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PRODUCT DISTANCE MATRIX OF A GRAPH AND SQUARED DISTANCE MATRIX OF A TREE

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Let G be a strongly connected, weighted directed graph. We define a product distance $\eta(i, j)$ for pairs i, j of vertices and form the corresponding product distance matrix. We obtain a formula for the determinant and the inverse of the product distance matrix. The edge orientation matrix of a directed tree is defined and a formula for its determinant and its inverse, when it exists, is obtained. A formula for the determinant of the (entry-wise) squared distance matrix of a tree is proved.

1. INTRODUCTION

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 $d(i, j)$, is defined to be the minimum length (the number of edges) of a path from i to j (or an ij-path). 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 $d(i, j)$ if $i \neq j$.

According to a well-known result due to Graham and Pollak [**7**], 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 [**6**]. These two results have generated considerable interest and a plethora of extensions and generalizations have been proved (see, for example, [**1–4**, **10**] and the references contained therein). Here we describe an early generalization due to Graham, Hoffman and Hosoya [**5**].

The set up of [**5**] is quite general and considers weighted, directed graphs. Let G be a directed graph with vertex set $V(G) = \{1, \ldots, n\}$. We assume G to be

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strongly connected. The weight of a directed path is defined to be the sum of the weights of the edges on the path and the distance $d(i,j)$ between two vertices i and j is the minimum weight of a directed path between i and j. The distance matrix of G is then defined as the $n \times n$ matrix D with its (i,j)-element equal to $d(i,j)$. Note that the distance matrix is not necessarily symmetric. Recall that a block of G is defined to be a maximal subgraph with no cut-vertices. For the purpose of defining blocks we consider the underlying undirected graph obtained from G. Let $B_1, \dots, B_p$ be the blocks of G. It was shown in [**5**] that the determinant of $D(G)$ depends only on the determinants of $D(B_1), \dots, D(B_p)$ but not in the manner in which the blocks are assembled. If A is a square matrix then $\operatorname{cof} A$ will denote the sum of the cofactors of A.

Theorem 1 (Graham, Hoffman, Hosoya)**.** *Let G be a directed, weighted, strongly connected graph and let $B_1, \dots, B_p$ be the blocks of G. Then*

(i) $\operatorname{cof} D(G) = \prod_{i=1}^{p} \operatorname{cof} D(B_i)$

(ii) $\det D(G) = \sum_{i=1}^{p} \det D(B_i) \prod_{j \neq i} \operatorname{cof} D(B_j)$.

If G is an undirected graph, then we may replace each edge of G by a pair of directed edges in each direction and get a directed graph. Theorem 1, applied to the directed graph, in fact gives a statement about the original undirected graph. Thus the formula for the determinant of the distance matrix of a tree can be obtained from (ii) of Theorem 1.

Let T be a tree with vertex set $\{1, \dots, n\}$. The exponential distance matrix of T is defined to be the $n \times n$ matrix E with (i,j)-element $q^{d(i,j)}$, where q is a parameter. It was shown in [**3**] that the determinant of E is $(1-q^2)^{n-1}$, which again is a function only of the number of vertices. The result was generalized to directed trees in [**4**] as follows. Replace each edge of T by a pair of directed edges in either direction. For each edge e in T, let the corresponding directed edges be assigned weights q_e, t_e. Define the product distance between vertices $i \neq j$ to be the product of the weights of the edges of the unique directed path from i to j. The product distance between a vertex to itself is defined to be 1. The product distance matrix E of T is the $n \times n$ matrix with its (i,j)-element equal to the product distance between i and j. With this notation we state the following result from [**4**].

Theorem 2. *Let T be a tree with vertex set $\{1, \dots, n\}$ and let E be the product distance matrix of T. Then* $\det E = \prod_{i=1}^{n-1} (1 - q_i t_i)$.

In this paper we extend Theorem 2 to arbitrary graphs in the spirit of Theorem 1. Thus we consider a product distance, to be precisely defined in the next section, on arbitrary graphs and obtain a formula for the determinant of the product distance matrix of the graph in terms of the determinants of the corresponding matrices of the blocks. It turns out that we also have a formula for the inverse, when it exists, of the product distance matrix. These results are obtained in the next section. In Section 3 we define the edge orientation matrix of a directed tree and obtain a formula for its determinant and inverse using the results on the product distance matrix.

In the final section we consider the entry-wise square of the distance matrix of a tree, which we refer to as the squared distance matrix of a tree. Using the results in Section 3, we obtain a formula for the determinant of the squared distance matrix as well as a formula for the sum of its cofactors. Both the determinant and the sum of cofactors turn out be functions of the degree sequence of the tree.

2. PRODUCT DISTANCE

Let G be a directed graph with vertex set $V(G) = \{1, \ldots, n\}$. We assume G to be strongly connected. Recall that a block of G is defined to be a maximal subgraph with no cut-vertices. For the purpose of defining blocks we consider the underlying undirected graph obtained from G.

