# A simple proof of the matrix-tree theorem, upward routes, and a matrix-tree-cycle theorem

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#### **Abstract**

The matrix-tree theorem states that the number of spanning trees in a graph is  $\det L'$ , where L' is the Laplacian matrix L of the graph, with any row and column deleted. We give a direct proof of the fact that  $\det(xI+L)$  is the generating function of spanning forests with k roots. The proof does not rely on the Cauchy-Binet formula, yet is arguably simpler than the standard proof, and applies to weighted & directed graphs as well.

The proof is based on a lemma that if A is the adjacency matrix of a graph where each vertex has at most one outgoing edge, then  $\det(I-A)=1$  if A is a forest and  $\det(I-A)=0$  otherwise. We generalize this lemma to any graph, in which case  $\det(I-xA)^{-1}$  is shown to be the generating function of *upward routes*.

Lastly, we generalize the matrix-tree theorem to a theorem about  $\det(A+L)$  where A is the adjacency matrix of a second graph, which reduces to counting spanning forests when A=xI but allows some cycles when A is not diagonal. The special case L=0 gives that  $\det(A)$  counts signed cycle covers. The all-minors matrix-tree theorem follows as a corollary. For instance, the fact that  $\det(L')$  counts spanning forests, where L' is L with any column i and row j deleted, follows by picking A to have  $A_{ij}=1$  and zero elsewhere.

#### 1 Introduction

Given finite sets of numbers  $T_1, \ldots, T_n \subset \mathbb{R}$ , we have the identity:

$$\left(\sum_{x_1 \in T_1} x_1\right) \cdots \left(\sum_{x_n \in T_n} x_n\right) = \sum_{x_1 \in T_1} \cdots \sum_{x_n \in T_n} x_1 \cdots x_n$$

On the right hand side, we get one term for every way of choosing  $(x_1, ..., x_n) \in T_1 \times \cdots \times T_n$ . Similarly, given finite sets of vectors  $T_1, ..., T_n \subset \mathbb{R}^k$ , we have the following identity, by multilinearity of the determinant:

$$\det\left(\sum_{v_1 \in T_1} v_1 \mid \cdots \mid \sum_{v_n \in T_n} v_n\right) = \sum_{v_1 \in T_1} \cdots \sum_{v_n \in T_n} \det(v_1 \mid \cdots \mid v_n)$$

Here  $\det(v_1|\dots|v_n)$  is the determinant of a matrix with those columns. We shall see that Kirchoff's theorem can be obtained by applying this identity to the Laplacian. The right hand side contains a nonzero term for each spanning forest, and all the other terms vanish.

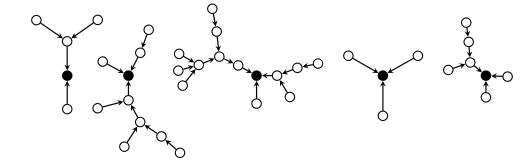


Figure 1: A forest with 5 roots.

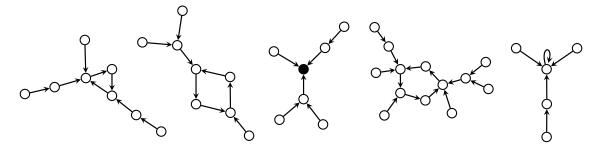


Figure 2: A 01-graph with one root. If we delete the third component, we obtain a 1-graph.

**Definition 1.1.** We define the concepts 1-graph, 01-graph, forest, root, and tree:

- A 1-graph is a directed graph where each vertex has 1 outgoing edge.
- A 01-graph is a directed graph where each vertex has 0 or 1 outgoing edges.
- A forest is a 01-graph with no cycles.
- The *roots* are vertices with 0 outgoing edges.
- A tree is a forest with one root.

See Figure 1 and Figure 2 for examples.

If we start at a vertex  $\nu$  in a 01-graph and keep following the unique outgoing edge, then we either loop in a cycle, or we end up at a vertex with no outgoing edges. Therefore a general 01-graph consists of roots and cycles, plus trees converging onto the roots and cycles. A 1-graph is a 01-graph with no roots, so regardless of where we start, we always end up in a cycle.

