MINORS OF TREE DISTANCE MATRICES

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Abstract. We prove that the principal minors of the distance matrix of a tree satisfy a combinatorial expression involving counts of rooted spanning forests of the underlying tree. This generalizes a result of Graham and Pollak. We also give such an expression for the case of edge-weighted trees.

Contents

1. Introduction

Suppose $G = (V, E)$ is a tree with n vertices. Let D denote the distance matrix of G. In [6], Graham and Pollak proved that

$$\det D = (-1)^{n-1} 2^{n-2} (n-1). \tag{1}$$

This identity is remarkable in that the result does not depend on the tree structure, beyond the number of vertices. The identity (1) was motivated by a problem in data communication, and inspired much further research on distance matrices.

The main result of this paper is to generalize (1) by replacing $\det D$ with any of its principal minors. For a subset $S \subset V(G)$, let $D[S]$ denote the submatrix consisting of the S-indexed rows and columns of D.

Theorem 1.1. *Suppose G is a tree with n vertices, and distance matrix D. Let $S \subset V(G)$ be a nonempty subset of vertices. Then*

$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \left((n-1)\, \kappa(G; S) - \sum_{\mathcal{F}_2(G;S)} (\deg^o(F, *) - 2)^2 \right), \tag{2}$$

where $\kappa(G; S)$ is the number of S-rooted spanning forests of G, $\mathcal{F}_2(G; S)$ is the set of $(S, *)$-rooted spanning forests of G, and $\deg^o(F, *)$ denotes the outdegree of the $*$-component of F.

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For definitions of $(S,*)$-rooted spanning forests and other terminology, see Section 2. When $S = V$ is the full vertex set, the set of V-rooted spanning forests is a singleton, consisting of the subgraph with no edges, so $\kappa(G;V) = 1$; and moreover the set $\mathcal{F}_2(G;V)$ of $(V,*)$-rooted spanning forests is empty. Thus (2) recovers the Graham–Pollak identity (1) when $S = V$.

1.1. **Weighted trees.** If $\{\alpha_e : e \in E\}$ is a collection of positive edge weights, the α-distance matrix $D^{(\alpha)}$ is defined by setting the (u,v)-entry to the sum of the weights α_e along the unique path from u to v. The relation (1) has an analogue for the weighted distance matrix,

$$\det D^{(\alpha)} = (-1)^{n-1} 2^{n-2} \sum_{e\in E} \alpha_e \prod_{e\in E} \alpha_e, \tag{3}$$

which was proved by Bapat–Kirkland–Neumann [1]. The weighted identity (3) reduces to (1) when taking all unit weights, $\alpha_e = 1$. We also prove the following weighted version of our main theorem.

Theorem 1.2. *Suppose $G = (V,E)$ is a finite, weighted tree with edge weights $\{\alpha_e : e \in E\}$, and corresponding weighted distance matrix $D = D^{(\alpha)}$. For any nonempty subset $S \subset V$, we have*

$$\det D^{(\alpha)}[S] = (-1)^{|S|-1} 2^{|S|-2} \left(\sum_{E(G)} \alpha_e \sum_{\mathcal{F}_1(G;S)} w(\overline{T}) - \sum_{\mathcal{F}_2(G;S)} (\deg^o(F,*) - 2)^2 w(\overline{F}) \right), \tag{4}$$

where $\mathcal{F}_1(G;S)$ is the set of S-rooted spanning forests of G, $\mathcal{F}_2(G;S)$ is the set of $(S,*)$-rooted spanning forests of G, $w(\overline{T})$ and $w(\overline{F})$ denote the α-weights of the forests T and F, and $\deg^o(F,*)$ is the outdegree of the $*$-component of F, as above.

Theorem 1.2 reduces to Theorem 1.1 when taking all unit weights, $\alpha_e = 1$.

1.2. **Applications.** Suppose we fix a tree distance matrix D. It is natural to ask, how do the expressions $\det D[S]$ vary as we vary the vertex subset S? To our knowledge there is no nice behavior among the determinants, but as S varies there is nice behavior of the "normalized" ratios $\det D[S]/\operatorname{cof} D[S]$ which we describe here.

Given a matrix A, let $\operatorname{cof} A$ denote the *sum of cofactors* of A, i.e.

$$\operatorname{cof} A = \sum_{i=1}^{|S|} \sum_{j=1}^{|S|} (-1)^{i+j} \det A_{i,j}$$

where $A_{i,j}$ is the submatrix of A that removes the i-th row and the j-th column. If A is invertible, then $\operatorname{cof} A$ is related to the sum of entries of the matrix inverse A^{-1} by a factor of $\det A$, i.e. $\operatorname{cof} A = (\det A)(\mathbf{1}^\intercal A^{-1} \mathbf{1})$. In [3], Bapat and Sivasubramanian showed the following identity for the sum of cofactors of a distance submatrix $D[S]$ of a tree,

$$\operatorname{cof} D[S] = (-2)^{|S|-1} \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}). \tag{5}$$

Using the Bapat–Sivasubramanian identity (5), an immediate corollary to Theorem 1.2 is the following result:

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \frac{1}{2} \left(\sum_{e\in E} \alpha_e - \frac{\sum_{F\in \mathcal{F}_2(G;S)} w(\overline{F})(\deg^o(F,*) - 2)^2}{\sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})} \right). \tag{6}$$

The expression (6) satisfies a monotonicity condition as we vary the vertex set $S \subset V(G)$.

Theorem 1.3 (Monotonicity of normalized principal minors)**.** *If $A, B \subset V(G)$ are nonempty subsets with $A \subset B$, then*

$$\frac{\det D[A]}{\operatorname{cof} D[A]} \leq \frac{\det D[B]}{\operatorname{cof} D[B]}.$$

The essential observation behind this result is that $\det D[S]/\operatorname{cof} D[S]$ is calculated via the following quadratic optimization problem: for all vectors $\mathbf{m} \in \mathbb{R}^S$,

$$\begin{aligned} \text{optimize objective function:} \quad & \mathbf{m}^\intercal D[S]\mathbf{m} \\ \text{with constraint:} \quad & \mathbf{1}^\intercal \mathbf{m} = 1. \end{aligned}$$

This result can be shown using Lagrange multipliers, and relies of knowledge of the signature of $D[S]$. For details, see Section 3.

If $S \subset V(G)$ is nonempty, the expression (6) immediately implies the bound

$$0 \leq \frac{\det D[S]}{\operatorname{cof} D[S]} \leq \frac{1}{2} \sum_{E(G)} \alpha_e.$$

We get refined bounds by making use of the monotonicity property, Theorem 1.3.

Theorem 1.4 (Bounds on principal minor ratios)**.** *Suppose $G = (V, E)$ is a finite, weighted tree with distance matrix $D^{(\alpha)}$.*

(a) If $\operatorname{conv}(S, G)$ denotes the subtree of G consisting of all paths between points of $S \subset V(G)$,

$$\frac{\det D^{(\alpha)}[S]}{\operatorname{cof} D^{(\alpha)}[S]} \leq \frac{1}{2} \sum_{E(\operatorname{conv}(S,G))} \alpha_e.$$

(b) If γ is a simple path between vertices $s_0, s_1 \in S$, then

$$\frac{1}{2} \sum_{e \in \gamma} \alpha_e \leq \frac{\det D^{(\alpha)}[S]}{\operatorname{cof} D^{(\alpha)}[S]}.$$

1.3. **Further questions.** A formula for the inverse matrix D^{-1} was found by Graham and Lovász in [5]. Namely,

$$D^{-1} = -\frac{1}{2} L + \frac{1}{2(n-1)} \mathbf{m}\mathbf{m}^\intercal$$

where L is the Laplacian matrix and $\mathbf{m}$ is the vector $\mathbf{m}_v = 2 - \deg v$. Does there exist a nice expression for the inverse of the matrix $D[S]$?

