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 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,

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

which was proved by Bapat–Kirkland–Neumann [1]. The weighted identity (3) reduces to (1) when taking all unit weights, $\alpha_e = 1$. We 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*

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

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 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.

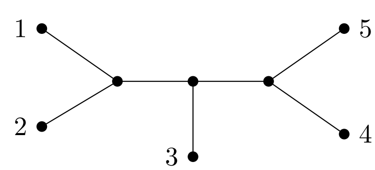


FIGURE 1. Tree with five leaves.

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 $(\det D[S])/(\operatorname{cof} D[S])$ 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 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,

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

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

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

[mention Devrient's thesis, Property 3.38] 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 $\mathbf{u}\in\mathbb{R}^S$,

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

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

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

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

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

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

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

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

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,

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

where L is the Laplacian matrix and $\mathbf{m}$ 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. $w(\overline{H}) = w(\overline{E(H)})$.

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.

If G is a tree, we let $\operatorname{conv}(S, G)$ 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.

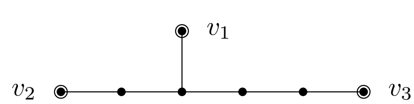
Given a set of vertices $S = \{v_1, v_2, \ldots, v_r\}$, an *$S$-rooted spanning forest* of G is a spanning forest which has exactly one vertex v_i in each connected component. Given $s \in S$ and a forest F, we let $F(s)$ denote the s-component of F.

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.

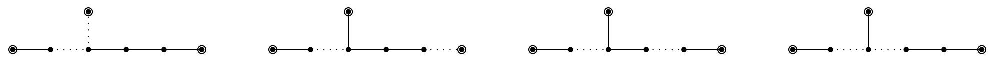


FIGURE 2. Some forests in $\mathcal{F}_1(G;S)$.

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 $L = BB^\intercal$. 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

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

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]. □

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

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

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.

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

(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

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

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

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

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 momemtum 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

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

(equivalent to Theorem 1.2), or more succinctly,

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

(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 $M[\bar{i}]$ "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 3.1 (Cauchy interlacing)**.** *Suppose M is a symmetric real matrix with ordered eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$, and the submatrix $M[\bar{i}]$ 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 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. □

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). □

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

$$(D^{(\alpha)})^{-1} \;=\; -\frac{1}{2}L^{(\alpha)} + \frac{1}{2}\Big(\sum_{e\in E}\alpha_e\Big)^{-1}\mathbf{m}\,\mathbf{m}^{\intercal} \tag{9}$$

where $\mathbf{m}$ 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

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

Hence $D^{(\alpha)}\mathbf{m} = \left(\sum_{e\in E}\alpha_e\right)\mathbf{1}$. 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 $\mathbf{u}^\intercal D\mathbf{u}\le 0$.
(b) If $\mathbf{u}\in\mathbb{R}^S$ is a vector whose coordinates sum to zero, then $\mathbf{u}^\intercal D[S]\mathbf{u}\le 0$.

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

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

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

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

4. Quadratic optimization

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

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

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*

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

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 $|S|\ge 2$. Proposition 3.5 implies that the objective function $\mathbf{u}\mapsto\mathbf{u}^\intercal D[S]\mathbf{u}$ is concave on the domain $\mathbf{1}^\intercal\mathbf{u} = 1$, 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 $\mathbf{1}$. By the theory of Lagrange multipliers, the optimal solution $\mathbf{u}^*$ is a vector satisfying

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

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

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

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

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

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

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

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

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

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 $\dfrac{\det D[S]}{\operatorname{cof} D[S]}$ behaves monotonically in S, and deduce further bounds on $\dfrac{\det D[S]}{\operatorname{cof} D[S]}$.