### 2 The matrix-tree theorem

We need a lemma that gives us an indicator function for forests.

**Lemma 2.1.** Let  $A_G$  be the adjacency matrix of a 1-graph G, then

$$\det(I - A_G) = \begin{cases} 1 & \text{if G is empty} \\ 0 & \text{if G is not empty} \end{cases}$$

*Proof.* If *G* is empty, we have a  $0 \times 0$  matrix, which has determinant 1. If *G* is not empty, then each column of  $I - A_G$  has one +1 diagonal entry and one -1 entry from  $A_G$ , so the sum of the rows is zero, so  $\det(I - A_G) = 0$ . This remains true in the presence of self loops.

**Lemma 2.2.** Let  $A_G$  be the adjacency matrix of a 01-graph G, then

$$\det(I - A_G) = \begin{cases} 1 & \text{if } G \text{ is a forest} \\ 0 & \text{if } G \text{ has a cycle} \end{cases}$$

*Proof.* We calculate the determinant by repeatedly performing Laplace expansion on a column i that corresponds to a root. The column of a root has a single +1 entry on the diagonal, so performing Laplace expansion along this column deletes column i and row i. Row i contains all the incoming edges of the root. Therefore, this operation corresponds to deleting root i and all its incoming edges from the graph. Deleting a root may create new roots. Repeating this process of deleting roots, the remaining 1-graph will be empty iff the original graph was a forest. Applying the previous lemma gives the desired result.

An alternative shorter proof using eigenvalues:

*Proof.* If *G* is a forest then  $A_G$  is nilpotent, so all its eigenvalues are 0, so all the eigenvalues of  $I - A_G$  are 1, so  $\det(I - A_G) = 1$ . If *G* has a cycle, then  $A_G$  has 1 as an eigenvalue (take the eigenvector that is 1 on the cycle and 0 elsewhere), so  $I - A_G$  has 0 as an eigenvalue, so  $\det(I - A_G) = 0$ .

We now fix  $n \times n$  matrices A and D over some commutative ring:

- An arbitrary matrix A of edge weights (with  $A_{ij}$  being the weight of edge  $i \rightarrow j$ )
- A diagonal matrix D of vertex weights (with  $D_{ii}$  being the weight of vertex i).

**Definition 2.1.** The Laplacian matrix *L* is defined as having columns:

$$L_i = \sum_j A_{ij} (e_i - e_j)$$

**Definition 2.2.** The weight of a forest *G* is:

$$w(G) = \prod_{i \in \text{roots}(G)} D_{ii} \prod_{(i \to j) \in \text{edges}(G)} A_{ij}$$

We're ready to state Kirchoff's theorem for multiple-root forests in weighted directed graphs.

**Theorem 2.1** (Kirchoff, Tutte). The determinant det(D+L) is the weight-sum of all forests on n vertices:

$$\det(D+L) = \sum_{forest\ G} w(G)$$

*Proof.* The *i*-th column of the matrix is  $(D+L)_i = D_{ii}e_i + \sum_i A_{ij}(e_i - e_j)$ , so

$$\det(D+L) = \det\begin{pmatrix} D_{11}e_1 & D_{22}e_2 \\ + & + \\ A_{11}(e_1-e_1) & + \\ + & + \\ A_{12}(e_1-e_2) & + \\ \vdots & \vdots & \\ A_{1n}(e_1-e_n) & A_{2n}(e_2-e_n) & \\ & \vdots & \\ & A_{nn}(e_n-e_n) & \\ & A_{nn}(e_n-e_n) & \\ & & \vdots & \\ & A_{nn}(e_n-e_n) & \\ & & \vdots & \\ & & A_{nn}(e_n-e_n) & \\ & & & \vdots & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & &$$

The first step is by the definition of L. In the middle step we expand the determinant by multilinearity: we sum over all possible ways to pick one term of each column. To choose a 01-graph on n vertices, is to choose for each vertex i (column i) whether to make i a root (term  $D_{ii}e_i$ ) or to give i an outgoing edge  $i \rightarrow j$  (term  $A_{ij}(e_i - e_j)$ ). Then we take the weights  $D_{ii}$  and  $A_{ij}$  out of the determinant, and we're left with  $w(G) \det(I - A_G)$ , where  $A_G$  is the adjacency matrix of the chosen 01-graph. The final step is applying lemma 2.2.