1.4. **Notation.** G a finite graph, loops and parallel edges allowed, possibly disconnected
$E(G)$ edge set of G
$V(G)$ vertex set of G
$\mathcal{F}_1(G; S)$ the set of S-rooted spanning forests of G
$\mathcal{F}_2(G; S)$ the set of $(S, *)$-rooted spanning forests of G

2. Graphs and matrices

For background on enumeration problems for graphs and trees, see Tutte [11, Chapter VI].

Let $G = (V, E)$ be a graph with edge weights $\{\alpha_e : e \in E\}$. For any edge subset $A \subset E$ we define the *weight* of A as $w(A) = \prod_{e \in A} \alpha_e$. We define the *co-weight* of A as $w(\overline{A}) = \prod_{e \notin A} \alpha_e$. By abuse of notation, if H is a subgraph of G, we use H to also denote its subset of edges $E(H)$, so e.g. $w(\overline{H}) = w(\overline{E(H)})$.

Let M be an $n \times n$ matrix. For a subset $S \subset \{1, \ldots, n\}$, let $M[S]$ denote the submatrix obtained by keeping the S-indexed rows and columns of M. Let $M[\overline{S}]$ denote the submatrix obtained by deleting the S-indexed rows and columns.

2.1. **Spanning trees and forests.** A *spanning tree* of a graph G is a subgraph which is connected, has no cycles, and contains all vertices of G. A *spanning forest* of a graph G is a subgraph which has no cycles and contains all vertices of G. Let $\kappa(G)$ denote the number of spanning trees of G, and let $\kappa_r(G)$ denote the number of r-component spanning forests.

Given a set of vertices $S = \{v_1, v_2, \dots, v_k\}$, an *$S$-rooted spanning forest* of G is a spanning forest which has exactly one vertex v_i in each connected component. An *$(S,*)$-rooted spanning forest* of G is a spanning forest which has $|S|+1$ components, where $|S|$ components each contain one vertex of S, and the additional component is disjoint from S. We call the component disjoint from S the *floating component*, following terminology in [8]. Given $s \in S$ and a forest F in $\mathcal{F}_1(G;S)$ or $\mathcal{F}_2(G;S)$, we let $F(s)$ denote the s-component of F, and let $F(*)$ denote the floating component (if $F \in \mathcal{F}_2$).

Let $\kappa(G;S)$ denote the number of S-rooted spanning forests of G, and let $\kappa_2(G;S)$ denote the number of $(S,*)$-rooted spanning forests. Let $\mathcal{F}_1(G;S)$ denote the set of S-rooted spanning forests of G, and let $\mathcal{F}_2(G;S)$ denote the set of $(S,*)$-rooted spanning forests of G. Note that $\kappa(G;S)$ is also the number of spanning trees of the quotient graph G/S, which "glues together" all vertices in S as a single vertex.

Let

$$\kappa_k(v_1|v_2|\cdots|v_k)$$

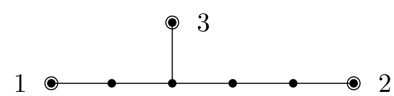
denote the number of k-component spanning trees which have a vertex v_i in each component. If $S = \{v_1, \dots, v_k\}$, then $\kappa_k(v_1|\cdots|v_k) = \kappa(G;S) = \kappa(G/S)$.

If u, v, w are vertices, then let

$$\kappa_2(uv|w)$$

denote the number of two-forests which have u, v in one component and w in the other component.

Example 2.1. Suppose G is the tree with unit edge lengths shown below.



Let S be the set of three leaf vertices. Then $\mathcal{F}_1(G;S)$ contains 11 forests, while $\mathcal{F}_2(G;S)$ contains 19 forests. Some of these are shown in Figures 1 and 2, respectively.

FIGURE 1. Some forests in $\mathcal{F}_1(G;S)$.

FIGURE 2. Some forests in $\mathcal{F}_2(G;S)$, with floating component highlighted.

2.2. **Laplacian matrix.** Given a graph $G = (V,E)$, consider an orientation on the edge set, which consists of a pair of functions head : $E \to V$ and tail : $E \to V$, such that head(e) and tail(e) are the endpoints of e. We abbreviate head(e) as e^+, and tail(e) as e^-.

The *incidence matrix* of G is the matrix $N \in \mathbb{R}^{V \times E}$ defined by

$$N_{v,e} = \mathbb{1}(v = e^+) - \mathbb{1}(v = e^-).$$

Let $L \in \mathbb{R}^{V \times V}$ denote the *Laplacian matrix* of G, which is defined by $L = NN^\intercal$. If G is a weighted graph with positive edge weights α_e for $e \in E$, let $L^{(\alpha)}$ denote the weighted Laplacian matrix of G, defined by

$$L^{(\alpha)} = N \begin{pmatrix} \alpha_1^{-1} & & \\ & \ddots & \\ & & \alpha_m^{-1} \end{pmatrix} N^\intercal.$$

It is clear that L and $L^{(\alpha)}$ are positive semidefinite.

Given $S \subset V$, let $L[\overline{S}]$ denote the matrix obtained from L by removing the rows and columns indexed by S. More generally, let $L[\overline{S}, \overline{T}]$ denote the matrix obtained from L by removing S-indexed rows and T-indexed columns. Recall that $\kappa(G; S)$ denotes the number of S-rooted spanning forests of G. The following theorem relates minors of the (weighted) Laplacian to (weighted) counts of rooted spanning forests.

Theorem 2.2 (Principal-minors matrix tree theorem)**.** *Let $G = (V, E)$ be a finite graph.*

(a) Let L denote the Laplacian matrix of G. Then for any nonempty vertex set $S \subset V$,

$$\det L[\overline{S}] = \kappa(G; S).$$

(b) Let $L^{(\alpha)}$ denote the weighted Laplacian matrix of G, with edge weights $\{\alpha_e\}$. Then for any nonempty vertex set $S \subset V$,

$$\det L^{(\alpha)}[\overline{S}] = \sum_{T \in \mathcal{F}_1(G;S)} w(T)^{-1} = \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}) \prod_{e \in E} \alpha_e^{-1}.$$

Proof. See Tutte [11, Section VI.6, Equation (VI.6.7)] or Chaiken [4] or Bapat [2, Theorem 4.7]. □

Next we recall a connection between minors of the Laplacian matrix and cofactor sums of the distance matrix, when G is a tree. The result is due to Bapat–Sivasubramanian [3]. Recall that $\operatorname{cof} M$ denotes the *sum of cofactors* of M, i.e. $\operatorname{cof} M = \sum_{i=1}^{n} \sum_{j=1}^{n} (-1)^{i+j} \det M[\overline{i}, \overline{j}]$.

Theorem 2.3 (Distance submatrix cofactor sums)**.** *Given a tree G with edge weights, let D be the weighted distance matrix of G, and L the weighted Laplacian matrix of G. Let $S \subset V(G)$ be a nonempty subset of vertices of G. Then*

$$\operatorname{cof} D^{(\alpha)}[S] = (-2)^{|S|-1} \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}).$$

Proof. Bapat and Sivasubramanian [3, Theorem 11] show that

$$\operatorname{cof} D^{(\alpha)}[S] = (-2)^{|S|-1} \left(\prod_{e \in E} \alpha_e \right) \det L[\overline{S}].$$

Then combine this equation with the matrix tree theorem, Theorem 2.2 (b). □

The following result is a direct consequence of theorems of Bapat–Kirkland–Neumann [1] and Bapat–Sivasubramanian [3].

Proposition 2.4. *Suppose D is the distance matrix of a weighted tree with edge weights $\{\alpha_e : e \in E\}$. Then*

$$\frac{\det D^{(\alpha)}}{\operatorname{cof} D^{(\alpha)}} = \frac{1}{2} \sum_{e \in E} \alpha_e.$$

Proof. Consider applying Theorem 2.3 with $S = V$. In this case $\mathcal{F}_1(G; V)$ consists of the forest with no edges, and for this forest $w(\overline{T})$ is the product of all edge weights. Thus

$$\operatorname{cof} D^{(\alpha)} = (-2)^{n-1} \prod_{e \in E} \alpha_e.$$

Combining this with the Bapat–Kirkland–Neuman formula (3) yields the result. □

2.3. **Tree splits and tree distance.** In this section we describe the tree splits associated to a tree, and use their associated indicator functions to give an expression for the tree distance.

