PRINCIPAL 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 trees with edge lengths. Our formulas can be expressed in terms of evaluations of Symanzik polynomials.

Contents

1. Introduction

[1]

Suppose $G = (V, E)$ is a tree with n vertices. Let D denote the *distance matrix* of G, defined by setting the (u, v)-entry to the length of the unique path from u to v. In [GP71], Graham and Pollak prove

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

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 $S \subseteq V$, let $D[S]$ denote the submatrix consisting of the S-indexed rows and columns of D.

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[1] [(Farbod) I say let's submit the paper to a journal around the same time as to arXiv...]

Theorem A. *Suppose G is a tree with n vertices whose distance matrix is D. Let $S \subseteq V$ be a nonempty subset of vertices. Then*

$$\det D[S] = (-1)^{|S|-1} 2^{|S|-2} \Big((n-1)\, \kappa(G;S) - \sum_{F \in \mathcal{F}_2(G;S)} (\operatorname{outdeg}(F,*) - 2)^2 \Big), \tag{2}$$

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 $\operatorname{outdeg}(F,*)$ *denotes the outdegree of the floating component of F.*

For definitions of rooted spanning forests as well as other terminology, see §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 $\kappa(G;V) = 1$. Moreover, the set $\mathcal{F}_2(G;V)$ of $(V,*)$-rooted spanning forests is empty. Thus Theorem A recovers the Graham–Pollak identity (1).

1.1. Trees with edge lengths.

Assume the tree G is endowed with a collection of positive real edge lengths $\alpha = \{\alpha_e \colon e \in E\}$. The *distance matrix* (with respect to α), which we will again denote by D, is defined by setting the (u,v)-entry to the sum of the edge lengths α_e along the unique path from u to v. The relation (1) has a generalization for the distance matrix for trees with edge lengths, proved by Bapat, Kirkland, and Neumann ([BKN05, Corollary 2.5]):

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

We, in fact, prove the following more general result. For a subset $A \subseteq E$ let the *weight* of A be $w(A) = \prod_{e \notin A} \alpha_e$.

Theorem B. *Suppose $G = (V,E)$ is a finite tree with edge lengths $\{\alpha_e \colon e \in E\}$, and the corresponding distance matrix D. For any nonempty subset $S \subseteq V$, we have*

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

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, $w(T)$ and $w(F)$ denote the weights of the forests T and F, and $\operatorname{outdeg}(F,*)$ *is the outdegree of the floating component of F, as above.*

See §2 for the other terminology used here.

Example. Suppose G is the tree with unit edge lengths shown in Figure 1, with five leaf vertices and three internal vertices. Let $S = \{1,2,3,4,5\}$ be the set of leaf vertices. The corresponding distance submatrix is

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

whose determinant is 864.

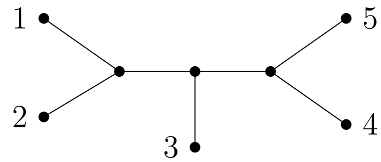

FIGURE 1. Tree with five leaves.

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 A,

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

1.2. **Normalized principal minors.** One may ask how 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 a "normalized" version 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 [BS11], Bapat and Sivasubramanian show the following identity for the sum of cofactors of a distance submatrix $D[S]$ of a tree with edge lengths $\{\alpha_e : e \in E\}$,

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

where $\mathcal{F}_1(G;S)$ denotes the set of S-rooted spanning forests of G (see §2 and Theorem 4.4). An immediate consequence of Theorem B, together with (5), is the identity

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

We will refer to $\det D[S]/\operatorname{cof} D[S]$ as the *normalized principal minor* corresponding to the subset S. It turns out normalized principal minors satisfy a monotonicity condition.

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

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

The essential observation behind this result is an intriguing connection to the theory of quadratic optimization; we will show the normalized principal minor $\det D[S]/\operatorname{cof} D[S]$ is calculated via the following 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 is obtained using the method of Lagrange multipliers, and relies of knowledge of the signature of $D[S]$. See §4.

Note, for a nonempty subset S, the expression in (6) implies the bound

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

We get refined bounds by making use of the monotonicity property, Theorem C. Let $\operatorname{conv}(S, G)$ denote the convex hull of S, i.e. the subtree of G consisting of all paths between points of S.

Theorem D (Bounds on principal minor ratios)**.** *Suppose $G = (V, E)$ is a finite tree with edge lengths $\{\alpha_e : e \in E\}$ and with distance matrix D.*

(a) For a nonempty subset $S \subseteq V$,

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

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

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

[2]

[2] [(Farbod) mention Devriendt thesis, e.g. Property 3.38?]

1.3. **Connection with Symanzik polynomials.** Recall, 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.