#### JJ: start with corollary immediately.

The classic form of Kirchoff's matrix tree theorem lets us count the number of spanning trees of an *undirected* and *unweighted* graph *G*. It is a special case of Theorem 2.1, as follows.

We interpret the undirected unweighted graph as a directed weighted graph where we insert two edges  $i \rightarrow j$  and  $j \rightarrow i$  of weight 1 for each undirected edge i - j. This makes the matrix A the adjacency matrix of G:

$$A_{ij} = \begin{cases} 1 & \text{if } \{i, j\} \in G \\ 0 & \text{otherwise} \end{cases}$$

The Laplacian L is still given by definition 2.1.

**Corollary 2.1.1** (Classic form of Kirchoff's theorem). Let L' be the Laplacian matrix L with the first row and column deleted. Then det(L') is the number of spanning trees of G.

*Proof.* Set the vertex weight  $D_{11} = 1$  for vertex 1 and  $D_{ii} = 0$  for the other vertices. Then on the one hand,  $\det(D+L) = \det(L')$  (since  $\det(L) = 0$ ), and on the other hand,  $\det(D+L)$  is the number of directed trees with 1 as the root, by theorem 2.1. Such trees are in bijective correspondence with undirected spanning trees of G, because we can turn a tree rooted at 1 into an undirected spanning tree by forgetting the direction of the edges, and we can turn an undirected spanning tree into a tree rooted at 1 by directing all the edges toward 1.

More generally, theorem 2.1 allows us to count the number of forests with a given number of roots. For our commutative ring we pick polynomials in x and set D = xI. Theorem 2.1 gives that the (slightly modified) characteristic polynomial  $\det(xI + L)$  of the Laplacian matrix L is the generating polynomial of forests with k roots.

It is essential that we consider directed forests. The correspondence between undirected spanning trees and directed spanning trees rooted at 1 fails to work as smoothly for k > 1. Thus it could be argued that Kirchoff's theorem is really a theorem about directed forests. The directed version was Tutte's contribution to the theorem.

# 3 A matrix-tree-cycle theorem

We shall now generalize the matrix-tree theorem about det(D+L) to a *matrix-tree-cycle theorem* by allowing D to be a general matrix. This theorem will express det(D+L) as a sum over 1-graphs with each edge labeled either with T (for tree) or with C (for cycle) but not both. We call such 1-graphs TC-labeled.

**Definition 3.1.** A TC-labeled 1-graph is called *tree-cyclic* if:

- 1. Each cycle has at least one C-edge (i.e., the T-edges form a forest)
- 2. Each C-edge lies on a cycle (i.e., edges not part of a cycle must be T-edges)

The cycle that a C-edge is a part of may use other C-edges as well as T-edges, but a cycle cannot consist solely of T-edges. Said differently: an 1-graph consists of a set of cycles and some extra edges converging onto those cycles. We obtain a valid tree-cyclic TC labeling as long as we obey two constraints: we must label at least one edge on each cycle with C, and we must label all the converging edges with T. The remaining cycle edges can be labeled with either C or T. Figure 3 contains an example of a tree-cyclic graph.

