrix of T is the $(n-1) \times (n-1)$ matrix H defined as follows. The rows and the columns of H are indexed by the edges of T. The (e, f)-element of H, denoted $h(e, f)$ is defined to be $1(-1)$ if the corresponding edges of T are similarly (oppositely) oriented. The diagonal elements of H are set to be 1.

We recall the following basic properties of H, proved in [6].

Lemma 10. *Let T be a directed tree on n vertices, let Δ, H and Q be, respectively, the squared distance matrix, the edge orientation matrix and the vertex-edge incidence matrix of T. Then (i) $\det H = 2^{n-2} \prod_{i=1}^{n} \tau_i$ and (ii) $Q'\Delta Q = -2H$.*

In the final result of this section we provide a simple formula for the inverse of the edge orientation matrix, when it exists.

Theorem 11. *Let T be a tree with $V(T) = \{1, \dots, n\}$ and let no vertex of T have degree 2. Then $H^{-1} = \frac{1}{2}Q'\hat{\tau}Q$.*

Proof. Since $\nu = \tilde{\tau}\mathbf{1} - L\hat{\tau}\mathbf{1}$, we have

$$\mathbf{1}'\nu = \mathbf{1}'\tilde{\tau}\mathbf{1} - \mathbf{1}'L\hat{\tau}\mathbf{1} = \sum_{i=1}^{n} \tau_i = 2. \tag{13}$$

By Theorem 7, we get

$$I = -\frac{1}{4}L\hat{\tau}L\Delta - \frac{\beta}{2}\nu\nu'\Delta. \tag{14}$$

Using (13) and Lemma 6, we see that $-\frac{\beta}{2}\nu\nu'\Delta$ is idempotent, and then it follows from (14) that $-\frac{1}{4}L\hat{\tau}L\Delta = I + \frac{\beta}{2}\nu\nu'\Delta$ is idempotent. Thus

$$\left(-\frac{1}{4}L\hat{\tau}L\Delta\right)\left(-\frac{1}{4}L\hat{\tau}L\Delta\right) = -\frac{1}{4}L\hat{\tau}L\Delta,$$

and hence

$$L\hat{\tau}L\Delta L\hat{\tau}L\Delta == -4L\hat{\tau}L\Delta. \tag{15}$$

From (15), after simplification, we get

$$(Q'\hat{\tau}Q)(Q'\Delta Q)(Q'\hat{\tau}Q) = -4Q'\hat{\tau}Q. \tag{16}$$

Since the rank of an idempotent matrix equals its trace, we see by taking the trace of both sides in (14) that the rank of $L\hat{\tau}L\Delta = n - 1$. Since Δ is nonsingular, rank $L\hat{\tau}L = n - 1$. Therefore rank $Q'\hat{\tau}Q \geq$ rank $QQ'\hat{\tau}QQ' =$ rank $L\hat{\tau}L = n - 1$. Thus $Q'\hat{\tau}Q$ is nonsingular. Furthermore, by Lemma 10, $Q'\Delta Q = -2H$. It follows from (16) that $Q'\hat{\tau}QH = 2I$ and the proof is complete. □

3. Inertia

Let A be a symmetric $n \times n$ matrix. Recall that the inertia of A, denoted $In(A)$, is the triple (π, ν, ϵ), where π, ν, ϵ are, respectively, the number of positive, negative and zero eigenvalues of A. In this section we determine the inertia of the squared distance matrix of a tree and the edge orientation matrix of a directed tree.

The next result and its extension given in Lemma 13 are well-known (see [9, pp. 282–284]).

Lemma 12 *(Sylvester's law of inertia). Let A be a symmetric $n \times n$ matrix and let S be a nonsingular $n \times n$ matrix. Then $In(A) = In(S'AS)$.*

Lemma 13. *Let A be a symmetric $n \times n$ matrix and let S be an $n \times m$ matrix. Let $In(A) = (\pi, \nu, \epsilon)$ and let $In(S'AS) = (\pi_1, \nu_1, \epsilon_1)$. Then $\pi \geq \pi_1$ and $\nu \geq \nu_1$.*

The next result is an easy consequence of the Cauchy Interlacing Principle (see [9, p. 242]).