Definition. *A product distance on G is a function $\eta : V(G) \times V(G) \to (-\infty, \infty)$ satisfying the following properties:*

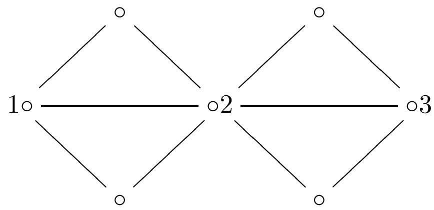
(i) $\eta(i, i) = 1, i = 1, \ldots, n.$

(ii) *If $i, j \in V(G)$ are vertices such that each directed path from i to j passes through the cut-vertex k, then $\eta(i, j) = \eta(i, k)\eta(k, j)$.*

Recall that a graph G is called a block graph if each block of G is a complete graph (a clique). We may construct a product distance on a block graph G as follows. We set $\eta(i, i) = 1, i = 1, \ldots, n$. If i, j belong to the same block, then $\eta(i, j)$ is set equal to any real number. If i, j are in different blocks of G, then there exists an ij-path, $i - k_1 - k_2 - \cdots - k_r - j$, where $k_1, \ldots, k_r$ (and possibly i, j as well) are cut-vertices. We set $\eta(i, j)$ to be the product $\eta(i, k_1)\eta(k_1, k_2) \cdots \eta(k_{r-1}, k_r)\eta(k_r, j)$.

Another way in which a product distance might arise is the following. Let G be a directed, strongly connected graph, which is not necessarily a block graph. We assume that each edge of G is assigned a positive weight. We set $\eta(i, i) = 1, i = 1, \ldots, n$. If e is an edge from i to j, then $\eta(i, j)$ is set equal to the weight of e. In general, for vertices i, j, set $\eta(i, j)$ equal to the minimum weight of a directed ij-path, where the weight of a path is defined to be the product of the weights of the edges in the path. It can be verified that this distance is a product distance in that it satisfies (i),(ii) in the definition.

We remark that it is important to have the weights as positive numbers in the preceding construction. Consider, for example, the following graph, with each edge carrying weight -1. Then $\eta(1, 2) = -1, \eta(2, 3) = -1$, whereas $\eta(1, 3) = -1$ and (ii) in the definition of product distance is violated.



Let G be a directed graph with $V(G) = \{1, \ldots, n\}$. Given a product distance η on G, the product distance matrix of G is the $n \times n$ matrix $E = ((e_{ij}))$, with rows and columns indexed by $V(G)$, and with $e_{ij} = \eta(i, j)$ for all i, j. We emphasize that the matrix E depends on the product distance function $\eta(i, j)$, though we suppress η in the notation and denote the matrix as E rather than E_η. The distance function will be clear from the context.

If G is an undirected graph, we may replace each edge by a pair of directed edges, oriented in either direction and obtain a directed graph, which we denote by $\tilde{G}$. A product distance may then be defined on $\tilde{G}$. If the product distance η on $\tilde{G}$ is symmetric, that is, if it satisfies $\eta(i, j) = \eta(j, i)$ for all i, j, then we may ignore the directed graph and work with G instead.

We show that the determinant of the product distance matrix equals the product of the determinants of the product distance matrices of the blocks in the graph. We first prove a preliminary result.

Lemma 3. *Let A be an $n \times n$ matrix with $a_{ii} = 1, i = 1, \ldots, n$. Let $j \in \{1, \ldots, n\}$ be fixed. For each $i \in \{1, \ldots, n\}, i \neq j$, subtract a_{ji} times the j-th column from the i-th column. From the resulting matrix, delete row j and column j and let B be the matrix obtained. Then* $\det A = \det B$.

Proof. Let C be the matrix obtained from A after subtracting a_{ji} times the j-th column from the i-th column, $i \in \{1, \ldots, n\}, i \neq j$. Clearly, $\det A = \det C$. Note that the j-th row of C is $(0, \ldots, 0, 1, 0, \ldots, 0)$, where the 1 occurs at the j-th place. Expanding $\det C$ along the j-th row we see that $\det C = \det B$ and the proof is complete.

Theorem 4. *Let G be a strongly connected, directed graph with $V(G) = \{1, \ldots, n\}$ and let $B_1, \ldots, B_p$ be the blocks of G. Let η be a product distance on G. Let E be the product distance matrix of G and let E_i be the product distance matrix of $B_i, i = 1, \ldots, p$. Then*

$$\det E = \prod_{i=1}^{p} \det E_i.$$

Proof. We prove the result by induction on p, the number of blocks of G. The base case when $p = 1$ is trivial and so we assume $p > 1$. Every such graph has a leaf block, which is a block with exactly one cut-vertex. Let B_k be a leaf block. We assume the unique cut-vertex of B_k to be 1, without loss of generality. Let

$H = G \setminus (B_k \setminus \{1\})$. We reorder the rows and the columns of E so that 1 appears first, followed by the vertices of H in any order, followed by the vertices of $B_k \setminus \{1\}$ in any order. We assume that B_k has s vertices. Let E_H be the distance matrix of H and let

$$E_H = \begin{bmatrix} 1 & a_2 & \cdots & a_t \\ b_2 & & & \\ \vdots & & P & \\ b_t & & & \end{bmatrix} \text{ and } E_k = \begin{bmatrix} 1 & f_2 & \cdots & f_s \\ g_2 & & & \\ \vdots & & Q & \\ g_s & & & \end{bmatrix}.$$

