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.

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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

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

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

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

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 floating 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,

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

which was proved by Bapat–Kirkland–Neumann [1]. The weighted identity (3) reduces to (1) when taking all unit weights, $\alpha_e = 1$. We 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 weighted distance matrix $D = D^{(\alpha)}$. For any nonempty subset $S \subset V$, we have

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

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 co-weights of the forests T and F, and $\deg^o(F,*)$ is the outdegree of the floating component of F, as above.

Theorem 1.2 reduces to Theorem 1.1 when taking all unit weights, $\alpha_e = 1$. We now demonstrate our main theorem on an example, in the unweighted case.

Example 1.3. Suppose G is the tree with unit edge weights shown in Figure 1, with five leaf vertices and three internal vertices. Let S denote the set of leaf vertices. The corresponding distance

submatrix is
$$D[S] = \begin{pmatrix} 0 & 2 & 3 & 4 & 4 \\ 2 & 0 & 3 & 4 & 4 \\ 3 & 3 & 0 & 3 & 3 \\ 4 & 4 & 3 & 0 & 2 \\ 4 & 4 & 3 & 2 & 0 \end{pmatrix}$$
, which has determinant 864.

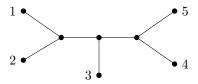


Figure 1. Tree with five leaves.

The tree G has 7 edges and 21 S-rooted spanning forests. There are 19 (S, *)-rooted spanning forests; of the floating components in these forests, 14 have outdegree three, 4 have outdegree four, and 1 has outdegree five. By Theorem 1.1,

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

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 $(\det D[S])/(\cot D[S])$ which we describe here.

Given a matrix A, let 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 the sum of entries of the matrix inverse A^{-1} multiplied 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,

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

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

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

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

Theorem 1.4 (Monotonicity of normalized principal minors). If $A, B \subset V(G)$ are nonempty subsets with $A \subset B$, then

$$\frac{\det D[A]}{\cot D[A]} \le \frac{\det D[B]}{\cot D[B]}.$$

[mention Devrient's thesis, Property 3.38] The essential observation behind this result is that $\det D[S]/\cot D[S]$ is calculated via the following quadratic optimization problem: for all vectors $\mathbf{u} \in \mathbb{R}^S$,

maximize objective function: $\mathbf{u}^{\mathsf{T}}D[S]\mathbf{u}$ with constraint: $\mathbf{1}^{\mathsf{T}}\mathbf{u} = 1$.

This result can be shown using Lagrange multipliers, and relies of knowledge of the signature of D[S]. For details, see Section 4.

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

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

We get refined bounds by making use of the monotonicity property, Theorem 1.4.

Theorem 1.5 (Bounds on principal minor ratios). Suppose G = (V, E) is a finite, weighted tree with distance matrix $D^{(\alpha)}$.

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

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

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

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

1.3. Further questions. It is natural to ask whether our results for trees may be generalized to arbitrary finite graphs. We address this in [9], which involves more technical machinery.

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

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

where L is the Laplacian matrix and **m** is the vector $\mathbf{m}_v = 2 - \deg v$. There is also a weighted version, see equation (9). Does there exist a nice expression for the inverse of the matrix D[S], or for the weighted version?

2. Graphs and spanning forests

For background on enumeration problems for graphs and trees, see Tutte [10, 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.

 $w(\overline{H}) = w(E(H)).$

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[S] denote the submatrix obtained by deleting the S-indexed rows and columns.

If G is a tree, we let conv(S,G) denote the subtree consisting of the union of all paths between vertices in S, which we call the *convex hull* of $S \subset G$.

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 $S = \{v_1, v_2, \dots, v_r\}$, an S-rooted spanning forest of G is a spanning forest which has exactly one vertex v_i in each connected component. Given $s \in S$ and a forest F, we let F(s) denote the s-component of F.

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].