Lemma 14. *Let A be a symmetric $n \times n$ matrix and let B be a principal submatrix of A of order $n - 1$. Let $In(A) = (\pi, \nu, \epsilon)$ and let $In(B) = (\pi_1, \nu_1, \epsilon_1)$. Then $\pi_1 \geq \pi - 1$ and $\nu_1 \geq \nu - 1$.*

We denote the column space of the matrix A by $\mathcal{C}(A)$. The next result, and its generalization given in Lemma 16, are well-known, see [4,11].

Lemma 15. *Let A be a symmetric $n \times n$ matrix partitioned as*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where A_{11} is square and nonsingular. Then

$$In(A) = In(A_{11}) + In(A_{22} - A_{21}A_{11}^{-1}A_{12}).$$

Lemma 16. *Let A be a symmetric $n \times n$ matrix partitioned as*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where A_{11} is square. Let $\mathcal{C}(A_{12}) \subset \mathcal{C}(A_{11})$ and $\mathcal{C}(A'_{21}) \subset \mathcal{C}(A_{11})$. Then $A_{21}A_{11}^{-}A_{12}$ is invariant with respect to the generalized inverse A_{11}^{-} of A, and furthermore,

$$In(A) = In(A_{11}) + In(A_{22} - A_{21}A_{11}^{-}A_{12}).$$

Lemma 17. *Let T be a tree and let v be a vertex of degree 2 in T. Let s and t be the neighbors of v in T. Replace column s of Δ by the sum of the columns s and t minus twice the column v. Then in the resulting matrix the column s is $(2, 2, \ldots, 2)'$.*

The following result is an immediate consequence of Lemma 17.

Lemma 18. *Let T be a tree and let v be a vertex of degree 2 in T. Let s and t be the neighbors of v in T. Let z be the vertex indexed by $V(T)$ with $z_s = z_t = -1$, $z_v = 2$ and all the remaining coordinates equal to zero. Then $\Delta z = 2\mathbf{1}$.*

Lemma 19. *Let T be a tree with vertex set $\{1, \ldots, n\}$ and let Δ be the squared distance matrix of T. Then the following assertions hold:*

(i) If T has no vertex of degree 2, then $\mathbf{1}'\Delta^{-1}\mathbf{1} < 0$.
(ii) If T has precisely one vertex of degree 2, then $\mathbf{1}'\Delta^{-1}\mathbf{1} = 0$.

Proof. (i). Since T has no vertex of degree 2, $\tau_i \neq 0$, $i = 1, \ldots, n$. By (i), Theorem 5,

$$\det \Delta = (-1)^n 4^{n-2} \prod_{i=1}^{n} \tau_i \left(2n - 1 - 2\sum_{i=1}^{n} \frac{1}{\tau_i}\right). \tag{17}$$

Let cof A denote the sum of the cofactors of the matrix A. By (ii), Theorem 5,

$$\text{cof } \Delta = (-1)^{n-1} 2 \cdot 4^{n-2} \prod_{i=1}^{n} \tau_i. \tag{18}$$

It follows from (17) and (18) that

$$\mathbf{1}'\Delta^{-1}\mathbf{1} = \frac{\text{cof } \Delta}{\det \Delta} = -2\left(2n - 1 - 2\sum_{i=1}^{n} \frac{1}{\tau_i}\right)^{-1}. \tag{19}$$

The result is clear when $n = 2$, so we assume $n \geq 3$. If T has $p \geq 2$ pendant vertices, then $\sum_{i=1}^{n} \frac{1}{\tau_i} = p - \alpha$ for some $\alpha > 0$. Then

$$2n - 1 - 2\sum_{i=1}^{n} \frac{1}{\tau_i} = 2n - 1 - 2(p - \alpha) = 2(n - p) + 2\alpha - 1 > 0,$$

since $2(n - p) \geq 1$. It follows from (19) that $\mathbf{1}'\Delta^{-1}\mathbf{1} < 0$.