Then

$$E = \left[\begin{array}{c|ccc|ccc} 1 & a_2 & \cdots & a_t & f_2 & \cdots & f_s \\ \hline b_2 & & & & b_2 f_2 & \cdots & b_2 f_s \\ \vdots & & P & & \vdots & \ddots & \vdots \\ b_t & & & & b_t f_2 & \cdots & b_t f_s \\ \hline g_2 & g_2 a_2 & \cdots & g_2 a_t & & & \\ \vdots & \vdots & \ddots & \vdots & & Q & \\ g_s & g_s a_2 & \cdots & g_s a_t & & & \end{array}\right].$$

For each $r \in B_k \setminus \{1\}$, subtract $d(1,r)$ times the first column of E from the r-th column. The resulting matrix has the form

$$\overline{E} = \left[\begin{array}{c|ccc|ccc} 1 & a_2 & \cdots & a_t & 0 & \cdots & 0 \\ \hline b_2 & & & & 0 & \cdots & 0 \\ \vdots & & P & & \vdots & \ddots & \vdots \\ b_t & & & & 0 & \cdots & 0 \\ \hline g_2 & g_2 a_2 & \cdots & g_2 a_t & & & \\ \vdots & \vdots & \ddots & \vdots & & \overline{Q} & \\ g_s & g_s a_2 & \cdots & g_s a_t & & & \end{array}\right].$$

Then

$$\det E = \det \overline{E} = (\det E_H)(\det \overline{Q}). \tag{1}$$

By Lemma 3, $\det \overline{Q} = \det E_k$, while by the induction assumption,

$$\det E_H = \prod_{i \neq k} \det E_i.$$

Substituting in (1) the result is proved. □

Our next objective is to obtain a formula for the inverse of the product distance matrix, when it is nonsingular, in terms of the inverses of the product distance matrices of the blocks.

Lemma 5. *Let A and B be matrices of order $m \times m$ and $n \times n$ respectively. Let $x, y \in \mathrm{Re}^m, u, v \in \mathrm{Re}^n$. Assuming that all inverses exist,*

$$\begin{bmatrix} 1 & x' \\ y & A \end{bmatrix}^{-1} = \begin{bmatrix} \alpha & -x'(A-yx')^{-1} \\ -\alpha A^{-1}y & (A-yx')^{-1} \end{bmatrix}, \tag{2}$$

$$\begin{bmatrix} 1 & u' \\ v & B \end{bmatrix}^{-1} = \begin{bmatrix} \beta & -\beta u'B^{-1} \\ -\beta B^{-1}v & B^{-1}+\beta B^{-1}vu'B^{-1} \end{bmatrix} \tag{3}$$

and

$$\begin{bmatrix} 1 & x' & u' \\ y & A & yu' \\ v & vx' & B \end{bmatrix}^{-1} = \begin{bmatrix} \alpha+\beta(u'B^{-1}v) & -x'(A-yx')^{-1} & -\beta u'B^{-1} \\ -\alpha A^{-1}y & (A-yx')^{-1} & 0 \\ -\beta B^{-1}v & 0 & B^{-1}+\beta B^{-1}vu'B^{-1} \end{bmatrix}, \tag{4}$$

where $\alpha = (1 - x'A^{-1}y)^{-1}$ and $\beta = (1 - u'B^{-1}v)^{-1}$.

Proof. A simple verification shows that

$$\begin{bmatrix} 1 & x' \\ y & A \end{bmatrix} \begin{bmatrix} \alpha & -x'(A-yx')^{-1} \\ -\alpha A^{-1}y & (A-yx')^{-1} \end{bmatrix}$$

equals the identity matrix and thus (2) is proved. The proofs of (3) and (4) are similar.

Theorem 6. *Let G be a strongly connected, directed graph with $V(G) = \{1, \ldots, n\}$ and let $B_1, \ldots, B_p$ be the blocks of G. Let η be a product distance on G. Let E be the product distance matrix of G and let E_i be the product distance matrix of $B_i, i = 1, \ldots, p$. Let E_i be nonsingular and let $N_i = E_i^{-1}, i = 1, \ldots, p$. Let M_i be the $n \times n$ matrix obtained by augmenting N_i with zero rows and columns corresponding to indices in $V(G) \setminus V(B_i), i = 1, \ldots, p$. Let R be the $n \times n$ diagonal matrix with its (i, i)-entry equal to $\delta_i - 1$ if i is contained in δ_i blocks. Then E is nonsingular and $E^{-1} = \sum_{i=1}^{p} M_i - R$.*

Proof. We set up the notation as in the proof of Theorem 4. The details are repeated here for convenience. We prove the result by induction on p, the number of blocks of G. The base case when $p = 1$ is trivial and so we assume $p > 1$. Every such graph has a leaf block, which is a block with exactly one cut-vertex. Let B_k be a leaf block. We assume the unique cut-vertex of B_k to be 1, without loss of generality. Let $H = G \setminus (B_k \setminus \{1\})$. We reorder the rows and the columns of E so that 1 appears first, followed by the vertices of H in any order, followed by the vertices of $B_k \setminus \{1\}$ in any order. We assume that B_k has s vertices. Let E_H be the distance matrix of H and let

$$E_H = \begin{bmatrix} 1 & a_2 & \cdots & a_t \\ b_2 & & & \\ \vdots & & P & \\ b_t & & & \end{bmatrix} \text{ and } E_k = \begin{bmatrix} 1 & f_2 & \cdots & f_s \\ g_2 & & & \\ \vdots & & Q & \\ g_s & & & \end{bmatrix}.$$

