### MINORS OF TREE DISTANCE MATRICES

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ABSTRACT. We prove a combinatorial formula for the principal minors of the distance matrix of a weighted tree. This generalizes a result of Graham and Pollak. The identity involves counts of rooted spanning forests of the underlying tree.

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### 1. Introduction

Suppose G = (V, E) is a tree with n vertices. Let D denote the distance matrix of G. In [4], Graham and Pollak proved that

eq:full-det

(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 (I) was motivated by a problem in data communication, and inspired much further research on distance matrices.

inspired much further research on distance matrices. The main result of this paper is to generalize (I) 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.

thm:main

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

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 \*-component of F.

For definitions of (S, \*)-rooted spanning forests and other terminology, see Section ??. Note that the quantity  $\deg^o(F, *)$  satisfies the bounds

$$1 \le \deg^o(F, *) \le |S|.$$

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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 (II) when S=V.

1.1. Weighted trees. If  $\{\alpha_e : e \in E\}$  is a collection of positive edge weights, the  $\alpha$ -distance matrix  $D_{\alpha}$  takes the distance along edge e to be  $\alpha_e$ . Namely, the (v, w)-entry of  $D_{\alpha}$  is the sum of the weights  $\alpha_e$  along the unique path from v to w. Then

eq:w-full-det

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

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

thm:w-main

**Theorem 2.** Suppose G = (V, E) is a finite, weighted tree with edge weights  $\{\alpha_e : e \in E\}$ , and corresponding weighted distance matrix  $D_{\alpha}$ . For any nonempty subset  $S \subset V$ , we have

eq:w-main

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

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

Theorem  $\frac{\text{thm:w-main}}{2 \text{ also reduces to Theorem}}$  taking all unit weights,  $\alpha_e = 1$ .

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  $\operatorname{convex}\ hull$  of  $S \subset G$ . To apply formula (2) or (2) "efficiently," we should replace G with this subtree  $\operatorname{conv}(S,G)$ . However, the formulas as stated are true even without this replacement due to cancellation of terms.

1.2. **Applications of the main theorem.** Given a matrix A, let cof A denote the sum of cofactors of A, i.e.

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

If A is invertible, then  $\operatorname{cof} A$  is related to the sum of entries of the matrix inverse  $A^{-1}$  by a factor of  $\det A$ , i.e.  $\operatorname{cof} A = (\det A)(\mathbf{1}^{\intercal}A^{-1}\mathbf{1})$ . In [2], Bapat and Sivasubramanian showed the following identity for the sum of cofactors of D[S].

eq:cof-trees

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

Using (??), an immediate corollary to Theorem thm:w-main 2 is the following identity.

**Theorem 3.** Suppose G = (V, E) is a finite, weighted tree with edge weights  $\{\alpha_e : e \in E\}$ . Let  $D = D_{\alpha}$  denote the weighted distance matrix of G. For any nonempty subset  $S \subset V$ , we have

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

where  $k(F, *) = 2 - \deg^{o}(F, *)$ .

# $\Diamond$ add remark / theorem that det/cof is achieved as result of optimization problem $\Diamond$

We remark that the calculation of det D[S] is related to the following quadratic optimization problem: for all vectors  $\mathbf{m} \in \mathbb{R}^{S}$ ,

optimize objective function:  $\mathbf{m}^{\mathsf{T}}D[S]\mathbf{m}$ 

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

The gradient of the objective function is  $2D[S]\mathbf{m}$ , and the gradient of the constraint is 1. By the theory of Lagrange multipliers, the optimal solution  $\mathbf{m}^*$  is a vector satisfying

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

It follows that the optimal objective value is

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

(The above computation uses the fact that D[S] is a symmetric matrix, and the given constraint  $\mathbf{1}^{\mathsf{T}}\mathbf{m} = 1$ .) On the other hand, assuming D[S] is invertible we have  $\mathbf{m}^* = \lambda(D[S]^{-1}\mathbf{1})$ , so that

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

**Proposition 4.** If D[S] is any matrix with rows and columns indexed by S, then any critical value of the optimization problem  $\diamondsuit$  cite above  $\diamondsuit$  is equal to  $\frac{\det D[S]}{\cot D[S]}$ , i.e.