A "momentum function" $p\colon V \to \mathbb{R}$ satisfies the constraint $\sum_{v \in V} p(v) = 0$. 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 $F = F_1 \cup F_2$. Note that it does not matter which component we label as F_1, since the momentum constraint implies that $\sum_{v \in F_1} p(v) = -\sum_{v \in F_2} p(v)$.

We note that the expressions in Theorem B and (6) are closely related to Symanzik polynomials. Let $\psi_{(G/S)}$ and $\varphi_{(G/S)}$ denote the first and second Symanzik polynomials of the quotient graph G/S. Let p_{can} be the momentum function defined by $p_{\text{can}}(v) = \deg(v) - 2$ for $v \notin S$ and $p_{\text{can}}(v_S) = -\sum_{v \notin S} p_{\text{can}}(v)$, where v_S denotes the vertex obtained by collapsing S to a vertex.

The identity in Theorem B can be written as follows

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

Furthermore, the equality in (6) can be written as

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

1.4. **Related work.** Karel, Amini, Brown, Khare, – maybe the new preprint, but be careful. [3] It is natural to ask how our results for trees may be generalized to arbitrary finite graphs. We address this in an upcoming paper [RSW23], which involves more technical machinery. [4]

The first Symanzik polynomial can be computed using Kirchhoff's celebrated matrix-tree theorem. The second Symanzik polynomial can similarly be calculated via determinant of the Generalized Laplacian matrix; see [?amini, Section 1.1] and [?brown, Theorem 7.1]. [5]

[3] [(Farbod) should we have a "related work" subsection? one awkward thing is to address the work after our work... but we can have the following paragraph, and also give Devriendt a better treatment...]

[4] [(Farbod) Harry: did you want to say something about phylogenetic stuff?]

[5] [(Farbod) give reference to Amini [?amini] and Brown [?brown] for compuational aspects, using determinants, of (second) Symanzik. Also: I believe Chenxi at some point thought one of Brown's identities might be related to our work...]

Structure of the paper. [6] In §2
In §3
In §4 Theorem C and Theorem D are proved in
In §5
In §6

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2. Graphs and spanning forests

Throughout, let $G = (V, E)$ be a finite graph with (positive, real) edge lengths $\{\alpha_e \colon e \in E\}$. A graph without edge lengths will be considered as a special case, with $\alpha_e = 1$ for all $e \in E$.

We assume all graphs in the paper are equipped with an implicit (arbitrary) orientation. This means we fix 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^-.

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.

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, that is, the component of F containing s.

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 [KKW15][7]. For an $(S, *)$-rooted spanning forest F, we let $F(*)$ denote the floating component. We sometimes refer to the floating component as the $*$-component of F. Again, for $s \in S$, we let $F(s)$ denote the s-component of F.

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.

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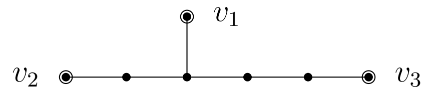
[6] [(Farbod) complete at the end...]

[7] [(Farbod) do we need "following terminology in...". kassel-kenyon-wu is used only for this sentence. if there is anything else about that paper that can be added, let's keep this and say more in the related work section]

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



Let S be the set of three leaf vertices. Then $\mathcal{F}_1(G;S)$ contains 11 forests, while $\mathcal{F}_2(G;S)$ contains 19 forests. Some of these are shown in Figure 2 and Figure 3, respectively.

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

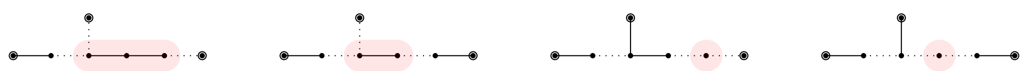


FIGURE 3. Some forests in $\mathcal{F}_2(G;S)$, with floating component highlighted.

Remark 2.2. Let q be a fixed vertex. Then $\mathcal{F}_1(G;\{q\})$ is the set of spanning trees of G, and $\mathcal{F}_2(G;\{q\})$ is the set of two-component spanning forests of G. Note that both these sets are independent of the choice of the vertex q, and were denoted by $\mathcal{F}_1(G)$ and $\mathcal{F}_2(G)$, respectively, in §1.3.

2.2. **Laplacian matrix.** The *incidence matrix* of a graph $G = (V, E)$ (endowed with an arbitrary orientation) 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 $\{\alpha_e : e \in E\}$ denote the edge lengths as before. The Laplacian matrix is defined by

$$L = B \begin{pmatrix} \alpha_1^{-1} & & \\ & \ddots & \\ & & \alpha_m^{-1} \end{pmatrix} B^\intercal. \tag{7}$$

It is clear that L is positive semidefinite.