Given a tree $G = (V, E)$ and an edge $e \in E$, the edge deletion $G \setminus e$ contains two connected components. Using the implicit orientation on $e = (e^+, e^-)$, we let $(G \setminus e)^+$ denote the component that contains endpoint e^+, and let $(G \setminus e)^-$ denote the other component. For any $e \in E$ and $v \in V$, we let $(G \setminus e)^v$ denote the component of $G \setminus e$ containing v, respectively $(G \setminus e)^{\overline{v}}$ for the component not containing v.

Tree splits can be used to express the path distance between vertices in a tree. Given an edge $e \in E$ and vertices $v, w \in V$, let

$$\delta(e; v, w) = \begin{cases} 1 & \text{if } e \text{ separates } v \text{ from } w, \\ 0 & \text{otherwise.} \end{cases}$$

In other words, $\delta(e; v, w) = 1$ if the vertices are in different components of the split $G \setminus e$, and $\delta(e; v, w) = 0$ if they are in the same component. Note that $\delta(e; v, v) = 0$ for any e and v.

We have the following perspectives on the function $\delta(e; v, w)$:

(i) If we fix e and v, then $\delta(e; v, -) : V(G) \to \{0, 1\}$ is the indicator function for the component $(G \setminus e)^{\overline{v}}$ of the tree split $G \setminus e$ not containing v.
(ii) On the other hand if we fix v and w, then $\delta(-; v, w) : E(G) \to \{0, 1\}$ is the indicator function for the unique $v \sim w$ path in G.

Proposition 2.5 (Weighted tree distance)**.** *For a tree $G = (V, E)$ with weights $\{\alpha_e : e \in E\}$, the weighted distance function satisfies*

$$D^{(\alpha)}(v, w) = \sum_{e \in E} \alpha_e \, \delta(e; v, w).$$

For an unweighted tree, we can express the tree distance $d(v, w)$ as the unweighted sum

$$d(v, w) = \sum_{e \in E(G)} \delta(e; v, w).$$

2.4. **Outdegree of rooted forest.** Given a vertex v in a graph, the *degree* $\deg(v)$ is the number of edges incident to v. A consequence of the "handshake lemma" of graph theory is that for any tree G, we have

$$\sum_{v \in V(G)} (2 - \deg(v)) = 2.$$

In this section we discuss some generalizations, which will be used later.

Given a connected subgraph $H \subset G$, we define the *outdegree* $\deg^o(H)$ as the number of edges which join H to its complement; i.e.

$$\deg^o(H) = \#\{e = (a, b) \in E : a \in V(H),\, b \notin V(H)\}.$$

We often use the following special case of the outdegree: given a rooted forest F in $\mathcal{F}_1(G; S)$ and $s \in S$, let $F(s)$ denote the s-component of F. We define the *outdegree* $\deg^o(F, s)$ as the number of edges which join $F(s)$ to a different component; i.e.

$$\deg^o(F, s) = \#\{e = (a, b) \in E : a \in F(s),\, b \notin F(s)\}. \tag{7}$$

If F is a forest in $\mathcal{F}_2(G; S)$, let $\deg^o(F, *)$ denote the outdegree of the floating component.

Lemma 2.6. *Suppose G is a tree.*
(a) If $H \subset G$ is a (nonempty) connected subgraph, then

$$\sum_{v \in V(H)} (2 - \deg(v)) = 2 - \deg^o(H).$$

(b) For any fixed edge e and fixed vertex u of G, we have

$$\sum_{v \in V(G)} (2 - \deg(v))\, \delta(e; u, v) = 1.$$

Proof. (a) This is straightforward to check by induction on $|V(H)|$, with base case $|V(H)| = 1$: if $H = \{v\}$ consists of a single vertex, then $\deg^o(H) = \deg(v)$.

(b) Recall that $(G \setminus e)^{\overline{u}}$ denotes the component of the tree split $G \setminus e$ that does not contain u. Its vertices are precisely those v that satisfy $\delta(e; u, v) = 1$. Since this component has a single edge separating it from its complement, $\deg^o((G \setminus e)^{\overline{u}}) = 1$ Using part (a), we have

$$\sum_{v \in V} (2 - \deg(v)) \delta(e; u, v) = \sum_{v \in (G \setminus e)^{\overline{u}}} (2 - \deg(v)) = 2 - \deg^o((G \setminus e)^{\overline{u}}) = 1. \qquad \square$$

2.5. **Distance matrix.** In this section we recall some results on the distance matrix of a tree.

Bapat–Kirkland–Neumann [1, Theorem 2.1] prove that

$$(D^{(\alpha)})^{-1} = -\frac{1}{2} L^{(\alpha)} + \frac{1}{2} \Big(\sum_{e \in E} \alpha_e \Big)^{-1} \mathbf{m}\, \mathbf{m}^\intercal \tag{8}$$

where $\mathbf{m}$ is the vector with components $\mathbf{m}_v = 2 - \deg v$.

Proposition 2.7. *Let D denote the weighted distance matrix of a tree, and L the weighted Laplacian matrix. Then*

$$D^{(\alpha)} = -\frac{1}{2} D^{(\alpha)} L^{(\alpha)} D^{(\alpha)} + \frac{1}{2} \left(\sum_{e \in E} \alpha_e \right) \mathbf{1}\mathbf{1}^\intercal.$$

Proof. Multiply (8) by the all-ones vector $\mathbf{1}$; since $L^{(\alpha)}\mathbf{1} = 0$ and $\mathbf{m}^\intercal \mathbf{1} = 2$, we obtain $(D^{(\alpha)})^{-1}\mathbf{1} = \Big(\sum_{e \in E} \alpha_e \Big)^{-1} \mathbf{m}$. Hence $D^{(\alpha)}\mathbf{m} = \big(\sum_{e \in E} \alpha_e \big) \mathbf{1}$. Then multiply (8) by $D^{(\alpha)}$ on both sides. $\square$

The unweighted version of (8) appeared earlier in Graham–Lovasz [5, Lemma 1].

Proposition 2.8. *Suppose D is the (weighted) distance matrix of a tree.*
(a) If $\mathbf{h} \in \mathbb{R}^V$ is a vector whose coordinates sum to zero, then $\mathbf{h}^\intercal D \mathbf{h} \leq 0$.
(b) If $\mathbf{h} \in \mathbb{R}^S$ is a vector whose coordinates sum to zero, then $\mathbf{h}^\intercal D[S] \mathbf{h} \leq 0$.

Proof. (a) By assumption $\mathbf{1}^\intercal \mathbf{h} = 0$. Using Proposition 2.7,

$$\mathbf{h}^\intercal D \mathbf{h} = -\frac{1}{2} \mathbf{h}^\intercal D L D \mathbf{h} + 0.$$

It is well-known that the Laplacian matrix is positive semidefinite, so $\mathbf{h}^\intercal D L D \mathbf{h} = (D\mathbf{h})^\intercal L (D\mathbf{h}) \geq 0$. Thus $\mathbf{h}^\intercal D \mathbf{h} \leq 0$ as claimed.

(b) This follows from (a) since $\mathbf{h}^\intercal D[S] \mathbf{h} = D$. $\square$

Later we will make use of the fact that a submatrix $D[S]$ of a distance matrix has nonzero determinant, as long as $|S| \geq 2$. We prove this fact in this section.

We first recall a result of Cauchy, which states that the eigenvalues of $M[\bar{i}]$ "interlace" the eigenvalues of M. Recall that $M[\bar{i}]$ denotes the matrix obtained from M by deleting the i-th row and column.