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*

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

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 $\dfrac{\det D[A]}{\operatorname{cof} D[A]} \leq \dfrac{\det D[B]}{\operatorname{cof} D[B]}$. By Corollary 4.5, 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 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 $\operatorname{conv}(S, G)$ denotes the subgraph of G which is the union of all paths between vertices in S. To see that

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

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

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

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 $\dfrac{\det D[S]}{\operatorname{cof} D[S]}$ is the maximum value of the function $\mathbf{u} \mapsto \mathbf{u}^\intercal D[S] \mathbf{u}$ 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.

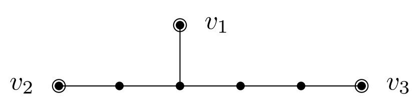
(i) Find a vector $\mathbf{m} \in \mathbb{R}^S$ such that $D[S]\mathbf{m} = \lambda \mathbf{1} \in \mathbb{R}^S$.

(ii) Compute the sum of entries of $\mathbf{m}$, i.e. $\mathbf{1}^\intercal \mathbf{m}$, and normalize $\mathbf{u}^* = \dfrac{\mathbf{m}}{\mathbf{1}^\intercal \mathbf{m}}$. This solves the optimization problem of Section 4.

(iii) Find the optimal objective value $\lambda^* = \dfrac{\lambda}{\mathbf{1}^\intercal \mathbf{m}}$.

(iv) Use the expression for $\operatorname{cof} D[S]$ in Theorem 4.3 to compute $\det D[S] = \lambda^* (\operatorname{cof} D[S])$.

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



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 $\mathbf{1}^\intercal \mathbf{m} = 22$.

(iii) We have $\lambda^* = \dfrac{\lambda}{\mathbf{1}^\intercal \mathbf{m}} = \dfrac{30}{11}$.
(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 $\mathbf{m}$ 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 $\mathbf{m}$ 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

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

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

Proposition 5.3. *Suppose S is nonempty. For the vector $\mathbf{m} = \mathbf{m}(G; S)$ defined above,*
(a) $\mathbf{1}^\intercal \mathbf{m} = 2 \sum_{T \in \mathcal{F}_1(G;S)} w(\overline{T})$*;*
(b) if all edge weights α_e are positive, $\mathbf{m}$ is nonzero.

Proof. (a) By Lemma 2.4 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 $\mathbf{1}^\intercal \mathbf{m}$,

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

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 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 $\mathbf{m}$ defined in (10) satisfies $\mathbf{1}^\intercal \mathbf{m} = 2\,\kappa(G; S)$.*

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

$$
\begin{aligned}
(D[S]\mathbf{m})_v &= \sum_{s\in S} d(v,s)\mathbf{m}_s \\
&= \sum_{s\in S}\left(\sum_{e\in E(G)} \alpha_e\, \delta(e;v,s)\right)\left(\sum_{T\in\mathcal{F}_1(G;S)} (2-\deg^o(T,s))w(\overline{T})\right) \\
&= \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{s\in S}\delta(e;v,s)(2-\deg^o(T,s))\right) \\
&= \sum_{T\in\mathcal{F}_1} w(\overline{T}) \sum_{e\in E} \alpha_e \left(\sum_{s\in S}\delta(e;v,s) \sum_{u\in T(s)} (2-\deg(u))\right). \qquad (11)
\end{aligned}
$$

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

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

Using this notation,

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

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

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

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

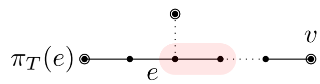
$$\delta(e;v,\pi_T(u)) - \delta(e;v,u) = \begin{cases} 0 & \text{if } \delta(e;\pi_T(u),u) = 0 \\ 1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 1 \\ -1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 0. \end{cases} \qquad (14)$$

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.



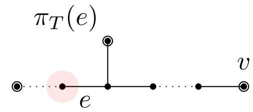


FIGURE 4. Edge $e \in T$ with $\delta(e; v, \pi_T(e)) = 1$ (left) and $\delta(e; v, \pi_T(e)) = 0$ (right). The floating component of $T \setminus e$ is highlighted.