Note that the incidence matrix depends on the choice of the orientation but the Laplacian matrix does not.

2.3. **Principal minors matrix-tree theorem.** For a subset $A \subseteq E$ we define the *weight* of A as

$$w(A) = \prod_{e \notin A} \alpha_e$$

and the *coweight* of A as

$$w'(A) = \prod_{e \in A} \alpha_e^{-1}.$$

Clearly,

$$w(A) = w'(A) \prod_{e \in E} \alpha_e \tag{8}$$

If H is a subgraph of G, we use H to also denote its subset of edges $E(H)$. So, for example, $w(H) = w\,(E(H))$.

Let

$$\kappa(G;S) = \sum_{T \in \mathcal{F}_1(G;S)} w'(T).$$

Remark 2.3. If G is a graph *without* edge lengths (so $\alpha_e = 1$ for all $e \in E$), then $\kappa(G;S)$ is simply the number of S-rooted spanning forests of G. In this case, $\kappa(G;S)$ is also the number of spanning trees of the quotient graph G/S, which "glues together" all vertices in S as a single vertex v_S.

The *(principal minors) matrix-tree theorem* gives a determinantal formula for computing $\kappa(G;S)$, which we now explain. Given $S \subseteq V$, let $L[\overline{S}]$ denote the matrix obtained from L by removing the rows and columns indexed by S.

Theorem 2.4. *Let $G = (V, E)$ be a finite graph with edge lengths $\{\alpha_e \colon e \in E\}$ For any nonempty vertex set $S \subseteq V$,*

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

Proof. See Tutte [Tut84, Section VI.6, Equation (VI.6.7)]. □

Note that the classical (Kirchhoff's) matrix-tree theorem is the special case, where S is a singleton.

2.4. **Tree splits and tree distance.** Fix a tree $G = (V, E)$ with edge lengths $\{\alpha_e \colon e \in E\}$ (and endowed with an arbitrary orientation). Given an edge $e \in E$, the edge deletion $G \setminus e$ contains two connected components. This phenomenon is referred to as a *tree split*.

Using the orientation on $e = (e^+, e^-)$, we let $(G \setminus e)^+$ denote the component that contains endpoint e^+, and let $(G \setminus e)^-$ denote the component that contains endpoint e^-. For any $e \in E$ and $v \in V$, we denote by $(G \setminus e)^v$ the component of $G \setminus e$ containing v, and $(G \setminus e)^{\overline{v}}$ the component not containing v.

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

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

Remark 2.5.

(i) $\delta(e; v, w) = 1$ 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.
(ii) $\delta(e; v, v) = 0$ for any edge e and vertex v.
(iii) If we fix an edge e and a vertex v, then $\delta(e; v, -) \colon V(G) \to \{0, 1\}$ is the indicator function for the component $(G \setminus e)^{\overline{v}}$ of the tree split $G \setminus e$ not containing v.
(iv) If we fix vertices v, w, then $\delta(-; v, w) \colon E(G) \to \{0, 1\}$ is the indicator function for the unique path between v and w.

Recall the distance between vertices v, w (with respect to edge lengths $\{\alpha_e \colon e \in E\}$), denoted by $d(v, w)$, is defined as the sum of the edge lengths α_e along the unique path from u to v.

Proposition 2.6. *For a tree $G = (V, E)$ with edge lengths $\{\alpha_e \colon e \in E\}$, the corresponding distance function satisfies*

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

Proof. This follows from Remark 2.5 (iv). □

2.5. **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 "handshaking lemma" in graph theory is that for any tree G, we have

$$\sum_{v \in V(G)} (2 - \deg(v)) = 2. \tag{9}$$

We next state a slight generalization (9), which will be useful later.

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

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

We define the *outdegree* of H in G as the number of edges in its edge boundary, $\mathrm{outdeg}(H) = |\partial H|$. Note that the edge boundary and outdegree do not depend on the implicit orientation on E.

We are especially interested in the following special cases. [8]Let G be a tree and $\emptyset \neq S \subseteq V$. For an S-rooted spanning forest F of G, and $s \in S$, we define the *outdegree* $\mathrm{outdeg}(F, s)$ as the number of edges which join $F(s)$ (the s-component of F) to a different component; i.e. outdegree of $F(s)$ in the tree G. Similarly, if F is a $(S, *)$-rooted spanning forest of G, we let $\mathrm{outdeg}(F, *)$ denote the outdegree of the floating component $F(*)$. [9]

Lemma 2.7. *Suppose G is a tree.*

[8][(Farbod) G is a tree now, right?]
[9][(Farbod) do we want an example here, perhaps continuing Example 2.1?]