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

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

$$\cot A = \sum_{i=1}^{|S|} \sum_{j=1}^{|S|} (-1)^{i+j} \det A_{ij}$$

**Theorem 5** (Monotonicity of principal minor ratios). If  $A, B \subset V(G)$  are nonempty subsets with  $A \subset B$ , then

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

**Theorem 6** (Bounds on principal minor ratios). Suppose G = (V, E) is a finite, weighted tree with distance matrix D.

(1) If  $S \subset V(G)$  is nonempty,

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

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

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

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

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

**Theorem 7** (Nonsingular minors). Let G be a finite tree with (weighted) distance matrix D, and let  $S \subset V(G)$  be a subset of vertices. If  $|S| \ge 2$  then  $\det D[S] \ne 0$ .

1.3. Previous work. A formula for the inverse matrix  $D^{-1}$  was found by Graham and Lovász in [3].

graphs-matrices

1.4. **Notation.** G a finite graph, loops and parallel edges allowed, possibly disconnected

E(G) edge set of G

V(G) vertex set of G

 $\kappa(G)$  number of spanning trees of G

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

 $\mathcal{F}_2(G)$  the set of 2-component forests of G

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

 $\mathcal{F}_2(G;S)$  the set of (S,\*)-rooted spanning forests of G

## 2. Graphs and matrices

For background on enumeration problems for graphs and trees, see Moon [5].

Given a graph G = (V, E) 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  $w(\overline{H})$  to denote  $w(\overline{E(H)})$ .

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  $S = \{v_1, v_2, \ldots, v_k\}$ , an S-rooted spanning forest of G is a spanning forest which has exactly one vertex  $v_i$  in each connected component. An (S, \*)-rooted spanning forest of G is a spanning forest which has |S| + 1 components, where |S| components each contain one vertex of S, and the additional component is disjoint from S. We call the component disjoint from S the "floating component."

Let

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

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

If u, v, w are vertices, then let

$$\kappa_2(uv|w)$$

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

**Example 8.** Suppose G is the tree with unit edge lengths shown below.



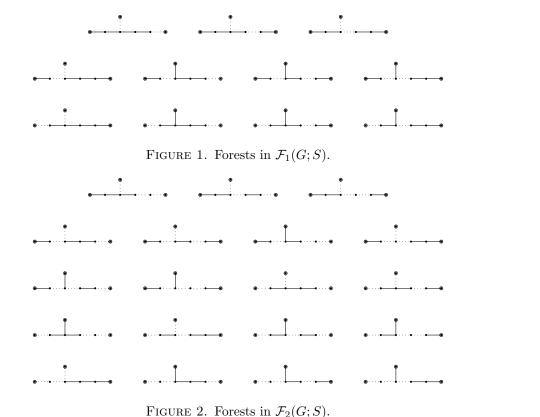
Let S be the set of three leaf vertices. Then  $\mathcal{F}_1(G;S)$  contains 11 forests, while  $\mathcal{F}_2(G;S)$  contains 19 forests. These are shown in Figures 1 and 2, respectively.

2.2. **Laplacian matrix.** Given a graph G = (V, E), let  $L \in \mathbb{R}^{V \times V}$  denote the *Laplacian matrix* of G. If G is a weighted graph with edge weights  $\alpha_e \in \mathbb{R}_{>0}$  for  $e \in E$ , let L denote the weighted Laplacian matrix of G.

Given  $S \subset V$ , let  $L[\overline{S}]$  denote the matrix obtained from L by removing the rows and columns indexed by S.

fig:1-forests

fig:2-forests



**Definition 9** (Weighted Laplacian matrix). Given a graph G = (V, E) and edge weights  $\{\alpha_e : e \in E\}$ , the weighted Laplacian matrix  $L_{\alpha} \in \mathbb{R}^{V \times V}$  is defined by

$$(L_{\alpha})_{v,w} = \begin{cases} 0 & \text{if } v \neq w \text{ and } (v,w) \notin E \\ \alpha_e^{-1} & \text{if } v \neq w \text{ and } (v,w) = e \in E \\ -\sum_{e \in N(v)} \alpha_e^{-1} & \text{if } v = w. \end{cases}$$

For any graph G, let  $\kappa(G)$  denote the number of spanning trees of G. The following theorem is due to Kirchhoff. For any graph G, let  $\kappa(G)$  denote the number of spanning trees of G.