Proposition 2.9 (Cauchy interlacing). *Suppose M is a symmetric real matrix with ordered eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$, and the submatrix $M[\bar{i}]$ has ordered eigenvalues $\mu_1 \leq \cdots \leq \mu_{n-1}$. Then*

$$\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \cdots \leq \mu_{n-1} \leq \lambda_n.$$

Proof. See Horn–Johnson [7, Theorem 4.3.17]. □

Lemma 2.10 (Bapat [2, Lemma 8.15]). *Suppose $D^{(\alpha)}$ is the (weighted) distance matrix of a tree with n vertices. Then $D^{(\alpha)}$ has one positive eigenvalue and $n-1$ negative eigenvalues.*

Proof. Lemma 8.15 of [2] is stated for a non-weighted distance matrix; however, the same argument applies to a weighted distance matrix by applying Bapat–Kirkland–Neumann's result (3) on the weighted distance matrix determinant [1, Corollary 2.5]. □

The following argument was communicated to the author by Bapat, via personal communication.

Proposition 2.11. *Suppose $D^{(\alpha)}$ is the weighted distance matrix of a tree $G = (V, E)$ and $S \subset V$ is a subset of size $|S| \geq 2$. Then*
(a) $D^{(\alpha)}[S]$ has one positive eigenvalue and $|S| - 1$ negative eigenvalues;
(b) $\det D^{(\alpha)}[S] \neq 0$.

Proof. (a) Let $n = |V|$; assume $n \geq 3$. We apply decreasing induction on the size of S. If $|S| = n-1$, then Lemma 2.10 and Cauchy interlacing imply that $D[S]$ has at most one positive eigenvalue, and at least one negative eigenvalue. Since all diagonal entries of $D[S]$ are zero, $D[S]$ has zero trace. Thus $D[S]$ has exactly one positive eigenvalue as claimed. The same argument applies for smaller S, as long as $|S| \geq 2$.

(b) This follows from (a), since the determinant is the product of eigenvalues. □

2.6. **Miscellaneous.**

Remark 2.12. A key step in the main proof is the use of the map

$$E(G) \times \mathcal{F}_1(G; S) \mapsto S \sqcup \{\text{error}\}$$

defined by

$$(e, T) \mapsto \begin{cases} s & \text{if } e \in T(s), \\ \text{error} & \text{if } e \notin T. \end{cases}$$

Remark 2.13. For a given spanning forest $F \in \mathcal{F}_2(G; S)$, there are exactly $\deg^o(F, *)$-many choices of pairs $(T, e) \in \mathcal{F}_1(G; S) \times E(G)$ such that $F = T \setminus e$. Consider the "deletion" map

$$E(G) \times \mathcal{F}_1(G; S) \to \mathcal{F}_2(G; S) \sqcup \mathcal{F}_1(G; S)$$

defined by

$$(e, T) \mapsto \begin{cases} T \setminus e & \text{if } e \in T, \\ T & \text{if } e \notin T. \end{cases}$$

For a forest F in $\mathcal{F}_2(G; S)$, the preimage under this map has $\deg^o(F, *)$ elements.

There is an associated "union" map

$$E(G) \times \mathcal{F}_2(G; S) \longrightarrow \mathcal{F}_1(G; S) \sqcup \mathcal{F}_2(G; S)$$

defined by

$$(e, F) \mapsto \begin{cases} F \cup e & \text{if } e \in \partial F, \\ F & \text{if } e \notin \partial F \end{cases}$$

For a forest T in $\mathcal{F}_1(G; S)$, the preimage under this map has $|E(T)|$-many elements.

3. Optimization: quadratic programming

In this section, we explain how the quantity $\dfrac{\det D[S]}{\operatorname{cof} D[S]}$ arises as the solution of a quadratic optimization problem.

Proposition 3.1. *If $D[S]$ is a principal submatrix of a distance matrix indexed by S, then*

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \max\{\mathbf{m}^\intercal D[S]\mathbf{m} : \mathbf{m} \in \mathbb{R}^S,\ \mathbf{1}^\intercal \mathbf{m} = 1\}$$

where $\operatorname{cof} D[S]$ *denotes the sum of cofactors of* $D[S]$.

Corollary 3.2. *If $D[S]$ is a principal submatrix of a distance matrix indexed by S, then*

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \max\{\mathbf{m}^\intercal D\mathbf{m} : \mathbf{m} \in \mathbb{R}^V,\ \mathbf{1}^\intercal \mathbf{m} = 1,\ \mathbf{m}_v = 0 \text{ if } v \notin S\}$$

where $\operatorname{cof} D[S]$ *denotes the sum of cofactors of* $D[S]$.

Proof. If $|S| = 1$ then $D[S]$ is the zero matrix and the statement is true trivially.

Now assume $|S| \geq 2$. Proposition 2.8 implies that the objective function is concave on the domain $\mathbf{1}^\intercal\mathbf{m} = 1$ so any critical point is a local maximum. The gradient of the objective function is $2D[S]\mathbf{m}$, and the gradient of the constraint is $\mathbf{1}$. By the theory of Lagrange multipliers, the optimal solution $\mathbf{m}^*$ is a vector satisfying

$$D[S]\mathbf{m}^* = \lambda \mathbf{1} \qquad \text{for some } \lambda \in \mathbb{R}.$$

The constant λ is in fact the optimal objective value, since

$$(\mathbf{m}^*)^\intercal D[S]\mathbf{m}^* = (D[S]\mathbf{m}^*)^\intercal \mathbf{m}^* = \lambda(\mathbf{1}^\intercal\mathbf{m}^*) = \lambda.$$

The above computation uses the fact that $D[S]$ is a symmetric matrix, and the given constraint $\mathbf{1}^\intercal\mathbf{m} = 1$.

On the other hand, since $D[S]$ is invertible (Proposition 2.11) we have $\mathbf{m}^* = \lambda(D[S]^{-1}\mathbf{1})$, so that

$$1 = \mathbf{1}^\intercal\mathbf{m}^* = \lambda(\mathbf{1}^\intercal D[S]^{-1}\mathbf{1}) = \lambda\frac{\operatorname{cof} D[S]}{\det D[S]}.$$

Thus the optimal objective value is $\lambda = \dfrac{\det D[S]}{\operatorname{cof} D[S]}$. □

Proof of Theorem 1.3. We are to show that for vertex subsets $A \subset B$, we have $\dfrac{\det D[A]}{\operatorname{cof} D[A]} \leq \dfrac{\det D[B]}{\operatorname{cof} D[B]}$. By Corollary 3.2, both values $\dfrac{\det D[A]}{\operatorname{cof} D[A]}$ and $\dfrac{\det D[B]}{\operatorname{cof} D[B]}$ arise from optimizing the same objective function, but the constraint for A is more strict. □

Proof of 1.4. (a) To see that

$$\frac{\det D[S]}{\operatorname{cof} D[S]} \leq \frac{1}{2}\sum_{E(\operatorname{conv}(S,G))} \alpha_e.$$

take B as the set of all vertices in $\operatorname{conv}(S, G)$. Then $S \subset B$, and by Proposition 2.4 we have

$$\frac{\det D[B]}{\operatorname{cof} D[B]} = \frac{1}{2}\sum_{E(\operatorname{conv}(S,G))} \alpha_e.$$

(b) Recall that γ is a simple path between vertices $s_0, s_1 \in S$. To see that

$$\frac{1}{2}\sum_{e\in\gamma} \alpha_e \leq \frac{\det D[S]}{\operatorname{cof} D[S]},$$

take A as the set of endpoints of $\{s_0, s_1\}$. Then $A \subset S$ by assumption, and by Proposition 2.4 we have

$$\frac{\det D[A]}{\operatorname{cof} D[A]} = \frac{1}{2} d(s_0, s_1) = \frac{1}{2} \sum_{e \in \gamma} \alpha_e. \qquad \square$$

4. Distance submatrices: Proofs

In this section we prove our main result, Theorem 1.2. Theorem 1.1 follows as an immediate corollary.

4.1. **Outline of proof.** Given a subset $S \subset V$ and distance submatrix $D[S]$, we will complete the following steps.

(i) Find vector $\mathbf{m} \in \mathbb{R}^S$ such that $D[S]\mathbf{m} = \lambda \mathbf{1} \in \mathbb{R}^S$.