(a) If $H \subseteq G$ is a nonempty connected subgraph then

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

(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 $\operatorname{outdeg}(H) = \deg(v)$.

(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 $\delta(e; u, v) = 1$ (see Remark 2.5 (iii)). Since this component has a single edge separating it from its complement, $\operatorname{outdeg}((G \setminus e)^{\overline{u}}) = 1$ Using part (a), we have

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

2.6. **Transitions between $\mathcal{F}_1(G; S)$ and $\mathcal{F}_2(G; S)$.** A key step in the proof of Theorem B 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

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

  Given $F \in \mathcal{F}_2(G; S)$, there are exactly $\operatorname{outdeg}(F, *)$ many choices of pairs $(e, T) \in E(G) \times \mathcal{F}_1(G; S)$ such that $F = T \setminus e$.

- Consider the "union map"

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

  defined by

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

  Given $T \in \mathcal{F}_1(G; S)$, 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[10]).

[10][(Farbod) this is confusing – T is not a spanning tree here... I suggest we just remove this parenthesis?]

3. Principal submatrices of D as bilinear forms

Let $G = (V, E)$ be a tree with edge lengths $\alpha = \{\alpha_e : e \in E\}$. The distance matrix (with respect to α) is symmetric, so it defines a symmetric bilinear forms on the vector space $\mathbb{R}^V$.

3.1. **Signature and invertibility.**

For a subset of vertices S with $|S| \geq 2$, the submatrix $D[S]$ has nonzero determinant. We give a proof in here, based on finding the signature of $D[S]$ as a bilinear form.

We first recall a celebrated result of Cauchy. Let $M[\bar{i}]$ 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 eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. Then the submatrix $M[\bar{i}]$ has eigenvalues $\mu_1 \leq \cdots \leq \mu_{n-1}$ satisfying*

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

Proof. See, for example, [HJ13, Theorem 4.3.17]. □

Lemma 3.2 ([Bap10, Lemma 8.15])**.** *Suppose D is the distance matrix of a tree with n vertices and edge lengths $\{\alpha_e : e \in E\}$. Then D has one positive eigenvalue and $n - 1$ negative eigenvalues.*

Remark 3.3. The proof in [Bap10] is by induction on the number of vertices, and uses Cauchy interlacing (Proposition 3.1). Lemma 8.15 in [Bap10] is actually stated for trees without edge lengths. However, the same argument applies to trees with edge lengths if one applies Bapat, Kirkland, Neumann's result [BKN05, Corollary 2.5] (see (3)).

The the following extension of Lemma 3.2 and its proof was communicated to the authors by Bapat (personal communication).

Lemma 3.4. *Suppose D is the distance matrix of a tree $G = (V, E)$ with edge lengths $\{\alpha_e : e \in E\}$. Let $S \subseteq V$ be a subset of size $|S| \geq 2$. Then $D[S]$ has one positive eigenvalue and $|S| - 1$ negative eigenvalues; In particular, $\det D[S] \neq 0$.*

Proof. We apply decreasing induction on the size of S. For $S = V$, we have 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 $S^+ \subseteq V$ 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 (Proposition 3.1) 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. □

3.2. **Negative definite hyperplane.** We next prove that any principal submatrix of D induces a negative semidefinite quadratic form on the hyperplane of zero-sum vectors.

Bapat, Kirkland, and Neumann ([BKN05, Theorem 2.1]) prove that

$$(D)^{-1} \;=\; -\frac{1}{2}L + \frac{1}{2}\Big(\sum_{e\in E}\alpha_e\Big)^{-1}\mathbf{m}\,\mathbf{m}^{\intercal} \tag{10}$$

where $\mathbf{m}$ is the vector with components $\mathbf{m}_v = 2 - \deg v$. The special case of of (10) for trees without edge lengths had appeared in an earlier work by Graham and Lovász ([GL78, Lemma 1]).

Remark 3.5. [11] To our knowledge, a generalization of (10), giving an expression for $D[S]^{-1}$ for a nonempty subset $S \subseteq V$, has not been obtained in the literature. This might be an interesting research problem.

Proposition 3.6. *Let D denote the distance matrix of a tree with edge lengths $\{\alpha_e \colon e \in E\}$. Let L be the Laplacian matrix. Then*

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

Proof. Multiply (10) by the all-ones vector $\mathbf{1}$; since $L\mathbf{1} = 0$ and $\mathbf{m}^{\intercal}\mathbf{1} = 2$ (see (9)), we obtain

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

Therefore,

$$D\mathbf{m} = \left(\sum_{e\in E}\alpha_e\right)\mathbf{1}. \tag{11}$$

The result now follows from multiplying (10) by D on both sides, and using (11). ☐

Proposition 3.7. *Suppose D is the distance matrix of a tree with edge lengths $\{\alpha_e \colon e \in E\}$.*

(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 3.6, we obtain

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

As is well-known that the Laplacian matrix is positive semidefinite (this readily follows from (7)). $\mathbf{u}^{\intercal}DLD\mathbf{u} = (D\mathbf{u})^{\intercal}L(D\mathbf{u}) \ge 0$. Thus $\mathbf{u}^{\intercal}D\mathbf{u} \le 0$ as claimed.