**Theorem 10** (All-minors matrix tree theorem). Let G = (V, E) be a finite graph, and let L denote the Laplacian matrix of G. Then for any nonempty vertex set  $S \subset V$ ,

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

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.

The following result is due to Bapat–Siviasubramanian.

**Theorem 11** (Distance matrix cofactor sums [2]). Given a tree G, let D be the distance matrix of G, and L the Laplacian matrix. Let  $S \subset V(G)$  be a nonempty subset of vertices of G. Then

$$\operatorname{cof} D[S] = (-2)^{|S|-1} \det L[\overline{S}].$$

2.3. Tree distance. For  $e \in E$  and  $v, w \in V$ , let

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

thm:matrix-tree

ec:tree-distance

(Note that  $\delta(e; v, v) = 0$  for any e and v.) Given an edge  $e \in E$  and vertices  $v, w \in V$ , let

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

We can express the tree distance d(v, w) as a sum over edges

$$d(v, w) = \sum_{e \in E(G)} \delta(e; v, w) \quad \text{where } \delta(e; v, w) = \begin{cases} 1 & \text{if } e \text{ lies on } v \sim w \text{ path,} \\ 0 & \text{otherwise.} \end{cases}$$

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

- If we fix v and w, then  $\delta(-;v,w):E(G)\to\{0,1\}$  is the indicator function for the unique v w path in G.
- On the other hand if we fix e and v, then the deletion  $G \setminus e$  has two connected components, and  $\delta(e; v, -): V(G) \to \{0, 1\}$  is the indicator function for the component of  $G \setminus e$  not containing v.

rop:distance-sum

**Proposition 12** (Weighted tree distance). For a tree G = (V, E) with weights  $\{\alpha_e : e \in E\}$ , the  $weighted\ distance\ function\ satisfies$ 

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

2.4. Principal cuts. 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  $e^+$ , respectively  $(G \setminus e)^-$  and endpoint  $e^-$ .

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  $(G \setminus e)^{\overline{v}} \diamondsuit \text{ or } (G \setminus e)^{-v} \diamondsuit \text{ for the component not containing } v.$ 

2.5. Outdegree of rooted forest. Given a rooted forest F in  $\mathcal{F}(G;S)$  and  $s \in S$ , let F(s) denote the s-component of F. We define the outdegree  $\deg^o(F,s)$  by

eq:outdeg

(5) 
$$\deg^{o}(F,s) = \#\{e = (a,b) \in E : a \in F(s), b \notin F(s)\}.$$

In words,  $\deg^o(F,s)$  is the number of edges which connect the s-component of F to a different component.

 $\#\{e \in E : e \text{ connects the } s\text{-component of } F \text{ to a different component}\}\$ 

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

lem:outdeg-sum

**Lemma 13.** Suppose G is a tree and  $H \subseteq G$  is a (nonempty) connected subgraph. Then

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

*Proof.* 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  $\deg^o(H) = \deg(v)$ .

## 3. Proofs

In this section we prove Theorem 2.

- Outline of proof: given a subset  $S \subset V$  and distance submatrix D[S], we will
- (i) Find vector  $\mathbf{m} \in \mathbb{R}^S$  such that  $D[S]\mathbf{m} = \lambda \mathbf{1} \in \mathbb{R}^S$ .
- (ii) Compute the sum of entries of  $\mathbf{m}$ , i.e.  $\mathbf{1}^{\mathsf{T}}\mathbf{m}$ .
- (iii) Using (i), relate the sum  $\mathbf{1}^{\mathsf{T}}\mathbf{m}$  to the sum of entries of the inverse matrix  $D[S]^{-1}$ :

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

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

(iv) Use known expression for cof D[S] to compute

$$\det D[S] = \lambda(\operatorname{cof} D[S]) \left(\mathbf{1}^{\mathsf{T}} \mathbf{m}\right)^{-1}.$$

The interesting part of this expression will turn out to be in the constant  $\lambda$ .