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

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

Thus

$$\begin{aligned} &(D[S]\mathbf{m})_v - \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in E} \alpha_e \\ (15) \qquad &= \sum_{T \in \mathcal{F}_1} w(\overline{T}) \sum_{e \in T} \alpha_e (2 - \deg^o(T \setminus e, *)) \Big(\mathbb{1}(\delta(e; v, \pi_T(e)) = 1) - \mathbb{1}(\delta(e; v, \pi_T(e)) = 0)\Big). \end{aligned}$$

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

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

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

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

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 Figures 5 and 6. Thus

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

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

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

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 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.

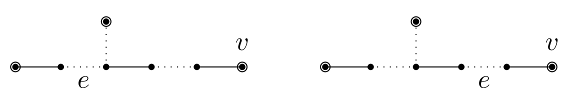


FIGURE 6. Edges $e \in \partial F(*)$ with $\delta(e; v, \pi_{(F\cup e)}(e)) = 1$ (left) and $\delta(e; v, \pi_{(F\cup e)}(e)) = 0$ (right).

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

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

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

$$\mathbf{1}^\intercal D[S]^{-1}\mathbf{1} = \frac{\operatorname{cof} D[S]}{\det D[S]}. \tag{17}$$

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

$$\mathbf{1}^\intercal D[S]^{-1} \mathbf{1} = \lambda^{-1} \mathbf{1}^\intercal \mathbf{m} = \frac{\operatorname{cof} D[S]}{(-1)^{|S|-1} 2^{|S|-1} \lambda}. \tag{18}$$

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

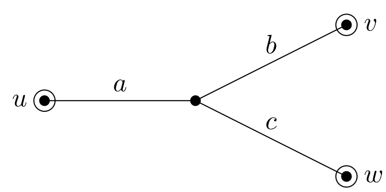
Proof of Theorem 1.1. Set all weights α_e to 1 in Theorem 1.2. In this case, the weights $w(\overline{T}) = 1$ and $w(\overline{F}) = 2$ for all forests T and F, and

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

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

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

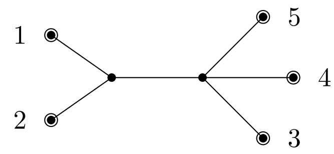
which has determinant $\det D[S] = -4(a+b+c)abc$.

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 $\det D[S] = 2(a+b)(a+c)(b+c) = 2\Big((a+b+c)(ab+ac+bc) - abc\Big)$. The "special vector" that satisfies $D[S]\mathbf{m} = \lambda \mathbf{1}$ in this example is $\mathbf{m} = \begin{pmatrix} ab+ac \\ ab+bc \\ ac+bc \end{pmatrix}$.

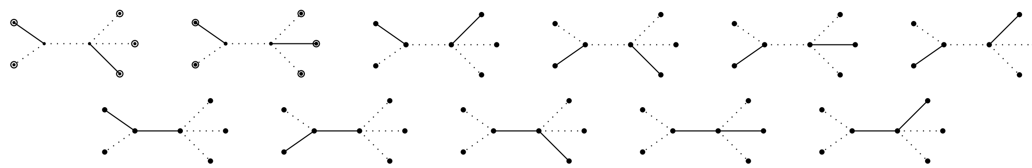
Example 6.2. Suppose G is the tree with unit edge weights shown below, with five leaf vertices.



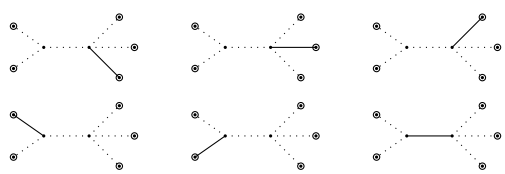
Let S denote the set of five leaf vertices. Then

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

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

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

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

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

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

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

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

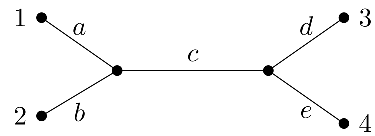


FIGURE 7. Tree with four leaves, and varying edge weights.

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