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

[11] [(Farbod) do we want to keep this remark? Could it be that Devriendt has already answered this?]

4. Quadratic optimization

Here, we explain how the quantity $\det D[S]/\mathrm{cof}\, D[S]$, introduced in §1.2 arises as the solution of a quadratic optimization problem.

Proposition 4.1. *Suppose D is the distance matrix of a tree with edge lengths $\{\alpha_e \colon e \in E\}$. If $D[S]$ is a principal submatrix of a distance matrix indexed by a nonempty subset S of vertices, then*

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

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

Assume $|S| \geq 2$. Proposition 3.7 (b) 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 $\mathbf{1}$.[12] 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

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

(The first equality is because $D[S]$ is symmetric, and the last equality is by the given constraint $\mathbf{1}^\intercal\mathbf{u} = 1$.)

On the other hand, $D[S]$ is invertible by Lemma 3.4. Therefore, we have $\mathbf{u}^* = \lambda(D[S]^{-1}\mathbf{1})$, so

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

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

Remark 4.2. If we consider G as a resistive electrical network, with each edge e representing a resistor of resistance α_e, then the optimal vector $\mathbf{u}^*$ has a physical interpretation as a current flow: it records the currents in the network when external current enters the network in the amount $(\deg(v)-2)/2$ for each $v \in V\backslash S$ [13], and exits from the nodes in S, and the network is grounded at all nodes in S. Indeed, we give an explicit combinatorial expression for $\mathbf{u}^*$, up to a normalizing constant, in (12). It is a classical result in network theory that this gives the current flow as described; see, for example, Tutte [Tut84, Section VI.6].

We 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.

[12][(Farbod) this could be clarified a bit]

[13][(Farbod) is it okay backslash S]

Corollary 4.3. *If $D[S]$ is a principal submatrix of a distance matrix indexed by S, then*

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

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 essentially due to Bapat and Sivasubramanian ([BS11]).

Recall from §1.2 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 4.4 (Distance submatrix cofactor sums)**.** *Let $G = (V, E)$ be a tree with edge lengths $\{\alpha_e \colon e \in E\}$, and let D be the distance matrix of G. Let $S \subseteq V$ be a nonempty subset of vertices. Then*

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

Proof. Bapat and Sivasubramanian ([BS11, Theorem 11]) show that

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

where L is the Laplacian matrix. Combine this identity with Theorem 2.4 and (8). □

The following result is a direct consequence of theorems of Bapat, Kirkland, Neumann ([BKN05]) and Bapat, Sivasubramanian ([BS11]).

Proposition 4.5. *Suppose D is the distance matrix of a tree with edge lengths $\{\alpha_e \colon e \in E\}$. Then*

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

Proof. Consider Theorem 4.4 with $S = V$. In this case $\mathcal{F}_1(G;V)$ is a singleton consisting of the forest T with no edges, so $w(T)$ is the product of all edge lengths. Thus

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

Combining this with (3) yields the result. □

4.2. **Monotonicity.** Using Proposition 4.1, we can now prove Theorem C and Theorem D.

Proof of Theorem C. By Corollary 4.3, both values

$$\frac{\det D[A]}{\operatorname{cof} D[A]} \quad \text{and} \quad \frac{\det D[B]}{\operatorname{cof} D[B]}$$

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. □

Proof of Theorem D. (a) To see

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

take B as the set of all vertices in $\operatorname{conv}(S, G)$. Then $S \subseteq B$, and apply Theorem C. By Proposition 4.5 we have

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

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

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

let $A = \{s_0, s_1\}$. Then $A \subseteq S$ by assumption. Now apply Theorem C. By Proposition 4.5 we have

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

5. Proof of Theorems A and B

In this section, we prove our main result, Theorem B. Theorem A is an immediate corollary.

5.1. **Outline of the proof.** [14]

In §4, we showed that $\det D[S]/\operatorname{cof} D[S]$ 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 $D[S]\mathbf{u}^* = \lambda \mathbf{1}$. Therefore, we can compute $\det D[S]$ via the following steps.