**Example 14.** Suppose G is a tree consisting of three paths joined at a central vertex. Let S consist of the central vertex, and the three endpoints of the paths. The corresponding submatrix of the distance matrix is

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

Following the steps outlined above:

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

- (ii) The sum of entries of  $\mathbf{m}$  is  $\mathbf{1}^{\intercal}\mathbf{m} = 2$ .
- (iii) We have

$$2 = \mathbf{1}^{\mathsf{T}} \mathbf{m} = \lambda (\mathbf{1}^{\mathsf{T}} D[S]^{-1} \mathbf{1}) = \lambda \frac{\operatorname{cof} D[S]}{\det D[S]}$$

(iv) The cofactor sum cof D[S] is -8abc, so the determinant is

$$\det D[S] = \lambda \frac{\cot A}{\mathbf{1}^{\mathsf{T}} \mathbf{m}} = (a+b+c)(-8abc)\frac{1}{2} = -4(a+b+c)abc.$$

3.1. Warmup case: S = V.

**Proposition 15.** Let G = (V, E) a tree, and consider the vector  $\mathbf{m} \in \mathbb{R}^V$  defined by

$$\mathbf{m}_v = 2 - \deg v$$
 for each  $v \in V$ .

Then  $\mathbf{1}^{\intercal}\mathbf{m} = \sum_{v \in V} (2 - \deg v) = 2$ .

*Proof.* For any graph, 
$$\sum_{v \in V} \deg v = 2|E|$$
. Since G is a tree,  $|E| = |V| - 1$ .

**Proposition 16.** Let  $\mathbf{m}$  be the vector defined above, and let D be the distance matrix of G. Then  $D\mathbf{m} = \lambda \mathbf{1}$  for some constant  $\lambda$ .

*Proof.* It suffices to show that for each edge e, with endpoints  $(e^+, e^-)$ , we have

$$(D\mathbf{m})_{(e^+)} = (D\mathbf{m})_{(e^-)}.$$

We compute

$$(D\mathbf{m})_{(e^+)} - (D\mathbf{m})_{(e^-)} = \sum_{v \in V} (d(v, e^+) - d(v, e^-))(2 - \deg v)$$
$$= \sum_{v \in (G \setminus e)^-} \alpha_e (2 - \deg v) - \sum_{v \in (G \setminus e)^+} \alpha_e (2 - \deg v)$$

since

eq:12-1

(6)

-distance-warmup

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

 $\lozenge$  TO DO: define notation  $(G \setminus e)^{\pm}$   $\diamondsuit$  For each sum in (B.1), we apply Proposition  $\diamondsuit$  cite  $\diamondsuit$  to obtain

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

The same identity applies to the sum over  $(G \setminus e)^+$ , so  $(D\mathbf{m})_{(e^+)} = (D\mathbf{m})_{(e^-)}$  as desired.

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

dfn:m-vector

**Definition 17.** Let  $\mathbf{m} = \mathbf{m}(G; S) \in \mathbb{R}^S$  be defined by

eq:m-vector

(7) 
$$\mathbf{m}_v = \sum_{T \in \mathcal{F}_1(G;S)} (2 - \deg^o(T,v)) w(T) \quad \text{for each } v \in S.$$

where  $\deg^o(T,v)$  is the outdegree of the v-component of T, (2.4).

Let 1 denote the all-ones vector.

**Proposition 18.** For **m** defined above,  $\mathbf{1}^{\intercal}\mathbf{m} = 2\sum_{T \in \mathcal{F}_1(G;S)} w(T)$ .

*Proof.* We have

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

In the second line we apply Lemma 9 and exchange the outer summations. To obtain the third line, we observe that the vertex sets of T(s) for  $s \in S$  form a partition of V, since T is an S-rooted spanning forest. Finally we again apply Lemma  $s \in S$  for the last equality, as  $s \in S$  for  $s \in S$ 

Corollary 19. If G is a graph with unit edge weights  $\alpha_e = 1$ , then the vector  $\mathbf{m}$  defined in  $(\stackrel{\text{leq:m-vector}}{\mathbb{I}^4})$  satisfies  $\mathbf{1}^{\mathsf{T}}\mathbf{m} = 2 \kappa(G; S)$ .