(ii) Compute the sum of entries of $\mathbf{m}$, i.e. $\mathbf{1}^\intercal \mathbf{m}$, and normalize

$$\mathbf{m}^* = \frac{\mathbf{m}}{\mathbf{1}^\intercal \mathbf{m}}.$$

This solves the optimization problem of Section 3.

(iii) The optimal objective value $(\mathbf{m}^*)^\intercal D[S]\mathbf{m}^* = \lambda^*$ is

$$\lambda^* = \frac{\lambda}{\mathbf{1}^\intercal \mathbf{m}}.$$

(iv) Using Theorem 3.1,

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \lambda^* = \frac{\lambda}{\mathbf{1}^\intercal \mathbf{m}}$$

where $\operatorname{cof} D[S]$ is the sum of cofactors of $D[S]$. Use expression for $\operatorname{cof} D[S]$ in Theorem 2.3 to compute $\det D[S]$.

It turns out that the entries of $\mathbf{m}$ are combinatorially meaningful, which also gives combinatorial meaning to the constant λ.

Example 4.1. Suppose G is a tree consisting of three paths joined at a central vertex. Let S consist of the central vertex, and the three endpoints of the paths. The corresponding submatrix of the distance matrix is

$$D[S] = \begin{bmatrix} 0 & a & b & c \\ a & 0 & a+b & a+c \\ b & a+b & 0 & b+c \\ c & a+c & b+c & 0 \end{bmatrix}.$$

Following the steps outlined above:

(i) The vector $\mathbf{m} = \begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ satisfies $D[S]\mathbf{m} = (a+b+c)\mathbf{1}$

(ii) The sum of entries of $\mathbf{m}$ is $\mathbf{1}^\intercal \mathbf{m} = 2$, so $\mathbf{m}^* = \frac{1}{2}\mathbf{m}$.

(iii) We have

$$\lambda^* = \frac{\lambda}{\mathbf{1}^\intercal \mathbf{m}} = \frac{a+b+c}{2}.$$

(iv) The cofactor sum $\operatorname{cof} D[S]$ is $-8abc$, so the determinant is

$$\det D[S] = (\lambda^*) \operatorname{cof} A = \frac{a+b+c}{2}(-8abc) = -4(a+b+c)abc.$$

4.2. **General case:** $S \subset V$**.** Fix a tree $G = (V, E)$ and a nonempty subset $S \subset V$.

Definition 4.2. Let $\mathbf{m} = \mathbf{m}(G; S)$ denote the vector in $\mathbb{R}^S$ be defined by

$$\mathbf{m}_v = \sum_{T \in \mathcal{F}_1(G;S)} (2 - \deg^o(T, v)) w(\overline{T}) \qquad \text{for each } v \in S. \tag{9}$$

where $\deg^o(T, v)$ is the outdegree of the v-component of T, (7).

Let $\mathbf{1}$ denote the all-ones vector.

Proposition 4.3. *For the vector* $\mathbf{m}$ *defined above,*

(a) $\mathbf{1}^\intercal \mathbf{m} = 2 \displaystyle\sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})$*;*

(b) if all edge weights α_e *are positive,* $\mathbf{m}$ *is nonzero.*

Proof. (a) By Lemma 2.6 we have

$$\mathbf{m}_s = \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})(2 - \deg^o(T, s)) = \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}) \left(\sum_{v \in T(s)} (2 - \deg(v)) \right).$$

Then exchange the order of summation in $\mathbf{1}^\intercal \mathbf{m}$,

$$\begin{aligned} \mathbf{1}^\intercal \mathbf{m} = \sum_{s \in S} \mathbf{m}_s &= \sum_{s \in S} \left(\sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}) \sum_{v \in T(s)} (2 - \deg(v)) \right) \\ &= \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}) \left(\sum_{s \in S} \sum_{v \in T(s)} (2 - \deg(v)) \right). \end{aligned}$$

Observe that the inner double sum is simply a sum over $v \in V$, since the vertex sets of $T(s)$ for $s \in S$ form a partition of V by definition of S-rooted spanning forest. Thus

$$\mathbf{1}^\intercal \mathbf{m} = \sum_{T \in \mathcal{F}_1} w(\overline{T}) \left(\sum_{v \in V} (2 - \deg(v)) \right) = \sum_{T \in \mathcal{F}_1} w(\overline{T}) \cdot 2$$

where we again apply Lemma 2.6 for the last equality, as $\deg^o(G) = 0$.

(b) If all edge weights are positive, then $w(\overline{T}) > 0$ for all T, and $\mathcal{F}_1(G; S)$ is nonempty as long as S is nonempty. Thus part (a) implies that $\mathbf{1}^\intercal \mathbf{m} > 0$. $\square$

Corollary 4.4. *If* G *is a graph with unit edge weights* $\alpha_e = 1$*, then the vector* $\mathbf{m}$ *defined in* (9) *satisfies* $\mathbf{1}^\intercal \mathbf{m} = 2\,\kappa(G; S)$*.*

Theorem 4.5. *With* $\mathbf{m} = \mathbf{m}(G; S)$ *defined as in* (9)*,* $D[S]\mathbf{m} = \lambda \mathbf{1}$ *for the constant*

$$\lambda = \sum_{E(G)} \alpha_e \sum_{\mathcal{F}_1(G;S)} w(\overline{T}) - \sum_{\mathcal{F}_2(G;S)} (2 - \deg^o(F, *))^2\, w(\overline{F}).$$

Proof. For $e \in E$ and $v, w \in V$, let $\delta(e; v, w)$ denote the function defined in Section 2.3. For any $v \in S$, we have

$$\begin{aligned}
(D[S]\mathbf{m})_v &= \sum_{s\in S} d(v,s)\mathbf{m}_s \\
&= \sum_{s\in S}\left(\sum_{e\in E(G)} \alpha_e\, \delta(e;v,s)\right)\left(\sum_{T\in\mathcal{F}_1(G;S)} (2-\deg^o(T,s))w(\overline{T})\right) \\
&= \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{s\in S} \delta(e;v,s)(2-\deg^o(T,s))\right) \\
&= \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{s\in S} \delta(e;v,s) \sum_{u\in T(s)} (2-\deg(u))\right). \qquad (10)
\end{aligned}$$

where in the last equality, we apply Lemma 2.6 to the subgraph $H = T(s)$.

We introduce additional notation to handle the double sum in parentheses in (10). Each S-rooted spanning tree T naturally induces a surjection $\pi_T : V \to S$, defined by

$$\pi_T(u) = s \qquad \text{if and only if} \qquad u \in T(s).$$

Using this notation,

$$(D[S]\mathbf{m})_v = \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{u\in V} (2-\deg(u))\delta(e;v,\pi_T(u))\right) \qquad (11)$$

We will compare the above expression with the one obtained after replacing $\delta(e; v, \pi_T(u))$ with $\delta(e; v, u)$. From Lemma 2.6 (b), we have $\sum_{u\in V}(2-\deg(u))\delta(e;v,u) = 1$. Thus

$$\sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e = \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{u\in V} (2-\deg(u))\delta(e;v,u)\right) \qquad (12)$$

By subtracting equation (12) from (11),

$$(D[S]\mathbf{m})_v - \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e = \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \sum_{u\in V} (2-\deg(u))\Big(\delta(e;v,\pi_T(u)) - \delta(e;v,u)\Big).$$

When $e \in E$ and $v \in V$ are fixed, $u \mapsto \delta(e; v, u)$ is the indicator function of one component of the principal cut $G \setminus e$. We have

$$\delta(e;v,\pi_T(u)) - \delta(e;v,u) = \begin{cases} 0 & \text{if } \delta(e;\pi_T(u),u) = 0 \\ 1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 1 \\ -1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 0 \end{cases} \qquad (13)$$

Now consider varying u over all vertices, when e, T, and v are fixed. We have the following three cases:

Case 1: if $e \notin T$, then u and $\pi_T(u)$ are on the same side of the principal cut $G \setminus e$, for every vertex u. In this case $\delta(e; v, \pi_T(\cdot)) - \delta(e; v, \cdot) = 0$.