As before, for an (S,*)-rooted spanning forest F, we let F(s) denote the s-component of F, and additionally let F(*) denote the floating component. (We may refer to the floating component as the *-component of F.)

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, i.e. $\kappa(G;S) = \kappa(G/S)$.

Example 2.1. Suppose G is the tree with unit edge weights 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 2 and 3, respectively.

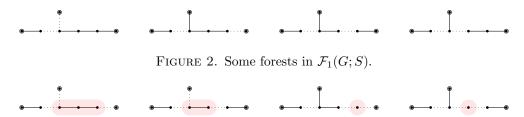


FIGURE 3. Some forests in $\mathcal{F}_2(G; S)$, with floating component highlighted.

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^- . We assume all graphs in the paper are equipped with an implicit orientation. The incidence matrix depends on the orientation, but the Laplacian matrix does not.

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

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

Here $\mathbb{1}(\cdot)$ denotes the indicator function. Let $L \in \mathbb{R}^{V \times V}$ denote the *Laplacian matrix* of G, which is defined by $L = BB^{\mathsf{T}}$. 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

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

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 the 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 $\{\alpha_e\}$. For any nonempty vertex set $S \subset V$,

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

where $\mathcal{F}_1 = \mathcal{F}_1(G; S)$ is the set of S-rooted spanning forests.

Proof. See Tutte [10, Section VI.6, Equation (VI.6.7)] or Chaiken [4] or Bapat [2, Theorem 4.7]. \Box

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 v, w are in different components of the tree 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 2.3 (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 forest components. 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

(7)
$$\sum_{v \in V(G)} (2 - \deg(v)) = 2.$$

In this section we state a generalization, Lemma 2.4 which will be used later.

Given a connected subgraph $H \subset G$, we define the *edge boundary* ∂H as the set of edges which join H to its complement; i.e.

$$\partial H = \{e = \{a, b\} \in E : a \in V(H), b \notin V(H)\}.$$

We define the *outdegree* of H as the number of edges in its edge boundary, $\deg^o(H) = |\partial H|$. (The edge boundary and outdegree do not depend on the implicit orientation on E.)

We often use the following special case of the outdegree: We define the *outdegree* $\deg^o(F, s)$ as the number of edges which join F(s) to a different component; i.e.

(8)
$$\deg^{o}(F, s) = |\{e = (a, b) \in E : a \in F(s), b \notin F(s)\}|.$$

(Recall that F(s) denotes the s-component of an S-rooted spanning forest F.) If F is a forest in $\mathcal{F}_2(G;S)$, let $\deg^o(F,*)$ denote the outdegree of the floating component and $\partial F(*)$ its edge boundary.

Lemma 2.4. 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

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

Remark 2.5. A key step in the proof of Theorem 1.2 uses the following "transition structure" which relates the S-rooted spanning forests $\mathcal{F}_1(G;S)$ with (S,*)-rooted spanning forests $\mathcal{F}_2(G;S)$, via the operations of edge-deletion and edge-union.

Consider the "deletion" map

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

defined by

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

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

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 spanning forest $T \in \mathcal{F}_1(G; S)$, there are exactly (|V| - 1)-many choices of pairs $(e, F) \in E(G) \times \mathcal{F}_2(G; S)$ such that $T = F \cup e$ (since |E(T)| = |V| - 1 for any spanning tree T).

2.5. **Symanzik polynomials.** We note that the expression in the main theorem, Theorem 1.2, is closely 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 the constraint $\sum_{v \in V} p(v) = 0$. 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 , since the momentum constraint implies that $\sum_{v \in F_1} p(v) = -\sum_{v \in F_2} p(v)$.

In terms of Symanzik polynomials, let ψ and φ denote the first and second Symanzik polynomials of the quotient graph G/S. Let p be the momentum function $p(v) = \deg(v) - 2$ for $v \notin S$. We have

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

(equivalent to Theorem 1.2), or more succinctly,

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

(equivalent to equation (6)).