**Theorem 20.** With  $\mathbf{m} = \mathbf{m}(G; S)$  defined as in  $([14], D[S]\mathbf{m} = \lambda \mathbf{1}$  for the constant

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

where  $\deg^{o}(F, w)$  is the out-degree of the w-component of F (as a spanning forest).

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

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

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

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

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

$$(8)$$

eq:14-1

Each S-rooted spanning tree T is naturally associated with a surjection  $\pi_T: V \to S$ , defined by

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

Using this notation,

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

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

We have

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

Summing the terms  $(2 - \deg(u))$  against the above over all vertices u, we have the following 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.

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

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



FIGURE 3. Edge  $e \in T(s_0)$  with  $\delta(e; v, s_0) = 1$  (left) and  $\delta(e; v, s_0) = 0$  (right).

Thus we obtain

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

Thus

$$\begin{aligned} & (D[S]\mathbf{m})(v) - \sum_{T \in \mathcal{F}_1} w(T) \sum_{e \in E} \alpha_e \\ & = \sum_{T \in \mathcal{F}_1} w(T) \sum_{s_0 \in S} \left( \sum_{\substack{e \in T(s_0) \\ \delta(e; v, s_0) = 1}} \alpha_e (2 - \deg^o(T \setminus e, *)) - \sum_{\substack{e \in T(s_0) \\ \delta(e; v, s_0) = 0}} \alpha_e (2 - \deg^o(T \setminus e, *)) \right). \end{aligned}$$

We now rewrite the above expression in terms of  $\mathcal{F}_2(G; S)$ , observing that the deletion  $T \setminus e$  is an (S, \*)-rooted spanning forest of G, if  $e \in T$ , and that the corresponding weights satisfy

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

Thus

$$\frac{(eq:1)}{(???)} = \sum_{F \in \mathcal{F}_2} w(F)(2 - \deg^o(F, *)) \sum_{T \in \mathcal{F}_1} \sum_{s_0 \in S} \left( \sum_{\substack{e \in T(s_0) \\ \delta(e; v, s_0) = 1}} \mathbb{1}(F = T \setminus e) - \sum_{\substack{e \in T(s_0) \\ \delta(e; v, s_0) = 0}} \mathbb{1}(F = T \setminus e) \right)$$

$$= \sum_{F \in \mathcal{F}_2} w(F)(2 - \deg^o(F, *)) \left( \#\{T \in \mathcal{F}_1 : F = T \setminus e \text{ for some } e \in T(s_0), \, \delta(e; v, s_0) = 1\} \right)$$

$$- \#\{T \in \mathcal{F}_1 : F = T \setminus e \text{ for some } e \in T(s_0), \, \delta(e; v, s_0) = 0\} \right)$$

Next, we 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  $\partial F(*)$ :

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

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

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

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

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. Thus

$$\#\{e \in \partial F(*) : \delta(e; v, F(*)) = 1\} = 1$$

and

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

Thus

$$(\stackrel{\text{leg:}1}{??}) = \sum_{F \in \mathcal{F}_2} w(F)(2 - \deg^o(F, *)) \Big( (\deg^o(F, *) - 1) - (1) \Big)$$

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

as desired.  $\Box$ 

Old proof. Regarding the vertex sets that appear in the last summation, we have

$$\bigcup_{\substack{s \in S \\ \delta(e;v,s)=1}} \{u \in T(s)\} = \begin{cases} \{u \in (G \setminus e)^{\overline{v}}\} & \text{if } e \notin T, \\ \{u \in (G \setminus e)^{\overline{v}}\} \cup (T \setminus e)(*) & \text{if } e \in T(s_0), \, \delta(e;v,s_0) = 0 \\ \\ \{u \in (G \setminus e)^{\overline{v}}\} \setminus (T \setminus e)(*) & \text{if } e \in T(s_0), \, \delta(e;v,s_0) = 1. \end{cases}$$

alternative:

$$\bigcup_{\substack{s \in S \\ \delta(e;v,s)=1}} \{w \in T(s)\} = \begin{cases} \{w \in V : \delta(e;v,w)=1\} & \text{if } e \not\in T, \\ \{w \in (G \setminus e)^{\overline{v}}\} \cup (T \setminus e)(*) & \text{if } e \in T, s_0(e,T) \in (G \setminus e)^v \\ \{w \in (G \setminus e)^{\overline{v}}\} \setminus (T \setminus e)(*) & \text{if } e \in T, s_0(e,T) \in (G \setminus e)^{\overline{v}}. \end{cases}$$

