### MINORS OF TREE DISTANCE MATRICES

### HARRY RICHMAN, FARBOD SHOKRIEH, AND CHENXI WU

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	1
2.	Graphs and spanning forests	4
3.	Distance minors: Preliminaries	8
4.	Quadratic optimization	Q
5.	Distance minors: Proofs	11
6.	Examples	16
Acknowledgements		18
References		18

## 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.

Date: v1, May 30, 2023 (Preliminary draft, not for circulation). 2020 Mathematics Subject Classification. Primary 05C50; Secondary 05C05, 05C12, 05C30, 31C15.

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  $\alpha$ -distance matrix  $D^{(\alpha)}$  is defined by setting the (u, v)-entry to the sum of the weights  $\alpha_e$  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.

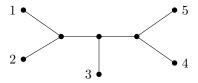


Figure 1. Tree with five leaves.

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 one, 4 have outdegree two, and 1 has outdegree three. 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

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

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  $\mathbf{u} \in \mathbb{R}^S$ ,

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

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  $\gamma$  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 [10], which involve 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 (8). 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 [11, Chapter VI].

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

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

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.

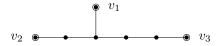
Given a set of vertices  $S = \{v_1, v_2, \dots, v_r\}$ , an S-rooted spanning forest of G is a spanning forest which has exactly one vertex  $v_i$  in each connected component. Given  $s \in S$  and a forest F, we let F(s) denote the s-component of F.

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.

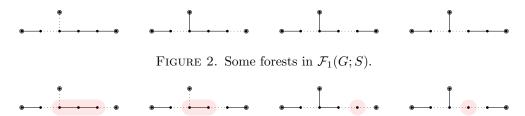


FIGURE 3. Some forests in  $\mathcal{F}_2(G; S)$ , with floating component highlighted.

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  $\alpha_e$  for  $e \in E$ , let  $L^{(\alpha)}$  denote the weighted Laplacian matrix of G, defined by

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

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

(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*  $\partial H$  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  $\psi$  and  $\varphi$  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  $M[\bar{i}]$  "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[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 assume by induction hypothesis that the claim holds for  $|S| = k \ge 3$ . If |S| = k - 1, Cauchy interlacing implies that D[S] has at most one positive eigenvalue, and at least one negative eigenvalue. Since all diagonal entries of D[S] are zero, D[S] has zero trace. Thus D[S] has exactly one positive eigenvalue as claimed.

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 (8) 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 (8) by the all-ones vector 1; since  $L^{(\alpha)}\mathbf{1} = 0$  and  $\mathbf{m}^{\dagger}\mathbf{1} = 2$ , 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 (8) 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  $\mathbf{u}^{\intercal}D[S]\mathbf{u} \leq 0$ .

*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

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

where 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 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  $\lambda$  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

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

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  $\alpha_e$ , 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 [11, 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

 $M[\overline{i},\overline{j}]$  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

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

*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

$$\frac{\det D[S]}{\cot D[S]} = \max\{\mathbf{u}^{\mathsf{T}} D\mathbf{u} : \mathbf{u} \in \mathbb{R}^{V}, \, \mathbf{1}^{\mathsf{T}} \mathbf{u} = 1, \, \mathbf{u}_{v} = 0 \, \text{if } v \notin S\}$$

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

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

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

(b) Recall that  $\gamma$  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  $\lambda$ .

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  $\lambda$ .

**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 (7)).

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  $\alpha_e$  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 (2.4) 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 (9) satisfies  $\mathbf{1}^{\mathsf{T}}\mathbf{m} = 2 \kappa(G; S)$ .

**Theorem 5.5.** With  $\mathbf{m} = \mathbf{m}(G; S)$  defined as in (9),  $D[S]\mathbf{m} = \lambda \mathbf{1}$  for the constant

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

*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 (10). 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 (12) from (11), 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 (13) by  $(2 - \deg(u))$  and summing over all vertices u, we obtain

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

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

$$w(\overline{F}) = \alpha_e \cdot w(\overline{T})$$
 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 (15) 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 (9). By Proposition 5.3 (a) and Theorem 4.3,

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

Theorem 5.5 states that  $D[S]\mathbf{m} = \lambda \mathbf{1}$  for some constant  $\lambda$ , 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 (16) with (17) gives the desired result,  $\det D[S] = (-1)^{|S|-1} 2^{|S|-1} \lambda$ .

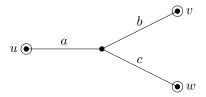
Proof of Theorem 1.1. Set all weights  $\alpha_e$  to 1 in Theorem 1.2. In this case, the weights  $w(\overline{T}) = 1$  and  $w(\overline{F}) = 2$  for all forests T and F, and

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

**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.

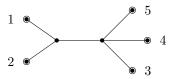
Next, suppose S consists of the leaf vertices  $\{u, v, w\}$ . Then

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

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  $\mathbf{m} = \begin{pmatrix} ab + ac \\ ab + bc \\ ac + bc \end{pmatrix}$ .

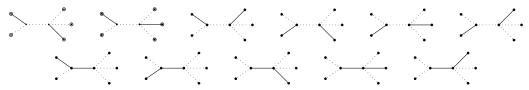
**Example 6.2.** Suppose G is the tree with unit edge weights shown below, with five leaf vertices.



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

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

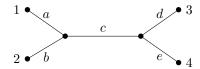


FIGURE 7. Tree with four leaves, and varying edge weights.

#### Acknowledgements

The authors would like to thank Ravindra Bapat for helpful discussion, in particular for providing a proof of Proposition 3.3.

#### References

- R. Bapat, S. J. Kirkland, and M. Neumann. On distance matrices and Laplacians. *Linear Algebra Appl.*, 401:193–209, 2005.
- [2] R. B. Bapat. Graphs and matrices. Universitext. Springer, London; Hindustan Book Agency, New Delhi, 2010.
- [3] R. B. Bapat and S. Sivasubramanian. Identities for minors of the Laplacian, resistance and distance matrices. Linear Algebra Appl., 435(6):1479–1489, 2011.
- [4] S. Chaiken. A combinatorial proof of the all minors matrix tree theorem. SIAM J. Algebraic Discrete Methods, 3(3):319–329, 1982.
- [5] R. L. Graham and L. Lovász. Distance matrix polynomials of trees. Adv. in Math., 29(1):60–88, 1978.
- [6] R. L. Graham and H. O. Pollak. On the addressing problem for loop switching. Bell System Tech. J., 50:2495— 2519, 1971.
- [7] R. A. Horn and C. R. Johnson. Matrix analysis. Cambridge University Press, Cambridge, second edition, 2013.
- [8] A. Kassel, R. Kenyon, and W. Wu. Random two-component spanning forests. Ann. Inst. Henri Poincaré Probab. Stat., 51(4):1457-1464, 2015.
- [9] D. H. Richman, F. Shokrieh, and C. Wu. The average cut size of a random two-forest, 2023. in preparation.
- [10] D. H. Richman, F. Shokrieh, and C. Wu. Capacity on metric graphs, 2023. in preparation.
- [11] W. T. Tutte. Graph theory, volume 21 of Encycl. Math. Appl. Cambridge University Press, Cambridge, 1984.