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

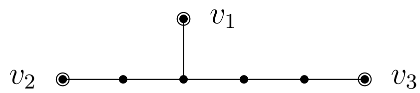
(ii) Compute the sum of entries of $\mathbf{m}$, i.e. $\mathbf{1}^\intercal \mathbf{m}$, and normalize $\mathbf{u}^* = \dfrac{\mathbf{m}}{\mathbf{1}^\intercal \mathbf{m}}$. This solves the optimization problem of §4.

(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 4.4 to compute $\det D[S] = \lambda^*(\operatorname{cof} D[S])$.

[14] [(Farbod) I was not happy with the subsection titles in this section, and my tweak hasn't helped...]

Example 5.1. [15] Suppose G is the tree with unit edge lengths 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 $\mathbf{m} = \begin{pmatrix} 5 & 8 & 9 \end{pmatrix}^\intercal$ 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 $\lambda^* = \lambda / \mathbf{1}^\intercal \mathbf{m} = 30/11$.
(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 (12)), which also gives combinatorial meaning to the constant λ.

5.2. **The proofs.** Fix a tree $G = (V, E)$ with edge lengths $\{\alpha_e \colon e \in E\}$ and a nonempty subset $S \subseteq V$. 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

$$\mathbf{m}_v = \sum_{T \in \mathcal{F}_1(G;S)} w(T)(2 - \operatorname{outdeg}(T, v)) \qquad \text{for each } v \in S. \tag{12}$$

where $\operatorname{outdeg}(T, v)$ is the outdegree of the v-component of T (see §2.5).

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

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

Proof. (a) By Lemma 2.7 we can express $\operatorname{outdeg}(T, s)$ as a sum over vertices in $T(s)$,

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

[15][(Farbod) should we keep this, drop it, or move it?]

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

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

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

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

where we apply equation (9) for the last equality.

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

Theorem 5.4. *With $\mathbf{m} = \mathbf{m}(G;S)$ defined as in (12), $D[S]\mathbf{m} = \lambda \mathbf{1}$ for the constant*

$$\lambda = \sum_{e\in E(G)} \alpha_e \sum_{T\in\mathcal{F}_1(G;S)} w(T) - \sum_{F\in\mathcal{F}_2(G;S)} w(F)\,(2-\operatorname{outdeg}(F,*))^2.$$

Proof. For $e \in E$ and $v, w \in V$, let $\delta(e; v, w)$ denote the function defined in §2.4. For any $v \in S$, we have

$$\begin{aligned}(D[S]\mathbf{m})_v &= \sum_{s\in S} d(v,s)\mathbf{m}_s \\ &= \sum_{s\in S} \left(\sum_{e\in E(G)} \alpha_e\, \delta(e;v,s) \right) \left(\sum_{T\in\mathcal{F}_1(G;S)} (2-\operatorname{outdeg}(T,s)) w(T) \right) \\ &= \sum_{T\in\mathcal{F}_1(G;S)} w(T) \sum_{e\in E} \alpha_e \left(\sum_{s\in S} \delta(e;v,s)(2-\operatorname{outdeg}(T,s)) \right) \\ &= \sum_{T\in\mathcal{F}_1(G;S)} w(T) \sum_{e\in E} \alpha_e \left(\sum_{s\in S} \delta(e;v,s) \sum_{u\in T(s)} (2-\deg(u)) \right). \qquad (13)\end{aligned}$$

The first equality follows from Proposition 2.6 and (12). The last equality follows from using Lemma 2.7 for the subgraph $H = T(s)$.

We introduce additional notation to handle the double sum in parentheses in (13). Each S-rooted spanning tree T naturally induces a surjection $\pi_T \colon V \to S$, defined by

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

Using this notation,

$$(D[S]\mathbf{m})_v = \sum_{T\in\mathcal{F}_1(G;S)} w(T) \sum_{e\in E} \alpha_e \left(\sum_{u\in V} (2-\deg(u))\delta(e;v,\pi_T(u)) \right) \tag{14}$$

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

$$\sum_{T\in\mathcal{F}_1(G;S)} w(T) \sum_{e\in E} \alpha_e = \sum_{T\in\mathcal{F}_1(G;S)} w(T) \sum_{e\in E} \alpha_e \left(\sum_{u\in V} (2-\deg(u))\delta(e;v,u) \right) \tag{15}$$

By subtracting equation (15) from (14), we obtain

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

We have

$$\delta(e;v,\pi_T(u)) - \delta(e;v,u) = \begin{cases} 0 & \text{if } \delta(e;\pi_T(u),u) = 0 \\ 1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 1 \\ -1 & \text{if } \delta(e;\pi_T(u),u) = 1 \text{ and } \delta(e;v,\pi_T(u)) = 0. \end{cases} \tag{16}$$

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.