3. Distance minors: Preliminaries

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

3.1. Signature and invertibility. Given a distance matrix D of a tree, the submatrix D[S] has nonzero determinant, as long as $|S| \geq 2$. We give a proof in this section, based on finding the signature of D[S] as a bilinear form. The argument in this section, particularly Proposition 3.3, was communicated to the authors by R. Bapat, via personal communication.

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

Proposition 3.1 (Cauchy interlacing). Suppose M is a symmetric real matrix with ordered eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$, and the submatrix M[i] has ordered eigenvalues $\mu_1 \leq \cdots \leq \mu_{n-1}$. Then

$$\lambda_1 \le \mu_1 \le \lambda_2 \le \dots \le \mu_{n-1} \le \lambda_n.$$

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

Lemma 3.2 (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. See Lemma 8.15 of [2]. The proof is by induction on the number of vertices, and uses Cauchy interlacing. \Box

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].

Proposition 3.3. 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) We apply decreasing induction on the size of S. If S=V, use Lemma 3.2. Now suppose |S|=k where $2\leq k< n$, and assume by induction hypothesis that the claim holds for all vertex subsets of size greater than k. Let $S^+\subset V$ be a set of k+1 vertices containing S. The inductive hypothesis states that $D[S^+]$ has k negative eigenvalues and one positive eigenvalue, so Cauchy interlacing from $D[S^+]$ implies that D[S] has at least k-1 negative eigenvalues. Since all diagonal entries of D[S] are zero, D[S] has zero trace. Thus the remaining eigenvalue of D[S] must be positive, as claimed.

(b) This follows from (a).
$$\Box$$

3.2. **Negative definite hyperplane.** In this section, we prove that a distance (sub)matrix induces a negative semidefinite quadratic form on the hyperplane of vectors whose coordinates sum to zero. This will be used in Section 4 on quadratic optimization.

Bapat-Kirkland-Neumann [1, Theorem 2.1] proved that

(9)
$$(D^{(\alpha)})^{-1} = -\frac{1}{2}L^{(\alpha)} + \frac{1}{2}\left(\sum_{e \in E} \alpha_e\right)^{-1} \mathbf{m} \, \mathbf{m}^{\mathsf{T}}$$

where **m** is the vector with components $\mathbf{m}_v = 2 - \deg v$. The unweighted version of (9) appeared earlier in Graham–Lovasz [5, Lemma 1].

Proposition 3.4. 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 (9) by the all-ones vector $\mathbf{1}$; since $L^{(\alpha)}\mathbf{1} = 0$ and $\mathbf{m}^{\intercal}\mathbf{1} = 2$, we obtain

$$(D^{(\alpha)})^{-1}\mathbf{1} = \left(\sum_{e \in E} \alpha_e\right)^{-1} \mathbf{m}.$$

Hence $D^{(\alpha)}\mathbf{m} = (\sum_{e \in E} \alpha_e) \mathbf{1}$. Then multiply (9) by $D^{(\alpha)}$ on both sides.

Proposition 3.5. Suppose D is the (weighted) distance matrix of a tree.

- (a) If $\mathbf{u} \in \mathbb{R}^V$ is a vector whose coordinates sum to zero, then $\mathbf{u}^{\intercal} D \mathbf{u} \leq 0$.
- (b) If $\mathbf{u} \in \mathbb{R}^S$ is a vector whose coordinates sum to zero, then $\mathbf{u}^{\mathsf{T}}D[S]\mathbf{u} \leq 0$.

Proof. (a) By assumption $\mathbf{1}^{\mathsf{T}}\mathbf{u} = 0$. Using Proposition 3.4,

$$\mathbf{u}^{\mathsf{T}}D\mathbf{u} = -\frac{1}{2}\mathbf{u}^{\mathsf{T}}DLD\mathbf{u} + 0.$$

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

(b) This follows from (a) since $\mathbf{u}^{\mathsf{T}}D[S]\mathbf{u} = \widetilde{\mathbf{u}}^{\mathsf{T}}D\widetilde{\mathbf{u}}$ where $\widetilde{\mathbf{u}}$ is the extension of \mathbf{u} by zeros.