Case 2: if $e \in T(s_0)$ and s_0 is separated from v by e, then $\delta(e; v, \pi_T(\cdot)) - \delta(e; v, \cdot)$ is the indicator function for the floating component of $T \setminus e$. See Figure 3, left.

Case 3: if $e \in T(s_0)$ and s_0 is on the same component as v from e, then $\delta(e; v, \pi_T(\cdot)) - \delta(e; v, \cdot)$ is the negative of the indicator function for the floating component of $T \setminus e$. See Figure 3, right.

FIGURE 3. Edge $e \in T(s_0)$ with $\delta(e; v, s_0) = 1$ (left) and $\delta(e; v, s_0) = 0$ (right). The floating component of $T \setminus e$ is highlighted.

Thus when multiplying the term (13) by $(2 - \deg(u))$ and summing over all vertices u, we obtain

$$\sum_{u \in V} (2 - \deg(u)) \Big(\delta(e; v, \pi_T(u)) - \delta(e; v, u) \Big) = \begin{cases} 0 & \text{if } e \notin T, \\ 2 - \deg^o(T \setminus e, *) & \text{if } e \in T(s_0) \text{ and } \delta(e; v, s_0) = 1, \\ -(2 - \deg^o(T \setminus e, *)) & \text{if } e \in T(s_0) \text{ and } \delta(e; v, s_0) = 0. \end{cases}$$

Thus

$$\begin{aligned} &(D[S]\mathbf{m})_v - \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e \\ &= \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in T} \alpha_e (2 - \deg^o(T \setminus e, *)) \Big(\mathbb{1}(\delta(e; v, \pi_T(e)) = 1) - \mathbb{1}(\delta(e; v, \pi_T(e)) = 0) \Big). \end{aligned} \tag{14}$$

We now rewrite the above expression in terms of $\mathcal{F}_2(G; S)$. For the rest of the argument, let

$$(\star) = (D[S]\mathbf{m})_v - \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e.$$

Observe in (14) that the deletion $T \setminus e$ is an $(S, *)$-rooted spanning forest of G, and that the corresponding weights satisfy

$$w(\overline{F}) = \alpha_e \cdot w(\overline{T}) \qquad \text{if} \qquad F = T \setminus e.$$

Note that $F = T \setminus e$ is equivalent to $T = F \cup e$, and in particular this only occurs when we choose the edge e to be in the floating boundary $\partial F(*)$.

Thus

$$\begin{aligned} (\star) &= \sum_{F \in \mathcal{F}_2} w(\overline{F})(2 - \deg^o(F, *)) \sum_{e \in \partial F} \Big(\mathbb{1}(\delta(e; v, \pi_{(F \cup e)}(e)) = 1) - \mathbb{1}(\delta(e; v, \pi_{(F \cup e)}(e)) = 0) \Big) \\ &= \sum_{F \in \mathcal{F}_2} w(\overline{F})(2 - \deg^o(F, *)) \Bigg(\#\{e \in \partial F : \delta(e; v, \pi_T(e)) = 1 \text{ for } T = F \cup e\} \\ &\qquad - \#\{e \in \partial F : \delta(e; v, \pi_T(e)) = 0 \text{ for } T = F \cup e\} \Bigg). \end{aligned}$$

Now for any $e \notin F$, let $\delta(e; v, F(*)) = \delta(e; v, x)$ for any $x \in F(*)$, i.e.

$$\delta(e; v, F(*)) = \begin{cases} 1 & \text{if } e \text{ lies on path from } v \text{ to } F(*), \\ 0 & \text{otherwise.} \end{cases}$$

The condition that $\delta(e; v, \pi_{(F \cup e)}(e)) = 1$ (respectively $\delta(e; v, \pi_{(F \cup e)}(e)) = 0$) is equivalent to $\delta(e; v, F(*)) = 0$ (respectively $\delta(e; v, F(*)) = 1$). For an illustration, compare Figure 4 and 5. Thus

$$\begin{aligned} (\star) = \sum_{F \in \mathcal{F}_2} w(\overline{F})(2 - \deg^o(F, *)) \Bigg(&\#\{e \in \partial F(*) : \delta(e; v, F(*)) = 0\} \\ &- \#\{e \in \partial F(*) : \delta(e; v, F(*)) = 1\} \Bigg). \end{aligned}$$

Finally, we observe that for any forest F in $\mathcal{F}_2(G;S)$, there is exactly one edge e in the boundary $\partial F(*)$ of the floating component which satisfies $\delta(e;v,F(*))=1$, namely the unique boundary edge on the path from the floating component $F(*)$ to v. Hence

$$\#\{e\in\partial F(*):\delta(e;v,F(*))=1\}=1 \qquad\text{and}\qquad \#\{e\in\partial(F,*):\delta(e;v,F(*))=0\}=\deg^o(F,*)-1.$$

Thus the previous expression $(\star)$ simplifies as

$$\begin{aligned}(\star) &= \sum_{F\in\mathcal{F}_2} w(\overline{F})(2-\deg^o(F,*))\Big((\deg^o(F,*)-1)-(1)\Big)\\ &= -\sum_{F\in\mathcal{F}_2} w(\overline{F})(2-\deg^o(F,*))^2.\end{aligned}$$

as desired. □

FIGURE 4. Edge $e\in\partial F(*)$ with $\delta(e;v,F(*))=0$ (left) and $\delta(e;v,F(*))=1$ (right). The floating component $F(*)$ is highlighted.

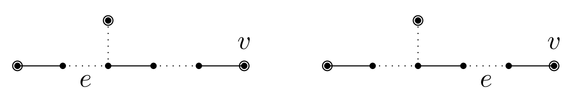


FIGURE 5. Edges $e\in\partial F(*)$ with $\delta(e;v,\pi_{(F\cup e)}(e))=1$ (left) and $\delta(e;v,\pi_{(F\cup e)}(e))=0$ (right).

Finally we can prove our main theorem: for any nonempty subset $S\subset V(G)$,

$$\det D[S]=(-1)^{|S|-1}2^{|S|-2}\left(\sum_{E(G)}\alpha_e\sum_{\mathcal{F}_1(G;S)}w(\overline{T})-\sum_{\mathcal{F}_2(G;S)}(\deg^o(F,*)-2)^2w(\overline{F})\right). \tag{15}$$

Proof of Theorem 1.2. First, suppose $|S|=1$. Then $D[S]$ is the zero matrix, and we must show that the right-hand side is zero. Since G is a tree, $\mathcal{F}_1(G;\{v\})$ consists of the tree G itself, with co-weight $w(\overline{G})=1$. Moreover, the subgraphs in $\mathcal{F}_2(G;\{v\})$ are precisely the tree splits $G\setminus e$, and for each $F=G\setminus e$ we have $w(\overline{F})=\alpha_e$ and $\deg^o(F,*)-2=-1$. This shows that the right-hand size of (15) is zero.