Then

$$E = \left[\begin{array}{c|ccc|ccc} 1 & a_2 & \cdots & a_t & f_2 & \cdots & f_s \\ \hline b_2 & & & & b_2 f_2 & \cdots & b_2 f_s \\ \vdots & & P & & \vdots & \ddots & \vdots \\ b_t & & & & b_t f_2 & \cdots & b_t f_s \\ \hline g_2 & g_2 a_2 & \cdots & g_2 a_t & & & \\ \vdots & \vdots & \ddots & \vdots & & Q & \\ g_s & g_s a_2 & \cdots & g_s a_t & & & \end{array}\right].$$

Let $\overline{R}$ be the matrix which is the same as R except that the $(1,1)$-element of $\overline{R}$ is $\delta_1 - 2$. By the induction assumption E_H is nonsingular and

$$\left[\begin{array}{cc} E_H^{-1} & 0 \\ 0 & 0 \end{array}\right] = \sum_{i \neq k} M_i - \overline{R}, \tag{5}$$

where the matrix on the left side of (5) is $n \times n$. We assume the matrix Q to be nonsingular. This will be true by perturbing the entries if necessary. The final result is then true without this assumption by a continuity argument. Let $f = (f_2, \ldots, f_s)', g = (g_2, \ldots, g_s)'$ and let $\beta = (1 - f'Q^{-1}g)^{-1}$. If we apply Lemma 5 to get a formula for E^{-1} and E_H^{-1}, then we see that
(6)

$$E^{-1} - \left[\begin{array}{cc} E_H^{-1} & 0 \\ 0 & 0 \end{array}\right] = \left[\begin{array}{c|ccc|c} \beta(f'Q^{-1}g) & 0 & \cdots & 0 & -\beta f'Q^{-1} \\ \hline 0 & & & & 0 \\ \vdots & & 0 & & \vdots \\ 0 & & & & 0 \\ \hline -\beta Q^{-1}g & 0 & \cdots & 0 & Q^{-1} + \beta Q^{-1}gf'Q^{-1} \end{array}\right].$$

Note that

$$M_k = \left[\begin{array}{c|ccc|c} \beta & 0 & \cdots & 0 & -\beta f'Q^{-1} \\ \hline 0 & & & & 0 \\ \vdots & & 0 & & \vdots \\ 0 & & & & 0 \\ \hline -\beta Q^{-1}g & 0 & \cdots & 0 & Q^{-1} + \beta Q^{-1}gf'Q^{-1} \end{array}\right]. \tag{7}$$

From (6), (7) we see that

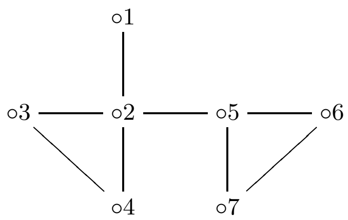
$$E^{-1} - \left[\begin{array}{cc} E_H^{-1} & 0 \\ 0 & 0 \end{array}\right] - M_k = \left[\begin{array}{cccc} -1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{array}\right] = \overline{R} - R. \tag{8}$$

Using (5), (8) we see that

$$E^{-1} = \sum_{i=1}^{p} M_i - R$$

and the proof is complete.

Example. Consider the graph G as shown. We make G into a directed graph by replacing each edge by two edges in either direction.



Let B_1, B_2, B_3, B_4 be the blocks with $V(B_1) = \{1, 2\}, V(B_2) = \{2, 3, 4\}, V(B_3) = \{2, 5\}$, $V(B_4) = \{5, 6, 7\}$. Let the distance matrices of the blocks be given by

$$E_1 = \begin{bmatrix} 1 & -2 \\ -3 & 1 \end{bmatrix}, E_2 = \begin{bmatrix} 1 & 3 & 4 \\ 2 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}, E_3 = \begin{bmatrix} 1 & 2 \\ 1 & 1 \end{bmatrix}, E_4 = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \\ 2 & 3 & 1 \end{bmatrix}.$$

Then the distance matrix of the corresponding product distance is seen to be

$$E = \begin{bmatrix} 1 & -2 & -6 & -8 & -4 & -8 & -12 \\ -3 & 1 & 3 & 4 & 2 & 4 & 6 \\ -6 & 2 & 1 & 1 & 4 & 8 & 12 \\ -3 & 1 & 0 & 1 & 2 & 4 & 6 \\ -3 & 1 & 3 & 4 & 1 & 2 & 3 \\ -3 & 1 & 3 & 4 & 1 & 1 & 1 \\ -6 & 2 & 6 & 8 & 2 & 3 & 1 \end{bmatrix}.$$

For example, the distance $d(1, 6)$ is given by the product $d(1, 2)d(2, 5)d(5, 6)$, which is $(-2)(2)(2) = -8$. We have

$$M_1 = \begin{bmatrix} -1/5 & -2/5 & 0 & 0 & 0 & 0 & 0 \\ -3/5 & -1/5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/6 & 1/2 & 1/6 & 0 & 0 & 0 \\ 0 & 1/6 & 1/2 & -7/6 & 0 & 0 & 0 \\ 0 & 1/6 & -1/2 & 5/6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, M_4 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2/3 & 7/3 & -1/3 \\ 0 & 0 & 0 & 0 & 1/3 & -5/3 & 2/3 \\ 0 & 0 & 0 & 0 & 1/3 & 1/3 & -1/3 \end{bmatrix}.$$

Finally, R is given by

$$R = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

We leave it to the reader to verify that $E^{-1} = M_1 + M_2 + M_3 + M_4 - R$, thereby verifying Theorem 6.