4. Quadratic optimization

In this section, we explain how the quantity $\frac{\det D[S]}{\cot D[S]}$ arises as the solution of the following quadratic optimization problem: for all vectors $\mathbf{u} \in \mathbb{R}^S$,

maximize objective function: $\mathbf{u}^{\mathsf{T}}D[S]\mathbf{u}$

with constraint: $\mathbf{1}^{\mathsf{T}}\mathbf{u} = 1$.

The statement is proved as Proposition 4.1.

Proposition 4.1. If D[S] is a principal submatrix of a distance matrix indexed by S, then

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

where $\cot D[S]$ 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 $|S| \ge 2$. Proposition 3.5 implies that the objective function $\mathbf{u} \mapsto \mathbf{u}^{\mathsf{T}} D[S] \mathbf{u}$ is concave on the domain $\mathbf{1}^{\mathsf{T}} \mathbf{u} = 1$, so any critical point is a local maximum. The gradient of the objective function is $2D[S]\mathbf{u}$, and the gradient of the constraint is 1. By the theory of Lagrange multipliers, the optimal solution \mathbf{u}^* is a vector satisfying

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

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

$$(\mathbf{u}^*)^{\mathsf{T}}D[S]\mathbf{u}^* = (D[S]\mathbf{u}^*)^{\mathsf{T}}\mathbf{u}^* = \lambda(\mathbf{1}^{\mathsf{T}}\mathbf{u}^*) = \lambda.$$

Here we use the fact that D[S] is symmetric, and the given constraint $\mathbf{1}^{\mathsf{T}}\mathbf{u} = 1$.

On the other hand, since D[S] is invertible (Proposition 3.3) we have $\mathbf{u}^* = \lambda(D[S]^{-1}\mathbf{1})$, so that

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

Thus the optimal objective value is $\lambda = \frac{\det D[S]}{\cot D[S]}$

Remark 4.2. If we consider G as a network of wires with each edge e containing a resistor of resistance α_e , then the optimal vector \mathbf{u}^* has a physical interpretation as current flow: it records the currents exiting at $s \in S$ when current enters the network in the amount $\frac{1}{2}(\deg(v) - 2)$ for each $v \in V$, and the network is grounded at all nodes in S.

We give an explicit combinatorial expression for \mathbf{u}^* , up to a normalizing constant, in Definition 5.2. It is a classical result in network theory that this gives the current flow; see Tutte [10, Section VI.6].

4.1. Cofactor sums. 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 cof M denotes the sum of cofactors of M, i.e. $\operatorname{cof} M = \sum_{i=1}^{n} \sum_{j=1}^{n} (-1)^{i+j} \operatorname{det} M[\overline{i}, \overline{j}]$ where

 $M[\bar{i},\bar{j}]$ denotes the matrix with the *i*-th row and *j*-th column deleted.

Theorem 4.3 (Distance submatrix cofactor sums). Given a tree G = (V, E) with edge weights, let $D^{(\alpha)}$ be the weighted distance matrix of G. Let $S \subset V$ be a nonempty subset of vertices. 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

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

where $L^{(\alpha)}$ is the weighted Laplacian matrix. 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 4.4. Suppose $D^{(\alpha)}$ is the distance matrix of a weighted tree with edge weights $\{\alpha_e : e \in E\}$. Then

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

Proof. Consider applying Theorem 4.3 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.

4.2. **Monotonicity.** As a consequence of Proposition 4.1, we show that the ratio $\frac{\det D[S]}{\cot D[S]}$ behaves

monotonically in S, and deduce further bounds on $\frac{\det D[S]}{\cot D[S]}$.