Next, suppose $|S|\geq 2$. Proposition 2.11 states that $D[S]$ is nonsingular, so we may use the inverse matrix identity

$$\mathbf{1}^\intercal D[S]^{-1}\mathbf{1}=\frac{\operatorname{cof} D[S]}{\det D[S]}. \tag{16}$$

Let $\mathbf{m}=\mathbf{m}(G;S)$ denote the vector (9). By Proposition 4.3 (a) and Theorem 2.3,

$$\mathbf{1}^\intercal\mathbf{m}=2\sum_{T\in\mathcal{F}_1(G;S)}w(\overline{T})=\frac{\operatorname{cof} D[S]}{(-1)^{1-|S|}2^{2-|S|}}.$$

Theorem 4.5 states that $D[S]\mathbf{m}=\lambda\mathbf{1}$ for some constant λ, which is nonzero since $D[S]$ is invertible and $\mathbf{m}$ is nonzero, c.f. Proposition 4.3 (b). Hence

$$\mathbf{1}^\intercal D[S]^{-1}\mathbf{1}=\lambda^{-1}\mathbf{1}^\intercal\mathbf{m}=\frac{\operatorname{cof} D[S]}{(-1)^{|S|-1}2^{|S|-1}\lambda}. \tag{17}$$

Comparing (16) with (17) gives the desired result, $\det D[S]=(-1)^{|S|-1}2^{|S|-1}\lambda$. □

Proof of Theorem 1.1. Set all weights α_e to 1 in Theorem 1.2. In this case, the weights $w(\overline{T}) = 1$ and $w(\overline{F}) = 2$ for all forests T and F, and

$$\sum_{e \in E} \alpha_e = n - 1, \qquad \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T}) = \kappa_1(G;S). \qquad \square$$

Remark 4.6. It is worth observing that depending on the chosen subset $S \subset V$, the distances appearing in the submatrix $D[S]$ may ignore a large part of the ambient tree G. We could instead replace G by the subtree $\mathrm{conv}(S, G)$ consisting of the union of all paths between vertices in S, which we call the *convex hull* of $S \subset G$. To apply formula (2) or (4) "efficiently," we should replace G on the right-hand side with the subtree $\mathrm{conv}(S, G)$. However, the formulas as stated are true even without this replacement due to cancellation of terms.

5. Physical interpretation

If we consider G as a network of wires with edge e containing a resistor of resistance α_e, which is grounded at all nodes in S, then the optimal vector $\mathbf{m}(G;S)$ defined in (9) has an interpretation as current flow: it records the currents exiting at $s \in S$ when current enters the vertices in the amount $\deg(v) - 2$ for each $v \notin S$.

5.1. **Alternate proof.** In the outline above, our first goal is to find a "special" vector $\mathbf{m} \in \mathbb{R}^S$ satisfying $D[S]\mathbf{m} = \lambda\mathbf{1}$. We can approach this first goal as follows: consider $\mathbb{R}^S$ inside the larger vector space $\mathbb{R}^V = \mathbb{R}^S \oplus \mathbb{R}^{V \setminus S}$, and let π_S denote the projection from $\mathbb{R}^V$ to $\mathbb{R}^S$. We wish to find vectors $\mathbf{n}(i) \in \mathbb{R}^V$ satisfying $\pi_S(D\mathbf{n}(i)) = \lambda_i\mathbf{1}$. OR, $D\mathbf{n}_i = \lambda_i \mathbf{1}^S \oplus (-)$. By finding sufficiently many such vectors $\mathbf{n}_i$, we can hope to find a linear combination that lies inside $\mathbb{R}^S \oplus \{0\}$.

Proposition 5.1. *Let $\mathbf{m} \in \mathbb{R}^V$ be the vector defined by $\mathbf{m}_v = 2 - \deg v$, and let D be the distance matrix of G. Then the entries of $D\mathbf{m}$ are constant on $V(G)$.*

Proof. It suffices to show that for each edge e, with endpoints (e^+, e^-), we have $(D\mathbf{m})_{(e^+)} = (D\mathbf{m})_{(e^-)}$. To compute $(D\mathbf{m})_{(e^+)} - (D\mathbf{m})_{(e^-)}$, first observe that the distance function on G satisfies

$$d(v, e^+) - d(v, e^-) = \begin{cases} \alpha_e & \text{if } v \text{ is closer to } e^- \text{ than } e^+, \\ -\alpha_e & \text{if } v \text{ is closer to } e^+ \text{ than } e^-. \end{cases}$$

Thus

$$\begin{aligned} (D\mathbf{m})_{(e^+)} - (D\mathbf{m})_{(e^-)} &= \sum_{v \in V} (d(v, e^+) - d(v, e^-))(2 - \deg v) \\ &= \sum_{v \in (G \setminus e)^-} \alpha_e (2 - \deg v) - \sum_{v \in (G \setminus e)^+} \alpha_e (2 - \deg v) \\ &= \alpha_e \left(\sum_{v \in (G \setminus e)^-} (2 - \deg v) - \sum_{v \in (G \setminus e)^+} (2 - \deg v) \right) \end{aligned} \tag{18}$$

For each sum in (18), we apply Lemma 2.6 to obtain

$$\sum_{v \in (G \setminus e)^-} (2 - \deg v) = (2 - \deg^o((G \setminus e)^-) = 1,$$

since each component of $(G \setminus e)$ has outdegree one. The same identity applies to the sum over $(G \setminus e)^+$, so $(D\mathbf{m})_{(e^+)} = (D\mathbf{m})_{(e^-)}$ as desired. $\square$

Proposition 5.2. *Fix $v \in V \setminus S$. Consider the vector $\mathbf{n} = \mathbf{n}(G; S, v) \in \mathbb{R}^V$ defined by*

$$\mathbf{n} = \sum_{T \in \mathcal{F}_1(G;S)} \Big(\boldsymbol{\delta}(v) - \boldsymbol{\delta}(\pi_T(v)) \Big).$$

Then $D\mathbf{n}$ is constant on S, i.e. $\pi_S(D\mathbf{n}) = \lambda\mathbf{1}$ for some λ.

Remark 5.3. For each $s \in S$, let $\mu(v, s)$ denote the current flowing to s when G is grounded at S and one unit of current enters G at v. Then

$$\mu(v, s) = \frac{1}{\kappa(G; S)}\mathbf{n}(v)_s.$$

Explicitly, if $s = s_j$, then

$$\mu(v, s_j) = \frac{\sum_{\mathcal{F}_1(G;S)} \mathbb{1}(\pi_T(v) = s_j)}{\kappa(G; S)} = \frac{\kappa_r(s_1|\cdots|s_j v|\cdots|s_r)}{\kappa(G; S))}$$

where $\kappa_r(s_1|\cdots|s_j v|\cdots|s_r)$ is the number of S-rooted spanning forests of G whose s_j-component contains v.

Proof sketch. For any $s, s' \in S$, consider tracking the value of $D\mathbf{n}$ along path from s to s'. The value of $D\mathbf{n}$ changes according to current flow in the corresponding network, i.e. $D\mathbf{n}$ records electrical potential. The set S is grounded by assumption, so $D\mathbf{n}$ takes the same value at s and s'. ☐

Theorem 5.4. *Let G be a tree, S a nonempty subset of vertices, and $D[S]$ the submatrix of the distance matrix of G. Suppose $\mathbf{m} = \mathbf{m}(G; S) \in \mathbb{R}^S$ is defined by (9);*

$$\mathbf{m}(G; S)_s = \sum_{T\in\mathcal{F}_1(G;S)} w(\overline{T}) \sum_{u\in T(s)} (2 - \deg u) = \sum_{T\in\mathcal{F}_1(G;S)} w(\overline{T})(2 - \deg^o(T, s)).$$

Then $D[S]\mathbf{m} = \lambda\mathbf{1}$ for some constant λ.

Proof. The vector $\mathbf{m} = \mathbf{m}(G; S)$ can be expressed as a linear combination of δ-vectors

$$\mathbf{m}(G; S) = \sum_{T\in\mathcal{F}_1(G;S)} w(\overline{T}) \sum_{u\in V}(2 - \deg(u))\boldsymbol{\delta}(\pi_T(u)).$$

Therefore

$$\begin{aligned}
\mathbf{m}(G; S) &= \sum_{T\in\mathcal{F}_1}\sum_{v\in V}(2 - \deg v)\boldsymbol{\delta}(v) - \sum_{T\in\mathcal{F}_1}\sum_{v\in V}(2 - \deg v)(\boldsymbol{\delta}(v) - \boldsymbol{\delta}(\pi_T(v)) \\
&= \kappa(G; S)\sum_{v\in V}(2 - \deg v)\boldsymbol{\delta}(v) - \sum_{v\in V\setminus S}(2 - \deg v)\mathbf{n}(G; S, v) \\
&= \kappa(G; S)\mathbf{m}(G; V) - \sum_{v\in V\setminus S}(2 - \deg v)\mathbf{n}(G; S, v).
\end{aligned}$$

◊ TODO: elaborate on this equation? ◊ From Proposition 5.1 we know that $D\mathbf{m}(G; V)$ is constant on V, and from Proposition 5.2 we know that for each $v \in V \setminus S$ the product $D\mathbf{n}(G; S, v)$ is constant on S. Hence by linearity, $D\mathbf{m}(G; S)$ is constant on S. ☐

Example 5.5. If

$$D[S \cup t] = \begin{bmatrix} 0 & a & b & c \\ a & 0 & a+b & a+c \\ b & a+b & 0 & b+c \\ c & a+c & b+c & 0 \end{bmatrix}$$

then

$$\begin{bmatrix} 0 & a & b & c \\ a & 0 & a+b & a+c \\ b & a+b & 0 & b+c \\ c & a+c & b+c & 0 \end{bmatrix} \begin{bmatrix} ab+ac+bc \\ -bc \\ -ac \\ -ab \end{bmatrix} = \begin{bmatrix} -3abc \\ -abc \\ -abc \\ -abc \end{bmatrix}$$

5.2. **Symanzik polynomials.** We note that the expression in the main theorem, Theorem 1.2, is related to Symanzik polynomials, which we recall here.