3. EDGE ORIENTATION MATRIX OF A TREE

Let T be a tree with $V(T) = \{1, \dots, n\}$. We assign an orientation to each edge of T. The distance between $i, j \in V(T)$ is defined to be the length (that is, the number of edges, ignoring direction) on the unique (undirected) ij-path. We set $d(i,i) = 0, i = 1, \dots, n$. Let D be the distance matrix of T. Thus the rows and the columns of D are indexed by $V(G)$, and for $i, j \in V(T)$, the (i,j)-element of D is $d(i,j)$. Let $e = (ij)$ and $f = (k\ell)$ be edges of T. We say that e and f are similarly oriented if $d(i,k) = d(j,\ell)$. 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.

Let Q be the directed vertex-edge incidence matrix of T. The rows and the columns of Q are indexed by $V(T)$ and $E(T)$ respectively. If $i \in V(G), e \in E(G)$, then the (i,e)-element of Q is 1 if i is the tail of e, -1, if i is the head of e, and 0 if i and e are not incident. Recall that $L = QQ'$ is the Laplacian of T.

We may define a weighted analogue of H when the tree has weights on the edges. Results analogous to those obtained in the section can be proved for the weighted version. However for simplicity, we consider the unweighted case.

Let T be a directed tree and let G be the line graph of T. Thus the vertex set of G is $V(G) = E(T)$. Two vertices of G are adjacent if the corresponding undirected edges of T have a vertex in common. Let $e = (ij)$ and $f = (k\ell)$ be edges of T, also viewed as vertices of G. With each edge of G we associate a weight as follows. If e and f are adjacent in G, then the corresponding edge joining e and f is assigned weight $1(-1)$ if e and f are similarly (oppositely) oriented. Let η be the product distance on G, which is well-defined since G is a block graph. (See the discussion in Section 2, following the definition of product distance.) Let $E = ((\eta(e,f)))$ be the product distance matrix of G. With these definitions we have the following.

Lemma 7. *Let T be a directed tree and let G be the line graph of T. Let H be the edge orientation matrix of T. Then $H = E$, the product distance matrix of G.*

Proof. Note that if e and f are adjacent in G, then the corresponding entry $h(e,f) = \eta(e,f)$ in view of the definition of H. If e and f are not adjacent, then there exists a path joining e and f in G. Let the shortest such path be $e = e_1, e_2, \ldots, e_k = f$. We prove the result by induction on the length of the path. The result is true when the length is 1. Assume the result to be true for paths of length less than $k-1$ and proceed by induction. Thus $\eta(e,f) = \eta(e_1,e_2)\eta(e_2,e_3)\cdots\eta(e_{k-1},e_k) = \eta(e_1,e_2)\eta(e_2,e_k)$, and by the induction assumption, this product equals $\eta(e_1,e_2)h(e_2,e_k) = \eta(e,e_2)h(e_2,f)$. First suppose that e and e_2 are similarly oriented. Then $\eta(e,e_2) = 1$. If e_2 and f are similarly oriented as well, then $h(e_2,f) = h(e,f) = 1$ and hence $\eta(e,f) = h(e,f)$. If e_2 and f are oppositely oriented, then $h(e_2,f) = h(e,f) = -1$ and again $\eta(e,f) = h(e,f)$. The case when e and e_2 are oppositely oriented is similar and the proof is complete.

Lemma 8. *Let S_t be the star on $t+1$ vertices. Let each edge of S_t be oriented and let X be the edge orientation matrix. Then* $\det X = 2^{t-1}(2-t)$.

Proof. Note that if we reverse the orientation of an edge, then the corresponding row and column of X both get multiplied by -1 and $\det X$ does not change. Thus we may assume that all the edges in S_t are oriented away from the center. Then

$$X = \begin{bmatrix} 1 & -1 & \cdots & -1 \\ -1 & 1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & 1 \end{bmatrix}.$$

The eigenvalues are: $2-t$ with multiplicity 1 and 2 with multiplicity $t-1$. Hence $\det X = 2^{t-1}(2-t)$ and the proof is complete.

Theorem 9. *Let T be a directed tree with $V(T) = \{1, \ldots, n\}$ and let H be the edge orientation matrix of T. Let $k_1, k_2, \ldots, k_n$ be the degree sequence of T. Then*

$$\det H = 2^{n-2} \prod_{i=1}^{n} (2-k_i). \tag{9}$$

Proof. We assume, without loss of generality, that vertices $1, \ldots, p$ are non-pendant vertices and that vertices $p+1, \ldots, n$ are pendant. Let G be the line graph of T and orient the edges of G as described earlier. As noted in Lemma 7, H is the product distance matrix of G. The blocks of G correspond to the stars in T and thus the blocks of G are the complete graphs with $k_1, \ldots, k_p$ vertices. From Theorem 4 and Lemma 8 it follows that

$$\det H = \prod_{i=1}^{p} 2^{k_i-1}(2-k_i). \tag{10}$$

We have

$$\sum_{i=1}^{p}(k_i-1) = \sum_{i=1}^{n}(k_i-1) = 2(n-1) - n = n-2. \tag{11}$$

Combining (10), (11) we obtain (9) and the proof is complete.