We first note the following restatement of Proposition 4.1, viewing \mathbb{R}^S as a subspace of \mathbb{R}^V where coordinates indexed by $V \setminus S$ are set to zero.

Corollary 4.5. If D[S] is a principal submatrix of a distance matrix indexed by S, then

$$\frac{\det D[S]}{\operatorname{cof} D[S]} = \max \{ \mathbf{u}^{\mathsf{T}} D \mathbf{u} : \mathbf{u} \in \mathbb{R}^{V}, \ \mathbf{1}^{\mathsf{T}} \mathbf{u} = 1, \ \mathbf{u}_{v} = 0 \ \textit{if} \ v \not\in S \}$$

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

Proof of Theorem 1.4. We are to show that for vertex subsets $A \subset B$, we have $\frac{\det D[A]}{\cot D[A]} \leq \frac{\det D[B]}{\cot D[B]}$

By Corollary 4.5, both values $\frac{\det D[A]}{\cot D[A]}$ and $\frac{\det D[B]}{\cot D[B]}$ arise from optimizing the same objective function on an affine subspace of \mathbb{R}^V , but the subspace for A is contained in the subspace for B. \square

Proof of 1.5. (a) Recall that conv(S,G) denotes the subgraph of G which is the union of all paths between vertices in S. To see that

$$\frac{\det D[S]}{\cot D[S]} \le \frac{1}{2} \sum_{E(\text{conv}(S,G))} \alpha_e,$$

take B as the set of all vertices in conv(S,G). Then $S \subset B$, and apply Theorem 1.4. By Proposition 4.4 we have

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

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

$$\frac{1}{2} \sum_{e \in \gamma} \alpha_e \le \frac{\det D[S]}{\cot D[S]},$$

take A as the set of endpoints of $\{s_0, s_1\}$. Then $A \subset S$ by assumption, and apply Theorem 1.4. By Proposition 4.4 we have

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

5. Distance minors: Proofs

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

- 5.1. Outline of proof. In Section 4, we showed that $\frac{\det D[S]}{\cot D[S]}$ is the maximum value of the function $\mathbf{u} \mapsto \mathbf{u}^{\mathsf{T}} D[S] \mathbf{u}$ on an affine hyperplane of \mathbb{R}^S , and that the maximum is achieved when $D[S] \mathbf{u}^* = \lambda \mathbf{1}$. We can thus compute $\det D[S]$ via the following steps.
 - (i) Find a 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. $\mathbf{1}^{\mathsf{T}}\mathbf{m}$, and normalize $\mathbf{u}^* = \frac{\mathbf{m}}{\mathbf{1}^{\mathsf{T}}\mathbf{m}}$. This solves the optimization problem of Section 4.
- (iii) Find the optimal objective value $\lambda^* = \frac{\lambda}{1^{\mathsf{T}}\mathbf{m}}$
- (iv) Use the expression for cof D[S] in Theorem 4.3 to compute det $D[S] = \lambda^*(\text{cof } D[S])$.

Example 5.1. Suppose G is the tree with unit edge weights shown below.

$$v_2 \quad \bullet \quad \bullet \quad v_3$$

 $v_2 \ \bullet - \bullet - \bullet \ v_3$ If S is the set of leaf vertices, the distance submatrix is $D[S] = \begin{pmatrix} 0 & 3 & 4 \\ 3 & 0 & 5 \\ 4 & 5 & 0 \end{pmatrix}$. Following the steps outlined above:

- (i) The vector $\mathbf{m} = \begin{pmatrix} 5 \\ 8 \\ 9 \end{pmatrix}$ satsifies $D[S]\mathbf{m} = \lambda \mathbf{1}$ for $\lambda = 60$.
- (ii) The sum of entries of \mathbf{m} is $\mathbf{1}^{\mathsf{T}}\mathbf{m} = 22$

(iii) We have $\lambda^* = \frac{\lambda}{\mathbf{1}^{\mathsf{T}}\mathbf{m}} = \frac{30}{11}$. (iv) The cofactor sum is $\operatorname{cof} D[S] = 44$, so $\det[S] = \lambda^*(\operatorname{cof} D[S]) = 120$.