(ii). Let v be the vertex of degree 2 in T and let s and t be the neighbors of v in T. Let z be the vertex indexed by $V(T)$ with $z_s = z_t = -1$, $z_v = 2$ and all the remaining coordinates equal to zero. By Lemma 18, $\Delta^{-1}\mathbf{1} = \frac{1}{2}z$. Thus $\mathbf{1}'\Delta^{-1}\mathbf{1} = \frac{1}{2}\mathbf{1}'z = 0$. $\square$

Theorem 20. *Let T be a tree with $n \geq 3$ vertices, p pendant vertices and q vertices of degree 2. Let Δ be the squared distance matrix of T. Then $In(\Delta)$ equals $(n-p, p, 0)$ if $q = 0$ and $(n-p-q+1, p, q-1)$ if $q \geq 1$.*

Proof. We induct on the number of vertices, with the case when T has 3 vertices being clear. Let w be a vertex of T adjacent to t pendant vertices in T where $t \geq 1$. Thus the degree of w is $t+1$, where w is adjacent to vertex u apart from the t pendant vertices. Without loss of generality, assume that the t pendant vertices are the vertices $1, 2, \dots, t$.

For $1 \leq i \leq t$, perform the following operations on Δ: replace row i by the sum of row i and row u minus twice the row w and similarly, replace column i by the sum of column i and column u minus twice the column w. By a repeated application of Lemma 17 with respect to the rows as well as the columns, we see that we obtain the matrix

$$\hat{\Delta} = \left[\begin{array}{c|c} 4(J-I) & 2J \\ \hline 2J & \Delta_1 \end{array}\right],$$

where Δ_1 is the squared distance matrix corresponding to the tree $\tilde{T} = T - \{1, 2, \dots, t\}$, the top left $X = 4(J-I)$ matrix is of order $t \times t$, and J denotes the matrix of all ones of the appropriate size. Note that $\hat{\Delta}$ is obtained from Δ by a sequence of elementary row operations, and the same sequence of elementary column operations. Thus $\hat{\Delta} = S'AS$ for a nonsingular matrix S and it follows by Lemma 12 that Δ and $\hat{\Delta}$ have the same inertia. We consider cases.

Case (i). $t = 1$ and T_1 has no vertex of degree 2. Then

$$\hat{\Delta} = \left[\begin{array}{c|c} 0 & 2\mathbf{1}' \\ \hline 2\mathbf{1} & \Delta_1 \end{array}\right].$$

By Lemma 15,

$$In(\hat{\Delta}) = In(\Delta_1) + In(-4(\mathbf{1}'{\Delta_1}^{-1}\mathbf{1})). \tag{20}$$

The tree T_1 has p pendant vertices and no vertices of degree 2. Therefore by the induction assumption, Δ_1 has p negative and $n-p-1$ positive eigenvalues. By Lemma 19, $\mathbf{1}'{\Delta_1}^{-1}\mathbf{1} < 0$. It follows from (20) that $\hat{\Delta}$ has p negative and $n-p$ positive eigenvalues, completing the proof in this case.

Case (ii). $t > 1$ and T_1 has precisely one vertex of degree 2. Then using the notation introduced earlier

$$\hat{\Delta} = \left[\begin{array}{c|c} 4(J-I) & 2J \\ \hline 2J & \Delta_1 \end{array}\right].$$

Note that Δ_1 is nonsingular and by Lemma 19, $\mathbf{1}'{\Delta_1}^{-1}\mathbf{1} = 0$. By Lemma 15,

$$In(\hat{\Delta}) = In(\Delta_1) + In(4(J-I)). \tag{21}$$

The tree T_1 has $n-t$ vertices of which $p-t+1$ are pendant vertices and 1 vertex is of degree 2. Therefore by the induction assumption, Δ_1 has $p-t+1$ negative and $n-p-1$ positive eigenvalues. Clearly, $J-I$ has $t-1$ negative and 1 positive eigenvalues. It follows from (21) that $\hat{\Delta}$ has p negative and $n-p$ positive eigenvalues, completing the proof in this case.