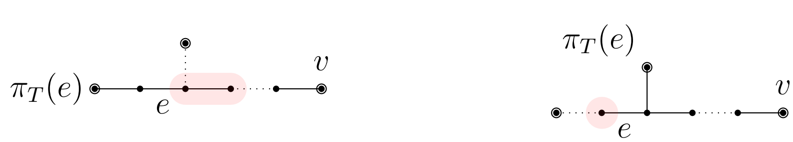


FIGURE 4. Edge $e \in T$ with $\delta(e;v,\pi_T(e)) = 1$ (left) and $\delta(e;v,\pi_T(e)) = 0$ (right). The floating component of $T \setminus e$ is highlighted.

Thus, when multiplying the term (16) by $(2-\deg(u))$ and summing over all vertices u, we obtain

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

Therefore

(17)
$$(D[S]\mathbf{m})_v-\sum_{T\in\mathcal{F}_1(G;S)}w(T)\sum_{e\in E}\alpha_e=\sum_{T\in\mathcal{F}_1(G;S)}w(T)\times$$
$$\sum_{e\in T}\alpha_e(2-\mathrm{outdeg}(T\setminus e,*))\Big(\mathbb{1}(\delta(e;v,\pi_T(e))=1)-\mathbb{1}(\delta(e;v,\pi_T(e))=0)\Big).$$

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

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

Observe in (17) that the deletion $T\setminus e$ is an $(S,*)$-rooted spanning forest of G, and that the corresponding weights satisfy

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

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

$$(\star)=\sum_{F\in\mathcal{F}_2}w(F)(2-\mathrm{outdeg}(F,*))\times$$
$$\sum_{e\in\partial F}\Big(\mathbb{1}(\delta(e;v,\pi_{(F\cup e)}(e))=1)-\mathbb{1}(\delta(e;v,\pi_{(F\cup e)}(e))=0)\Big)$$
$$=\sum_{F\in\mathcal{F}_2}w(F)(2-\mathrm{outdeg}(F,*))\Bigg(\#\{e\in\partial F\colon\delta(e;v,\pi_T(e))=1\text{ for }T=F\cup e\}$$
$$-\#\{e\in\partial F\colon\delta(e;v,\pi_T(e))=0\text{ for }T=F\cup e\}\Bigg).$$

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. Therefore

$$(\star) = \sum_{F\in\mathcal{F}_2} w(F)(2 - \operatorname{outdeg}(F,*))\Big(\#\{e \in \partial F(*) \colon \delta(e; v, F(*)) = 0\} - \#\{e \in \partial F(*) \colon \delta(e; v, F(*)) = 1\}\Big).$$

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

$$\#\{e \in \partial F(*) \colon \delta(e; v, F(*)) = 1\} = 1, \qquad \text{and}$$
$$\#\{e \in \partial F(*) \colon \delta(e; v, F(*)) = 0\} = \operatorname{outdeg}(F,*) - 1.$$

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

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

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.

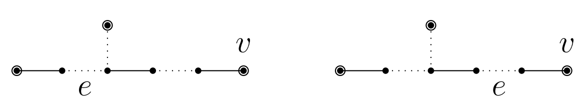


FIGURE 6. Edges $e \in \partial F(*)$ with $\delta(e; v, \pi_{(F\cup e)}(e)) = 1$ (left) and $\delta(e; v, \pi_{(F\cup e)}(e)) = 0$ (right).

Proof of Theorem B. 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 weight $w(G) = 1$. 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 $w(F) = \alpha_e$ and $\operatorname{outdeg}(F, *) - 2 = -1$. This shows that the right-hand side of (4) is zero.

Next, suppose $|S| \geq 2$. Lemma 3.4 states that $D[S]$ is nonsingular, so we may use the inverse matrix identity

$$\mathbf{1}^\intercal D[S]^{-1}\mathbf{1} = \frac{\operatorname{cof} D[S]}{\det D[S]}. \tag{18}$$

Let $\mathbf{m} = \mathbf{m}(G; S)$ denote the vector (12). By Proposition 5.3 (a) and Theorem 4.4,

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

Theorem 5.4 states that $D[S]\mathbf{m} = \lambda \mathbf{1}$ for some constant λ, which is nonzero since $D[S]$ is invertible (see Lemma 3.4) and $\mathbf{m}$ is nonzero (see Proposition 5.3 (b)). Hence

$$\mathbf{1}^\intercal D[S]^{-1}\mathbf{1} = \lambda^{-1}\mathbf{1}^\intercal \mathbf{m} = \frac{\operatorname{cof} D[S]}{(-1)^{|S|-1} 2^{|S|-1} \lambda}. \tag{19}$$

Comparing (18) with (19) gives the desired result, $\det D[S] = (-1)^{|S|-1} 2^{|S|-1} \lambda$. □

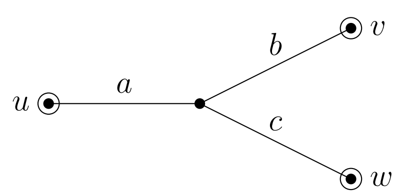
Proof of Theorem A. Set all lengths α_e to 1 in Theorem B. In this case, the weights $w(T) = 1$ and $w(F) = 2$ for all forests T and F, and

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

Remark 5.5. [16] It is worth observing that depending on the chosen subset $S \subseteq V$, 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. 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.