Here  $T \setminus e$  is a (S, \*)-rooted forest, i.e.  $T \setminus e \in \mathcal{F}_2(G; S)$ , and  $\deg^o(T \setminus e, *)$  refers to the out-degree of the floating component of  $T \setminus e$ . These cases correspond to

$$\sum_{s \in S \cap (G \setminus e)^{\overline{v}}} (2 - \deg^o(T, s)) = \begin{cases} 1 & \text{if } e \notin T, \\ 1 - (2 - \deg^o(T \setminus e, *)) & \text{if } s_0(e, T) \in (G \setminus e)^{\overline{v}}, \\ 1 + (2 - \deg^o(T \setminus e, *)) & \text{if } s_0(e, T) \in (G \setminus e)^v \end{cases}$$

From (3.2) we have

$$(D[S]\mathbf{m})_v = \sum_{e \in E} \alpha_e \sum_{T \in \mathcal{F}_1} w(T)(1 - f(v, e, T))$$
$$(D[S]\mathbf{m})_v = \sum_{T \in \mathcal{F}_1} w(T) \left( \sum_{e \notin T} \alpha_e + \sum_{s_0 \in S} \sum_{e \in T(s_0)} \alpha_e (1 - f(T, v, e, s_0)) \right)$$

where

$$f(T, v, e, s_0) = \begin{cases} 0 & \text{if } e \notin T \\ 2 - \deg^o(T \setminus e, *) & \text{if } \delta(e; v, s_0) = 0 \\ -(2 - \deg^o(T \setminus e, *)) & \text{if } e \in T(s_0) \text{ for some } s_0 \in S \text{ with } \delta(e; v, s_0) = 1 \end{cases}$$

FIGURE 5. Components rooted in  $S(G \setminus e)^{\overline{v}}$ .

# $\Diamond$ MOVE TO REMARK? If $e \in \text{conv}(G,S)$ , then $S(G \backslash e)^{\overline{v}}$ is nonempty and $\Diamond$

**Remark 21.** The set  $\mathcal{F}_2(G; S)$  of (S, \*)-rooted spanning forests of G can be partitioned into two types: "active" and "inactive".

$$\mathcal{F}_2(G/S) = \mathcal{F}_2^{in}(G;S) \sqcup \mathcal{F}_2^{out}(G;S),$$

where

$$\mathcal{F}_{2}^{in}(G; S) = \{ F \in \mathcal{F}_{2}(G; S) \text{ such that } \deg^{o}(*, F) \geq 2 \},$$
  
 $\mathcal{F}_{2}^{out}(G; S) = \{ F \in \mathcal{F}_{2}(G; S) \text{ such that } \deg^{o}(*, F) = 1 \}.$ 

Remark 22. A key step in the above proof is the use of the map

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

defined by

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

**Remark 23.** For a given spanning forest  $F \in \mathcal{F}_2(G; S)$ , there are exactly  $\deg^o(F, *)$ -many choices of pairs  $(T, e) \in \mathcal{F}_1(G; S) \times E(G)$  such that  $F = T \setminus e$ . Consider the "deletion" map

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

defined by ...

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

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

There is an associated "union" map

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

defined by

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

**Proposition 24.** Let G = (V, E) be a tree, and  $S \subset V$ . Suppose we label  $S = \{s_1, \ldots, s_r\}$  and  $V \setminus S = \{t_1, \ldots, t_{n-r}\}$ . For each  $t_i \in V \setminus S$ , consider  $\mathbf{f}_i \in \mathbb{R}^V$  defined by

Example 25. If

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

then

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

#### 4. Physical interpretation

If we consider G as a network of wires with each edge containing a unit resistor, which is grounded at all nodes in S, then  $\mathbf{m}_S$  records the currents flowing to S when current is added on  $V \setminus S$  in the amount  $2 - \deg v$  for each  $v \notin S$ .