It turns out that the entries of **m** are combinatorially meaningful (see Definition 5.2), which also gives combinatorial meaning to the constant λ .

5.2. **General case.** Fix a tree G = (V, E) with edge weights $\{\alpha_e : e \in E\}$ and a nonempty subset $S \subset V$. We first define a vector **m** which satisfies the relation $D[S]\mathbf{m} = \lambda \mathbf{1}$ for some λ .

Definition 5.2. Let $\mathbf{m} = \mathbf{m}(G; S)$ denote the vector in \mathbb{R}^S be defined by

(10)
$$\mathbf{m}_v = \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})(2 - \deg^o(T,v)) \quad \text{for each } v \in S.$$

where $w(\overline{T})$ is the co-weight of T (see Section 2.4) and $\deg^o(T,v)$ is the outdegree of the v-component of T (see Section 2.4, equation (8)).

Let 1 denote the all-ones vector.

Proposition 5.3. Suppose S is nonempty. For the vector $\mathbf{m} = \mathbf{m}(G; S)$ defined above,

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

(b) if all edge weights α_e are positive, **m** is nonzero.

Proof. (a) By Lemma 2.4 we can express $\deg^o(T,s)$ as a sum over vertices in T(s),

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

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

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

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 $S\text{-}\mathrm{rooted}$ spanning forest. Thus

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

where we apply equation (7) for the last equality.

(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 $\mathbf{1}^{\intercal}\mathbf{m} > 0$.

Corollary 5.4. If G is a graph with unit edge weights $\alpha_e = 1$, then the vector **m** defined in (10) satisfies $\mathbf{1}^{\mathsf{T}}\mathbf{m} = 2 \kappa(G; S)$.

Theorem 5.5. With $\mathbf{m} = \mathbf{m}(G; S)$ defined as in (10), $D[S]\mathbf{m} = \lambda \mathbf{1}$ for the constant

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

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

$$(D[S]\mathbf{m})_{v} = \sum_{s \in S} d(v, s)\mathbf{m}_{s}$$

$$= \sum_{s \in S} \left(\sum_{e \in E(G)} \alpha_{e} \,\delta(e; v, s)\right) \left(\sum_{T \in \mathcal{F}_{1}(G; S)} (2 - \deg^{o}(T, s))w(\overline{T})\right)$$

$$= \sum_{T \in \mathcal{F}_{1}} w(\overline{T}) \sum_{e \in E} \alpha_{e} \left(\sum_{s \in S} \delta(e; v, s)(2 - \deg^{o}(T, s))\right)$$

$$= \sum_{T \in \mathcal{F}_{1}} w(\overline{T}) \sum_{e \in E} \alpha_{e} \left(\sum_{s \in S} \delta(e; v, s) \sum_{u \in T(s)} (2 - \deg(u))\right).$$

$$(11)$$

where in the last equality, we apply Lemma 2.4 to the subgraph H = T(s).

We introduce additional notation to handle the double sum in parentheses in (11). Each S-rooted spanning tree T naturally induces a surjection $\pi_T: V \to S$, defined by

$$\pi_T(u) = s$$
 if and only if $u \in T(s)$.