Given a graph $G = (V, E)$, the *first Symanzik polynomial* is the homogeneous polynomial in edge-indexed variables $\underline{x} = \{x_e : e \in E\}$ defined by

$$\psi_G(\underline{x}) = \sum_{T \in \mathcal{F}_1(G)} \prod_{e \notin T} x_e,$$

where $\mathcal{F}_1(G)$ denotes the set of spanning trees of G.

Consider a "momentum" function $p : V \to \mathbb{R}$ which satisfies $\sum_{v \in V} p(v) = 0$. Then the second Symanzik polynomial is

$$\varphi_G(p; \underline{x}) = \sum_{F \in \mathcal{F}_2(G)} \left(\sum_{v \in F_1} p(v) \right)^2 \prod_{e \notin F} x_e,$$

where $\mathcal{F}_2(G)$ is the set of two-component spanning forests of G, and F_1 denotes one of the components of F. It doesn't matter which component we label as F_1, due to the momemtum constraint $\sum_{v \in V} p(v) = 0$.

Theorem statement:

$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \left(\sum_{E(G)} \alpha_e \sum_{\mathcal{F}_1(G;S)} w(\overline{T}) - \sum_{\mathcal{F}_2(G;S)} (\deg^o(F, *) - 2)^2 w(\overline{F}) \right).$$

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \frac{1}{2} \left(\sum_{e \in E} \alpha_e - \frac{\sum_{F \in \mathcal{F}_2(G;S)} w(\overline{F}) (\deg^o(F, *) - 2)^2}{\sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})} \right)$$

In terms of Symanzik polynomials, let ψ and φ denote the first and second Symanzik polynomials of the quotient graph G/S. We have

$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \left(\sum_{E(G)} \alpha_e \, \psi_{(G/S)}(\underline{\alpha}) - \phi_{(G/S)}(p; \underline{\alpha}) \right).$$

and

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \frac{1}{2} \left(\sum_{e \in E} \alpha_e - \frac{\varphi_{(G/S)}(p; \underline{\alpha})}{\psi_{(G/S)}(\underline{\alpha})} \right)$$

with momentum function $p(v) = \deg(v) - 2$ for $v \notin S$.

6. Examples

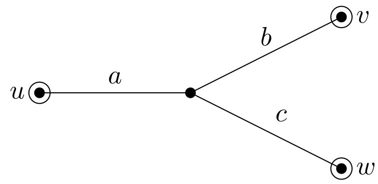
Example 6.1. Suppose G is a tree consisting of three paths joined at a central vertex. Let S consist of the central vertex, and the three endpoints of the paths. The corresponding minor of the distance matrix is

$$D[S] = \begin{bmatrix} 0 & a & b & c \\ a & 0 & a+b & a+c \\ b & a+b & 0 & b+c \\ c & a+c & b+c & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & a & b & c \\ a & -a & a & a \\ b & b & -b & b \\ c & c & c & -c \end{bmatrix} \sim \begin{bmatrix} 0 & a & b & c \\ a & -2a & 0 & 0 \\ b & 0 & -2b & 0 \\ c & 0 & 0 & -2c \end{bmatrix}.$$

The determinant is

$$\det D[S] = -4(a + b + c)abc.$$

Example 6.2. Suppose Γ is a tripod with lengths a, b, c and corresponding leaf vertices u, v, w.



Let $S = \{u, v, w\}$. Then

$$D[S] = \begin{bmatrix} 0 & a+b & a+c \\ a+b & 0 & b+c \\ a+c & b+c & 0 \end{bmatrix}.$$

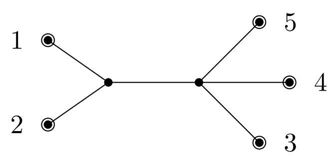
and

$$\det D[S] = 2(a+b)(a+c)(b+c) = 2\left((a+b+c)(ab+ac+bc) - abc\right).$$

The "special vector" that satisfies $D[S]\mathbf{m} = \lambda \mathbf{1}$ in this example is

$$\mathbf{m} = \begin{bmatrix} a(b+c) & b(a+c) & c(a+b) \end{bmatrix}^{\intercal}.$$

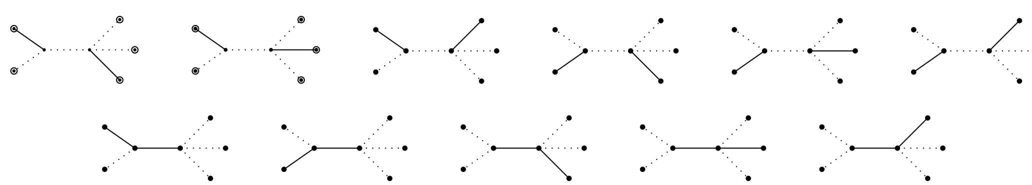
Example 6.3. Suppose G is the tree with unit edge lengths shown below, with five leaf vertices.



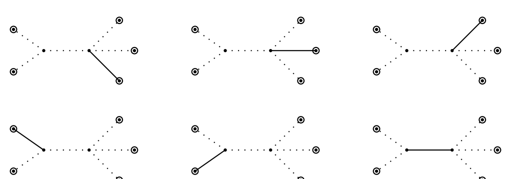
Let S denote the set of five leaf vertices. Then

$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 3 & 3 \\ 2 & 0 & 3 & 3 & 3 \\ 3 & 3 & 0 & 2 & 2 \\ 3 & 3 & 2 & 0 & 2 \\ 3 & 3 & 2 & 2 & 0 \end{bmatrix}.$$

There are 11 forests in $\mathcal{F}_1(G; S)$:



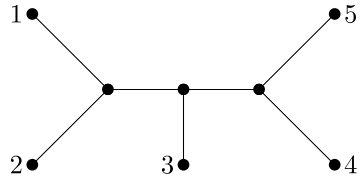
There are 6 forests in $\mathcal{F}_2(G; S)$:



and

$$\det D[S] = 368 = (-1)^4 2^3 \left(6 \cdot 11 - (3 \cdot 1^2 + 2 \cdot 2^2 + 1 \cdot 3^2)\right)$$

Example 6.4. Suppose G is the tree with unit edge lengths shown below, with five leaf vertices and three internal vertices.



Let S denote the set of five leaf vertices. Then

$$D[S] = \begin{bmatrix} 0 & 2 & 3 & 4 & 4 \\ 2 & 0 & 3 & 4 & 4 \\ 3 & 3 & 0 & 3 & 3 \\ 4 & 4 & 3 & 0 & 2 \\ 4 & 4 & 3 & 2 & 0 \end{bmatrix}$$

and

$$\det D[S] = 864 = (-1)^4 2^3 \left(7 \cdot 21 - (14 \cdot 1^2 + 4 \cdot 2^2 + 1 \cdot 3^2)\right)$$

7. Further work

It is natural to ask whether these results for trees may be generalized to arbitrary finite graphs. We address this in [10], which involve more technical machinery.
See [9].

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