4.1. Alternate proof. Let 1 denote the all-ones vector. When we choose a subset  $S \subset V(G)$ , we no longer have a single "obvious" replacement for  $\mathbf{m}$  inside  $\mathbb{R}^S$ . Instead, we can take an average over S-rooted spanning forests.

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

prop:n-vector

**Proposition 26.** Suppose  $v \in V \setminus S$ . For each  $s_j \in S$ , let  $\mu(v, s_j) = current$  flowing to  $s_j$  when unit current enters G at v and G is grounded at S. Explicitly,

$$\begin{split} \mu(v,s) &= \frac{\# \ of \ S\text{-}rooted \ spanning forests of } G \ whose \ s_{j}\text{-}component \ contains } v}{\# \ of \ S\text{-}rooted \ spanning forests of } G \\ &= \frac{\sum_{\mathcal{F}_{1}(G/S)} \mathbb{1}(v \in T(s))}{\kappa(G/S)} \\ &= \frac{\kappa_{r}(s_{1}|\cdots|s_{j}v|\cdots|s_{r})}{\kappa_{r}(s_{1}|\cdots|s_{r})} \end{split}$$

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

$$\mathbf{n}_v = 1, \quad \mathbf{n}_s = -\mu(v, s) \text{ if } s \in S, \quad \mathbf{n}_w = 0 \text{ if } w \notin S \cup v$$

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

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

**Theorem 27.** Let G be a tree, S a nonempty subset of vertices, and D[S] the corresponding submatrix of the distance matrix. Suppose  $\mathbf{m} = \mathbf{m}(G;S) \in \mathbb{R}^S$  is defined by (I4);

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

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

*Proof.* Note that

$$\mathbf{m}(G; S) = \kappa(G/S) \left( \sum_{v \in V} (2 - \deg v) \boldsymbol{\delta}(v) - \sum_{v \in V \setminus S} (2 - \deg v) \mathbf{n}(G; S, v) \right)$$
$$= \kappa(G; S) \left( \mathbf{m}(G; V) - \sum_{v \in V \setminus S} (2 - \deg v) \mathbf{n}(G; S, v) \right)$$

♦ TODO: elaborate on this equation ↑ From Proposition 13 we know that  $D\mathbf{m}(G; V)$  is constant on V, and from Proposition 21 we know that  $D\mathbf{n}(G; S, v)$  is constant on S. Hence by linearity,  $D\mathbf{m}(G; S)$  is constant on S.

### 5. Examples

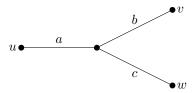
**Example 28.** Suppose G is a tree consisting of three paths joined at a central vertex. Let S consist of the central vertex, and the three endpoints of the paths. The corresponding minor of the distance matrix is

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

The determinant is

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

**Example 29.** Suppose  $\Gamma$  is a tripod with lengths a, b, c and corresponding leaf vertices u, v, w.



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

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

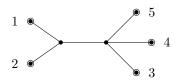
and

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

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

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

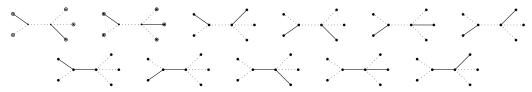
**Example 30.** Suppose  $\Gamma$  is the tree with unit edge lengths shown below, with five leaf vertices.



Let S denote the set of five leaf vertices. Then

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

Forests in  $\mathcal{F}_1(G;S)$ :

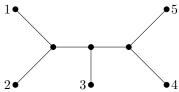


Forests in  $\mathcal{F}_2(G;S)$ :

and

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

**Example 31.** Suppose  $\Gamma$  is the tree with unit edge lengths shown below, with five leaf vertices and three internal vertices.



Let S denote the set of five leaf vertices. Then

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

and

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

6. Further work

See [6].

# 6.1. Symanzik polynomials.

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