Case (iii). $t = 1$ and T_1 has $r > 1$ vertices of degree 2. Then

$$\hat{\Delta} = \left[\begin{array}{c|c} 0 & 2\mathbf{1}' \\ \hline 2\mathbf{1} & \Delta_1 \end{array}\right].$$

In this case, Δ_1 is singular. By Lemma 18, $\mathbf{1} \in \mathcal{C}(\Delta_1)$ and for any generalized inverse Δ_1^-,

$$\begin{aligned} 4\mathbf{1}'\Delta_1^-\mathbf{1} &= z'\Delta_1\Delta_1^-\Delta_1 z \\ &= z'\Delta_1 z \\ &= \begin{pmatrix} -1 & 2 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 2 \\ -1 \end{pmatrix} \\ &= 0. \end{aligned} \tag{22}$$

It follows from Lemma 16 and (22) that

$$In(\hat{\Delta}) = In(\Delta_1) + In(0). \tag{23}$$

The tree T_1 has $n-1$ vertices of which p are pendant vertices and r vertices are of degree 2. Therefore by the induction assumption, Δ_1 has p negative and $r-1$ zero eigenvalues. It follows from (23) that $\hat{\Delta}$ has p negative and r zero eigenvalues. Since T has $r+1$ vertices of degree 2, the proof is complete in this case.

Case (iv). $t > 1$ and T_1 has $r > 1$ vertices of degree 2. The proof in this case is similar to the one in *Case (ii)* and is omitted. This completes the proof. □

Lemma 21. *Let T be a directed tree on n vertices and let H be the edge orientation matrix of T. If T has q vertices of degree 2, then rank $H = n-1-q$.*

Proof. If $q = 0$, then by Lemma 10(i), H is nonsingular and the result is proved. Therefore we assume $q \geq 1$. We prove the result by induction on n, with the case $n = 2$ being easy. So let $n \geq 3$. Let v be a vertex of degree 2 in T and let s and t be the neighbors of v in T. Let $e = (sv)$, $f = (vt)$ be the edges of T, which we assume to be similarly oriented, without loss of generality. Then the columns of H indexed by e and f are identical. Let z be the vector indexed by $E(T)$ with $z_e = -z_f = 1$ and with the other coordinates of z being zero. Then $Hz = 0$. Each degree 2 vertex thus gives rise to a null vector of H and these vectors must necessarily be independent. Thus H has at least q zero eigenvalues and hence rank $H \leq n - 1 - q$. Let T_1 be the tree obtained from T by removing vertex v and replacing edges e and f by the single edge (st). Let H_1 be the edge orientation matrix of H. Then H_1 is a principal submatrix of H. Since T_1 has $q-1$ degree 2 vertices, by the induction assumption rank $H_1 = n - 2 - (q - 1) = n - 1 - q$. Since rank $H \geq \operatorname{rank} H_1 = n - 1 - q$, it follows that rank $H = n - 1 - q$ and the proof is complete. □

Theorem 22. *Let T be a directed tree with n vertices, p pendant vertices and q vertices of degree 2. Let H be the edge orientation matrix of T. Then $In(H)$ equals $(p - 1, n - p, 0)$ if $q = 0$ and $(p - 1, n - p - q, q)$ if $q \geq 1$.*

Proof. First let $q = 0$. By Theorem 20, $In(\Delta) = (n - p, p, 0)$. By Lemma 10, H is nonsingular and hence $In(H) = (r, n - 1 - r, 0)$ for some $r \geq 0$. By Lemma 10(ii) and Lemma 13, $r \leq p$ and $n - 1 - r \leq n - p$. Thus $In(H)$ equals either $(p, n - p - 1, 0)$ or $(p - 1, n - p, 0)$. By Lemma 10(i), the determinant of H has the same sign as $(-1)^{n-p}$ and hence $In(H) = (p - 1, n - p, 0)$.

Now let $q \geq 1$. By Theorem 20, $In(\Delta) = (n-p-q+1, p, q-1)$. By Lemma 21, H has q zero eigenvalues and hence $In(H) = (r, n-1-r-q, q)$ for some $r \geq 0$. By the induction assumption, $In(H_1) = (p - 1, n - p - q, q - 1)$ and hence by Lemma 14, $r \geq p - 1$ and $n-1-r-q \geq n-p-q$. It follows that $r = p-1$ and hence $In(H) = (p-1, n-p-q, q)$. This completes the proof. □

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