Using this notation,

(12)
$$(D[S]\mathbf{m})_v = \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e \left(\sum_{u \in V} (2 - \deg(u)) \delta(e; v, \pi_T(u)) \right)$$

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 2.4 (b), we have $\sum_{u \in V} (2 - \deg(u)) \delta(e; v, u) = 1$. Thus

(13)
$$\sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e = \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e \left(\sum_{u \in V} (2 - \deg(u)) \delta(e; v, u) \right)$$

By subtracting equation (13) from (12), we obtain

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

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

(14)
$$\delta(e; v, \pi_T(u)) - \delta(e; v, u) = \begin{cases} 0 & \text{if } \delta(e; \pi_T(u), u) = 0\\ 1 & \text{if } \delta(e; \pi_T(u), u) = 1 \text{ and } \delta(e; v, \pi_T(u)) = 1\\ -1 & \text{if } \delta(e; \pi_T(u), u) = 1 \text{ and } \delta(e; v, \pi_T(u)) = 0. \end{cases}$$

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 $e \in T$ and $\pi_T(e)$ 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 4, left.

Case 3: if $e \in T$ and $\pi_T(e)$ 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 4, right.



FIGURE 4. Edge $e \in T$ with $\delta(e; v, \pi_T(e)) = 1$ (left) and $\delta(e; v, \pi_T(e)) = 0$ (right). The floating component of $T \setminus e$ is highlighted.

Thus when multiplying the term (14) by $(2 - \deg(u))$ and summing over all vertices u, we obtain

$$\sum_{u \in V} (2 - \deg(u)) \Big(\delta(e; v, \pi_T(u)) - \delta(e; v, u) \Big) = \begin{cases} 0 & \text{if } e \not\in T, \\ 2 - \deg^o(T \setminus e, *) & \text{if } e \in T(s_0) \text{ and } \delta(e; v, s_0) = 1, \\ -(2 - \deg^o(T \setminus e, *)) & \text{if } e \in T(s_0) \text{ and } \delta(e; v, s_0) = 0. \end{cases}$$

Thus

$$(D[S]\mathbf{m})_{v} - \sum_{T \in \mathcal{F}_{1}} w(\overline{T}) \sum_{e \in E} \alpha_{e}$$

$$= \sum_{T \in \mathcal{F}_{1}} w(\overline{T}) \sum_{e \in T} \alpha_{e} (2 - \deg^{o}(T \setminus e, *)) \Big(\mathbb{1}(\delta(e; v, \pi_{T}(e)) = 1) - \mathbb{1}(\delta(e; v, \pi_{T}(e)) = 0) \Big).$$

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

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

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

$$(\star) = \sum_{F \in \mathcal{F}_2} w(\overline{F})(2 - \deg^o(F, *)) \sum_{e \in \partial F} \left(\mathbb{1}(\delta(e; v, \pi_{(F \cup e)}(e)) = 1) - \mathbb{1}(\delta(e; v, \pi_{(F \cup e)}(e)) = 0) \right)$$

$$= \sum_{F \in \mathcal{F}_2} w(\overline{F})(2 - \deg^o(F, *)) \left(\#\{e \in \partial F : \delta(e; v, \pi_T(e)) = 1 \text{ for } T = F \cup e\} \right)$$

$$- \#\{e \in \partial F : \delta(e; v, \pi_T(e)) = 0 \text{ for } T = F \cup e\} \right).$$

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 Figures 5 and 6. Thus

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

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

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

Thus the previous expression (\star) simplifies as

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

as desired.



FIGURE 5. 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 6. 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 $S \subset V(G)$,

(16)
$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \left(\sum_{E(G)} \alpha_e \sum_{\mathcal{F}_1(G;S)} w(\overline{T}) - \sum_{\mathcal{F}_2(G;S)} w(\overline{F}) (\deg^o(F,*) - 2)^2 \right).$$

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 (16) is zero

Next, suppose $|S| \ge 2$. Proposition 3.3 states that D[S] is nonsingular, so we may use the inverse matrix identity

(17)
$$\mathbf{1}^{\mathsf{T}}D[S]^{-1}\mathbf{1} = \frac{\operatorname{cof}D[S]}{\det D[S]}.$$

Let $\mathbf{m} = \mathbf{m}(G; S)$ denote the vector (10). By Proposition 5.3 (a) and Theorem 4.3,

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

Theorem 5.5 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 5.3 (b). Hence

(18)
$$\mathbf{1}^{\mathsf{T}}D[S]^{-1}\mathbf{1} = \lambda^{-1}\mathbf{1}^{\mathsf{T}}\mathbf{m} = \frac{\cot D[S]}{(-1)^{|S|-1}2^{|S|-1}\lambda}.$$

Comparing (17) with (18) gives the desired result, $\det D[S] = (-1)^{|S|-1} 2^{|S|-1} \lambda$.