Corollary 10. *H is nonsingular if and only if no vertex in T has degree* 2.

Proof. The result easily follows from (9).

When H is nonsingular, we may construct H^{-1} using Theorem 6. We proceed to explain the construction. For positive integers p, q, we define J_{pq} to be the $p \times q$ matrix of all ones.

Lemma 11. *Let p, q be positive integers with $p + q \geq 3$ and let*

$$A = \begin{pmatrix} 2I_p - J_p & J_{pq} \\ J_{qp} & 2I_q - J_q \end{pmatrix}.$$

Then

$$A^{-1} = \frac{1}{2(p+q-2)} \begin{pmatrix} (p+q-2)I_p - J_p & J_{pq} \\ J_{qp} & (p+q-2)I_q - J_q \end{pmatrix}.$$

Proof. It is easily verified by multiplication that the product of the two matrices is I.

For each star of T write the inverse of the corresponding principal submatrix of H and put zeros elsewhere. The principal submatrix corresponding to a star has the same form as the matrix A in Lemma 11, after a relabeling of rows and columns and thus its inverse can readily be written down using Lemma 11. Add all such matrices. Then for each edge which is not a pendant edge, add 1 to the corresponding diagonal position. The resulting matrix is the inverse of H. The proof follows from Theorem 6.

Example. Consider the tree T as shown.

$$\begin{tikzcd}
\circ 2 & \circ 5 \arrow[d, "iv"] & \circ 8 \arrow[d, "vii"] & \\
\circ 1 \arrow[u, "i"] \arrow[r, "iii"] & \circ 4 \arrow[r, "vi"] & \circ 7 \arrow[d, "viii"] & \circ 10 \arrow[l, "ix"'] \\
\circ 3 \arrow[u, "ii"] & \circ 6 \arrow[u, "v"] & \circ 9 &
\end{tikzcd}$$

For convenience, we have labeled the edges with roman numerals. The edge orientation matrix H is given by

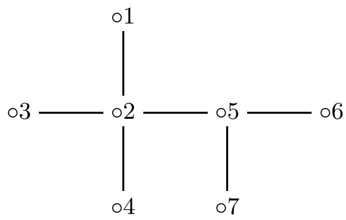
$$\begin{bmatrix}
1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 \\
-1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\
-1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 \\
-1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1
\end{bmatrix}.$$

There is no vertex of degree 2 in T and hence H is nonsingular. The tree has 3 stars, which we denote by S_1, S_2, S_3 with vertex sets $V(S_1) = \{1,2,3,4\}, V(S_2) = \{1,4,5,6,7\}$ and $V(S_3) = \{4,7,8,9,10\}$. We may obtain H^{-1} from the inverses of the principal submatrices corresponding to S_1, S_2, S_3 as described earlier.

4. SQUARED DISTANCE MATRIX OF A TREE

Let T be a tree with vertex set $\{1,2,\ldots,n\}$. Let D be the distance matrix of T and let Δ be obtained by squaring each element of D. We will refer to $\Delta = (f_{ij})_{1\le i,j\le n}$ as the squared distance matrix of T. The main objective of this section is to prove a formula for $\det\Delta$. It turns out that $\det\Delta$ depends only on the degree sequence of T.

Example. Consider the tree T as shown.



Then the squared distance matrix of T is:

$$\Delta = \begin{bmatrix} 0 & 1 & 4 & 4 & 4 & 9 & 9 \\ 1 & 0 & 1 & 1 & 1 & 4 & 4 \\ 4 & 1 & 0 & 4 & 4 & 9 & 9 \\ 4 & 1 & 4 & 0 & 4 & 9 & 9 \\ 4 & 1 & 4 & 4 & 0 & 1 & 1 \\ 9 & 4 & 9 & 9 & 1 & 0 & 4 \\ 9 & 4 & 9 & 9 & 1 & 4 & 0 \end{bmatrix}.$$

We first prove some results connecting Δ with Q and H defined after orienting each edge of T.

Lemma 12. *Let T be a tree with vertex set $\{1,2,\ldots,n\}$. Assign an orientation to each edge of T and let Q and H be the incidence matrix and the edge orientation matrix, respectively. Let Δ be the squared distance matrix of T. Then $Q'\Delta Q = -2H$.*

Proof. Let e and f be edges of T where e is directed from i to j and f is directed from k to ℓ. Then the (e,f)-element of $Q'\Delta Q$ is given by

$$d(i,k)^2 + d(j,\ell)^2 - d(i,\ell)^2 - d(j,k)^2. \tag{12}$$

We must consider cases. First suppose that e and f are similarly oriented, so that $d(i,k) = d(j,\ell)$. As a subcase, assume that j is on the path from i to k.