**Definition 3.2.** The sign of a TC-labeled 1-graph *G* is:

$$(-1)^G = (-1)^{\text{#cycles} + \text{#C-edges}}$$

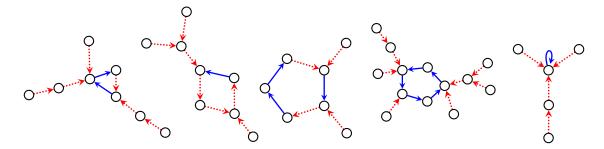


Figure 3: A tree-cyclic 1-graph. T-edges are red dotted edges, and C-edges are solid blue edges.

where #cycles is the number of cycles of G and #C-edges is the total number of C-labeled edges in G. Alternatively, each cycle with an odd number of C-edges does not affect the sign, and each cycle with an even number of C-edges flips the sign. Compare this with the sign of a permutation graph, for which a cycle with an odd number of edges does not affect the sign, and a cycle with an even number of edges flips the sign. The sign of a TC-labeled 1-graph can thus be determined by the same method, except that we consider only C-edges. The graph G in fig. 3 has sign  $(-1)^G = -1$  because there is one cycle with an even number of C-edges (the first component).

We associate a matrix  $M_G$  with a TC-labeled 1-graph G. This matrix will play the role that  $I - A_G$  played in the matrix-tree theorem.

**Definition 3.3.** The matrix  $M_G$  is defined as having columns:

$$(M_G)_i = \begin{cases} e_j & \text{if the outgoing edge } i \to j \text{ has label C} \\ e_i - e_j & \text{if the outgoing edge } i \to j \text{ has label T} \end{cases}$$

The following lemma generalizes lemma 2.2 used in the proof of the matrix-tree theorem.

**Lemma 3.1.** *The determinant of*  $M_G$  *is given by:* 

$$\det(M_G) = \begin{cases} (-1)^G & \text{if } G \text{ is tree-cyclic} \\ 0 & \text{otherwise} \end{cases}$$

*Proof.* Calculate the determinant in steps:

- 1. Perform Laplace expansion on vertices with no predecessors. This makes the determinant zero if the successor is a C-edge, and deletes the corresponding vertex if the successor is a T-edge.
- 2. We are now left with a disjoint set of cycles. If there is a cycle consisting solely of T-edges, the determinant is zero because the corresponding rows sum to zero.
- 3. We are now left with a disjoint set of cycles where each cycle has at least one C-edge. Use the C-edges to turn the T-edges into C-edges by row operations. The determinant obtains a -1 sign for each such switch.
- 4. We are now left with a disjoint set of cycles where each cycle consists solely of C-edges. In other words, a permutation matrix. The determinant of a permutation matrix is  $(-1)^{\text{#cycles+#edges}}$

If there was a C-edge not part of a cycle we have obtained 0 in step 1, and if there was a cycle among T-edges we have obtained 0 in step 2. For the remaining graphs, we have obtained a -1 sign for each T-edge in the cycles, so together with  $(-1)^{\text{#cycles}+\text{#edges}}$  we are left with  $(-1)^{\text{#cycles}+\text{#C-edges}} = (-1)^G$ .  $\square$ 

We now fix  $n \times n$  matrices A and D over some commutative ring:

• An arbitrary matrix *A* of weights for T-edges (with  $A_{ij}$  being the weight of edge  $i \xrightarrow{T} j$ )

- An arbitrary matrix D of weights for C-edges (with  $D_{ij}$  being the weight of edge  $i \xrightarrow{C} j$ )
- As before, the Laplacian *L* is given by  $L_i = \sum_i A_{ij} (e_i e_j)$

**Definition 3.4.** The weight of a TC-labeled graph *G* is:

$$w(G) = \prod_{\text{C-edge } (i \to j) \in G} D_{ij} \prod_{\text{T-edge } (i \to j) \in G} A_{ij}$$

We're ready to state the matrix-tree-cycle theorem.