[16][(Farbod) perhaps drop this remark, or change and move it to introduction?]

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

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

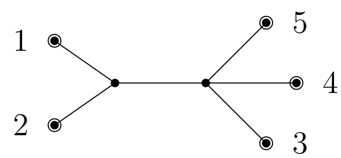
which has determinant

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

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

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

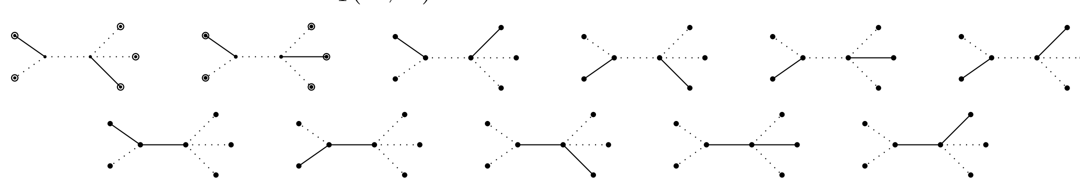
Example 6.2. Suppose G is the tree with unit edge lengths shown below, with five leaf vertices.



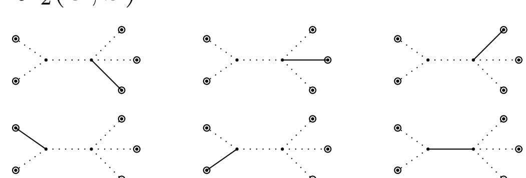
Let S denote the set of five leaf vertices. Then

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

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 $\mathbf{m} = \begin{pmatrix} 5 & 5 & 4 & 4 & 4 \end{pmatrix}^\intercal$.

Example 6.3. Suppose G is the tree with edge lengths 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 $\mathbf{m} = \begin{pmatrix} abd & +abe & +acd & +ace & +ade & & & -bde \\ abd & +abe & & & -ade & +bcd & +bce & +bde \\ abd & -abe & +acd & & +ade & +bcd & & +bde \\ -abd & +abe & & +ace & +ade & & +bce & +bde \end{pmatrix}$

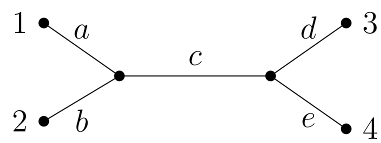


FIGURE 7. Tree with four leaves, and varying edge lengths.

The determinant of the distance submatrix is

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

References

[Bap10] R. B. Bapat, *Graphs and matrices*, Universitext, Springer, London; Hindustan Book Agency, New Delhi, 2010. MR2797201

[BKN05] R. Bapat, S. J. Kirkland, and M. Neumann, *On distance matrices and Laplacians*, Linear Algebra Appl. **401** (2005), 193–209. MR2133282

[BS11] R. B. Bapat and Sivaramakrishnan Sivasubramanian, *Identities for minors of the Laplacian, resistance and distance matrices*, Linear Algebra Appl. **435** (2011), no. 6, 1479–1489. MR2807165

[GL78] R. L. Graham and L. Lovász, *Distance matrix polynomials of trees*, Adv. in Math. **29** (1978), no. 1, 60–88. MR480119

[GP71] R. L. Graham and H. O. Pollak, *On the addressing problem for loop switching*, Bell System Tech. J. **50** (1971), 2495–2519. MR289210

[HJ13] Roger A. Horn and Charles R. Johnson, *Matrix analysis*, Second, Cambridge University Press, Cambridge, 2013. MR2978290

[KKW15] Adrien Kassel, Richard Kenyon, and Wei Wu, *Random two-component spanning forests*, Ann. Inst. Henri Poincaré Probab. Stat. **51** (2015), no. 4, 1457–1464. MR3414453

[RSW23] D. H. Richman, F. Shokrieh, and C. Wu, *Capacity on metric graphs*, 2023. in preparation.

[Tut84] W. T. Tutte, *Graph theory*, Encycl. Math. Appl., vol. 21, Cambridge University Press, Cambridge, 1984 (English).

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