Then $d(i,\ell)-1 = d(j,k)+1 = d(i,k)$. If we set $d(i,k) = d(j,\ell) = \alpha$, then $d(i,\ell) = \alpha+1$ and $d(j,k) = \alpha-1$. It follows that the expression in (12) equals $2\alpha^2-(\alpha+1)^2-(\alpha-1)^2 = -2$, which is the (e,f)-element of $-2H$. The other subcase when j is not on the (i,k)-path, as well as the case when e and f are oppositely oriented, are handled similarly and the proof is complete.

Lemma 13. *Let T be a tree with vertex set $\{1,2,\dots,n\}$. Let Δ be the squared distance matrix of T and let $k_1,\dots,k_n$ be the degree sequence of T. Let $\tau_i = 2-k_i, i=1,\dots,n$. Then*

$$\operatorname{cof}\Delta = (-1)^{n-1}2\cdot 4^{n-2}\prod_{i=1}^{n}\tau_i. \tag{13}$$

Proof. Assign an orientation to each edge of T and let Q and H be the incidence matrix and the edge orientation matrix, respectively. Let adj A denote the adjoint (the transpose of the cofactor matrix) of the square matrix A. By Lemma 12, $Q'\Delta Q = -2H$. Let γ_i denote the determinant of the $(n-1)\times(n-1)$ submatrix of Q obtained by deleting its i-th row, $i=1,\dots,n$. We claim that $(-1)^i\gamma_i$ is the same for all i. To see this, fix $1\le i<n$, and let $\tilde{Q}$ be the matrix obtained from Q by first replacing its i-th row by the sum of the i-th and the $(i+1)$-th rows and then deleting the $(i+1)$-th row. The sum of the elements in any column of $\tilde{Q}$ is zero and hence $\det\tilde{Q}=0$. However $\det\tilde{Q} = \gamma_i+\gamma_{i+1}$ and hence $\gamma_i = -\gamma_{i+1}$. This proves the claim. It is well-known that Q is totally unimodular (see, for example, [**1**, p.13]) and hence the common value of $(-1)^{\gamma_i}$ is ±1. Let $\Delta(i,j)$ denote the submatrix obtained by deleting row i and column j of Δ. A simple application of the Cauchy-Binet formula shows that

$$\begin{aligned}\det(Q'\Delta Q) &= \sum_{i=1}^{n}\sum_{j=1}^{n}\gamma_i\gamma_j\det(\Delta(i,j))\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}(-1)^i\gamma_i(-1)^j\gamma_j(-1)^{i+j}\det(\Delta(i,j))\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}(-1)^{i+j}\det(\Delta(i,j)) = \mathbf{1}'\text{adj }\Delta\mathbf{1}\end{aligned} \tag{14}$$

It follows from $Q'\Delta Q = -2H$ and (14) that

$$\mathbf{1}'(\text{adj }\Delta)\mathbf{1} = \det(-2H) = (-2)^{n-1}\det H. \tag{15}$$

By Theorem 9,

$$\det H = 2^{n-2}\prod_{i=1}^{n}(2-k_i) = 2^{n-2}\prod_{i=1}^{n}\tau_i. \tag{16}$$

Since $\operatorname{cof}\Delta = \mathbf{1}'(\text{adj }\Delta)\mathbf{1}$, the proof is complete in view of (15) and (16).

Lemma 14. *Let T be a tree and let v be a vertex of degree two 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 $(2, 2, \ldots, 2)'$.*

Proof. After performing this elementary column operation, consider the entry in row w of Col_s. The entry will be $f'_{w,s} = d^2_{w,s} - 2d^2_{w,v} + d^2_{w,t}$. If w is not the vertex v, then assume that $f_{w,s} = (d-1)^2$, $f_{w,v} = d^2$ and $f_{w,t} = (d+1)^2$ for some positive integer d, i.e., we assume that w is closer to s than to t. The other case where w is closer to t is proved analogously and hence omitted. It is clear that $f'_{w,s} = 2$. It is easy to see that when $w = v$, again $f'_{v,s} = 2$, completing the proof.

Corollary 15. *Let T be a tree on n vertices and let T have two distinct vertices a and b both having degree two. Then,* $\det \Delta = 0$.

Proof. Let the neighbors of a and b be s, t and y, z respectively. The four vertices s, t, y, z need not be distinct. However at least two of these four vertices must be at distance at least 3, which we assume to be s and y, without loss of generality. We apply the elementary column operations in Lemma 14 to both the vertices s and y, after which the columns s and y both change to $(2, 2, \ldots, 2)'$. Clearly, this operation leaves $\det \Delta$ unchanged. Since two columns are now identical, $\det \Delta = 0$.

The following result is easily proved using the multilinear property of the determinant (see, for example, [**1**, p.97]).

Lemma 16. *Let A be an $n \times n$ matrix. Then for any real α,*

$$\det(A + \alpha J) = \det A + \alpha \mathit{cof}\, A.$$

The following is the main result of this section.

Theorem 17. *Let T be a tree with $V(T) = \{1, \ldots, n\}$ and let Δ be the squared distance matrix of T. Let $k_1, k_2, \ldots, k_n$ be the degree sequence of T. Let $\tau_i = 2 - k_i, i = 1, \ldots, n$. Then*

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

Proof. We induct on the number of vertices, with the case when T has at most 3 vertices being clear. First suppose that T has two vertices both with degree 2. Then by Corollary 15, $\det \Delta = 0$. Also the right side of (17) is also zero and the result is proved. Therefore we assume that T has at most one vertex of degree 2. Then we may assume that there exists a vertex w of T adjacent to at least two pendant vertices. Let w be adjacent to t pendant vertices in T where $t \geq 2$. 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 $1, 2, \ldots, t$.