**Theorem 3.1.** The determinant det(D + L) is the signed weight-sum of tree-cyclic graphs:

$$\det(D+L) = \sum_{tree-cyclic\ G} (-1)^G w(G)$$

*Proof.* The *i*-th column of the matrix is  $(D+L)_i = \sum_j D_{ij}e_j + \sum_j A_{ij}(e_i-e_j)$ , so

$$\det(D+L) = \det \begin{pmatrix} D_{11}e_1 & D_{21}e_1 & & & D_{n1}e_1 \\ + & + & & + \\ \vdots & \vdots & & \vdots \\ + & D_{1n}e_n & D_{2n}e_n & & & \\ + & D_{2n}e_n & + & & & \\ + & A_{21}(e_1-e_1) & + & & & \\ + & & \vdots & & & \\ + & & & + & \\ \vdots & & \vdots & & & \\ + & & + & & \\ A_{1n}(e_1-e_n) & A_{2n}(e_2-e_n) & & & A_{nn}(e_n-e_n) \end{pmatrix} = \underbrace{\sum_{TC\text{-1-graph } G} w(G) \det(M_G)}_{TC\text{-1-graph } G} = \underbrace{\sum_{TC\text{-1-graph } G} w(G) \det(M_G)}_{TC\text{$$

In the middle step we have again expanded the determinant by multilinearity: we sum over all possible ways to pick one term of each column. To choose a TC-labeled 1-graph on n vertices, is to choose for each vertex i (column i) an outgoing edge  $i \rightarrow j$  and a label C (term  $D_{ij}e_j$ ) or T (term  $A_{ij}(e_i-e_j)$ ) for this edge. The final step is applying lemma 3.1.

The matrix-tree theorem is recovered by taking D to be diagonal. In that case, the number of cycles and the number of C-edges is equal, so  $(-1)^{\text{#cycles}+\text{#C-edges}} = 1$  and there are no signs involved. Each C-labeled self-loop corresponds to a root.

If we take A = 0 we get the fact that det(D) is the sum of signed cycle covers. A cycle cover of n vertices is a choice of edges such that each vertex has precisely one incoming and one outgoing edge, and its sign is the sign of the permutation that this graph depicts.

By taking  $D_{ij} = 1$  for some i, j and zero elsewhere, we also ensure that the sign  $(-1)^G = 1$ , because in this case we have one C-edge and one cycle. Thus,  $\det(D + L)$  will be the number of spanning trees rooted at i. The choice of j does not matter. By developing the determinant and using  $\det(L) = 0$  we see that this is equal to  $\det(L')$  where L' is obtained from L by deleting row i and column j. Theorem 2.1 was only able to establish this for i = j.

By taking more off-diagonal entries of D to be nonzero, and by taking the corresponding rows and columns to be zero in A (and thus in L), we obtain the all-minors matrix-tree theorem.

## 4 Upward routes

We now know that when A is the adjacency matrix of a 01-graph, then  $\det(I - A) = 1$  if G is a forest and  $\det(I - A) = 0$  if G has a cycle. One naturally wonders about the value of  $\det(I - A)$  when A is an arbitrary adjacency matrix. The goal of this section is a combinatorial interpretation of  $\det(I - xA)$  and  $\det(I - xA)^{-1}$  for an arbitrary adjacency matrix, which generalizes the lemma to arbitrary graphs.

**Definition 4.1.** Given a directed graph *G* with an order on the vertices, we define (*strictly*) *upward loops* and (*strictly*) *upward routes*:

- An *upward loop* at vertex *i* is a walk from *i* to *i* that does not visit vertices lower than *i*.
- A *strictly upward loop* at vertex *i* is a walk from *i* to *i* that only visits vertices higher than *i* (except at the start/endpoint of the walk, where it does visit *i* itself).
- A (strictly) upward route is a choice of (strictly) upward loop at each vertex.