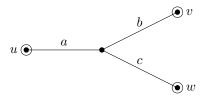
Proof of Theorem 1.1. Set all weights α_e to 1 in Theorem 1.2. In this case, the weights $w(\overline{T}) = 1$ and $w(\overline{F}) = 2$ for all forests T and F, and

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

Remark 5.6. 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 $\operatorname{conv}(S,G)$ 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 $\operatorname{conv}(S,G)$. However, the formulas as stated are true even without this replacement due to cancellation of terms.

6. Examples

Example 6.1. Suppose G is a tree consisting of three edges joined at a central vertex.



First, suppose S = V. The corresponding distance matrix is

$$D[V] = \begin{pmatrix} 0 & a & b & c \\ a & 0 & a+b & a+c \\ b & a+b & 0 & b+c \\ c & a+c & b+c & 0 \end{pmatrix},$$

which has determinant det D[S] = -4(a+b+c)abc.

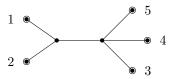
Next, suppose S consists of the leaf vertices $\{u, v, w\}$. Then

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

which has determinant det D[S] = 2(a+b)(a+c)(b+c) = 2((a+b+c)(ab+ac+bc) - abc). The

"special vector" that satisfies
$$D[S]\mathbf{m} = \lambda \mathbf{1}$$
 in this example is $\mathbf{m} = \begin{pmatrix} ab + ac \\ ab + bc \\ ac + bc \end{pmatrix}$.

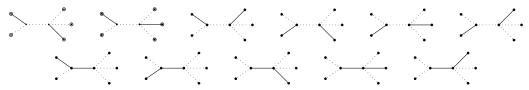
Example 6.2. Suppose G is the tree with unit edge weights shown below, with five leaf vertices.



Let S denote the set of five leaf vertices. Then

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

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



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

The determinant of the distance submatrix is

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

and the special vector is $\mathbf{m} = \begin{pmatrix} 5 \\ 5 \\ 4 \\ 4 \end{pmatrix}$.

Example 6.3. Suppose G is the tree with edge weights shown in Figure 7, with four leaf vertices and two internal vertices. Let S denote the set of four leaf vertices. Then

$$D[S] = \begin{pmatrix} 0 & a+b & a+c+d & a+c+e \\ a+b & 0 & b+c+d & b+c+e \\ a+c+d & b+c+d & 0 & d+e \\ a+c+e & b+c+e & d+e & 0 \end{pmatrix}$$

$$(a+c+e \quad b+c+e \quad d+e)$$
and $\mathbf{m} = \begin{pmatrix} abd & +abe & +acd & +ace & +ade & & -bde \\ abd & +abe & & -ade & +bcd & +bce & +bde \\ abd & -abe & +acd & & +ade & +bcd & & +bde \\ -abd & +abe & & +ace & +ade & & +bce & +bde \end{pmatrix}$
The determinant of the distance submatrix is

The determinant of the distance submatrix is

$$\det D[S] = (-1)^3 2^2 \Big((a+b+c+d+e) \cdot (abd+abe+acd+ace+ade+bcd+bce+bde) \\ - (1^2 (abcd+abce+acde+bcde) + 2^2 (abde)) \Big).$$

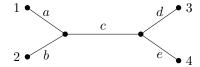


FIGURE 7. Tree with four leaves, and varying edge weights.

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