For $1 \le i \le t$, 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. This will result in

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

where Δ_1 is the squared distance matrix corresponding to the tree $\tilde{T} = T - \{1, 2, \ldots, t\}$, 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. It is easy to see that $\det X = (-1)^{t-1}4^t(t-1)$ and that $\mathbf{1}'X^{-1}\mathbf{1} = \dfrac{t}{4(t-1)}$. We equivalently write $\det X = (-4)^t(1-t)$.

By the Schur complement formula (see [**1**, p.4]) we get,

$$\det \Delta = (\det X) \det \left(\Delta_1 - \frac{t}{t-1} J\right). \tag{18}$$

It follows from (18) and Lemma 16 that

$$\det \Delta = (-1)^t 4^t (1-t) \left(\det \Delta_1 - \frac{t}{t-1} \operatorname{cof} \Delta_1\right). \tag{19}$$

In T, let $\tau = (\tau_1, \ldots, \tau_n)'$. Since $\tau_i = 1, i = 1, \ldots, t$ and $\tau_w = 1 - t$, we may write $\tau = (1, 1, \ldots, 1, (1-t), z')'$ where z is the vector consisting of $\tau_i, i = t+2, \ldots, n$. We write the vector of τ_i where i is a vertex of $\tilde{T}$ as $\tilde{\tau}' = (1, z')'$. Note that the first component in $\tilde{\tau}$ is 1 since w is a pendant vertex in $\tilde{T}$.

Let

$$A = \sum_{i=t+1}^{n} \prod_{j \neq i} \tilde{\tau}_j \qquad B = \sum_{i=1}^{n} \prod_{j \neq i} \tau_j \quad \text{and} \quad C = \prod_{i=1}^{n} \tau_i.$$

Note that A is defined for $\tilde{T}$, while B, C are defined for T. We claim that

$$A = \frac{B}{1-t} + \frac{t^2 - 2t}{(1-t)^2} C. \tag{20}$$

The claim is justified as follows. First suppose that no vertex of T has degree 2. Then

$$A = \prod_{i=t+1}^{n} \tilde{\tau}_i \sum_{j=t+1}^{n} \frac{1}{\tilde{\tau}_j}, \tag{21}$$

$$B = \prod_{i=1}^{n} \tau_i \sum_{j=1}^{n} \frac{1}{\tau_j} \qquad \text{and} \qquad C = (1-t) \prod z_i. \tag{22}$$

Note that

$$\sum_{i=1}^{n} \frac{1}{\tau_i} = t + \frac{1}{1-t} + \sum \frac{1}{z_i}. \tag{23}$$

Using (21), (22), (23), we get (20). If T has a vertex of degree 2, then we may assume, without loss of generality, that $z_1 = 0$. In that case $A = \prod_{i\neq 1} z_i, B = (1-t)\prod_{i\neq 1} z_i$ and $C = 0$, and again (20) is proved.

By induction hypothesis and using (20),

$$\begin{aligned}\det \Delta_1 &= (-1)^{n-t}4^{n-t-2}\left\{\frac{2(n-t)-1}{1-t}C - 2A\right\} \\ &= (-1)^{n-t}4^{n-t-2}\left\{\frac{2n(1-t)+3t-1}{(1-t)^2}C - \frac{2B}{1-t}\right\}.\end{aligned} \tag{24}$$

By Lemma 13,

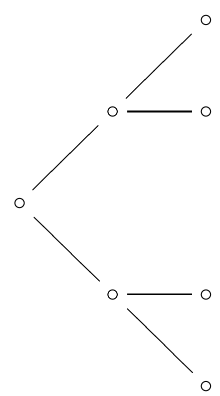
$$\frac{t}{t-1}\operatorname{cof}\Delta_1 = \frac{t}{t-1}(-1)^{n-t-1}4^{n-t-2}\frac{2C}{1-t} = (-1)^{n-t}4^{n-t-2}\frac{2t.C}{(1-t)^2}. \tag{25}$$

It follows from (24),(25) that

$$\det \Delta_1 - \frac{t}{t-1}\operatorname{cof}\Delta_1 = (-1)^{n-t}4^{n-t-2}\left\{\frac{(2n-1)C}{1-t} - \frac{2B}{1-t}\right\}. \tag{26}$$

Plugging in (26) into (19), we see that $\det \Delta = (-1)^n 4^{n-2}\{(2n-1)C - 2B\}$, completing the proof. $\square$

The complete binary tree BT_n with $2^n - 1$ vertices is the tree with a root vertex having degree 2, and is such that each vertex has either two or zero children (see, for example, [**9**, p.51]). It is easy to see that BT_n has 2^{n-1} pendant vertices. Below, we illustrate BT_3.



As a simple consequence of Theorem 17 we have the following.

Corollary 18. *Let T be the complete binary tree BT_{m+1} with $n = 2^{m+1}-1$ vertices. Let Δ be the squared distance matrix of T. Then* $\det \Delta = (-1)^m 2.4^{n-2}$.

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