Let  $f_i(x)$  be the generating function of strictly upward loops of length k at vertex i. Then

$$f_i^*(x) = (1 - f_i(x))^{-1}$$

is the generating function of upward loops of length k at vertex i, because an upward loop splits uniquely into a sequence of strictly upward loops. Furthermore, the generating functions f(x) and  $f^*(x)$  of (strictly) upward routes of k edges are given by:

$$f(x) = \prod_{i=1}^{n} f_i(x)$$
  $f^*(x) = \prod_{i=1}^{n} f_i^*(x)$ 

Recall Cramer's rule:

**Theorem 4.1.** (Cramer's rule) Let A be an invertible matrix and let  $A_{[i,j]}$  be the matrix A with column i and row j deleted, then:

$$(A^{-1})_{ij} = \frac{\det(A_{[i,j]})}{\det(A)}$$

From this, we get the following lemma that allows us to calculate  $det(A)^{-1}$  in terms of entries of inverses of submatrices of A:

**Lemma 4.1.** Given a matrix A, provided both sides are defined,

$$\det(A)^{-1} = \prod_{i=0}^{n-1} ((A_{[1...i,1...i]})^{-1})_{11}$$

where  $A_{[1...i,1...i]}$  is the matrix A with the first i rows and columns deleted.

Proof. Cramer's rule implies:

$$\det(A)^{-1} = A_{1,1}^{-1} \cdot \det(A_{[1,1]})^{-1}$$

Continuing this by induction, we get:

$$\begin{split} \det(A)^{-1} &= A_{1,1}^{-1} \cdot \det(A_{[1,1]})^{-1} \\ &= A_{1,1}^{-1} \cdot (A_{[1,1]})_{11}^{-1} \cdot \det(A_{[1..2,1..2]})^{-1} \\ &= \cdots \\ &= A_{1,1}^{-1} \cdot (A_{[1,1]})_{11}^{-1} \cdot (A_{[1..2,1..2]})_{1,1}^{-1} \cdot \cdots (A_{[1..n-1,1..n-1]})_{1,1}^{-1} \cdot 1 \end{split}$$

**Lemma 4.2.** The generating function of upward loops at vertex i is  $((I - xA)_{[1...i-1,1...i-1]})_{11}^{-1}$ .

*Proof.* Given an adjacency matrix B,  $(I-xB)^{-1}=I+xB+x^2B^2+\cdots$  is the matrix generating function of walks, so  $(I-xB)_{11}^{-1}$  is the generating function of loops from vertex 1 to 1. To obtain upward loops at vertex i in A we take  $B=(I-xA)_{[1...i-1,1...i-1]}$  with the first i-1 rows and columns deleted.  $\square$ 

We combine these lemmas to obtain:

**Theorem 4.2.** The generating function of upward routes with k edges is  $det(I - xA)^{-1}$ .

*Proof.* Combine the preceding two lemmas with  $f^*(x) = \prod_{i=1}^n f_i^*(x)$ .

**Corollary 4.2.1.** The number of upward routes of k edges does not depend on the order of the vertices.

*Proof.* If we permute the order of the vertices by a permutation *P*, the generating function

$$\det(I - xPAP^{-1}) = \det(P(I - xA)P^{-1}) = \det(I - xA)$$

stays the same. A bijective proof is left as an exercise:)

**Corollary 4.2.2.** For an arbitrary adjacency matrix *A*,

$$\det(I - xA) = \prod_{i=1}^{n} (1 - f_i(x))$$

where  $f_i(x)$  is the generating function of strictly upward loops at vertex *i*.

*Proof.* Use the relationship between the generating functions:

$$\det(I - xA) = f^*(x)^{-1} = \prod_{i=1}^n f_i^*(x)^{-1} = \prod_{i=1}^n (1 - f_i(x))$$

Note that  $\det(I-xA)$  is a polynomial, even though  $f_i(x)$  is a power series. If we take the coefficient of  $x^k$  of Corollary 4.2.2, then modulo sign conventions we obtain precisely Theorems 1&2 from [Rot01] about clow sequences (clow sequences are equivalent to strictly upward routes). Corollary 4.2.2 is equivalent to Theorem 2 from [Rot01], but is stated directly in terms of the polynomials, rather than in terms of their coefficients.

Lemma 2.2 follows from corollary 4.2.2, which gives us a third proof of the lemma:

**Corollary 4.2.3.** Let  $A_G$  be the adjacency matrix of a 01-graph G, then

$$\det(I - A_G) = \begin{cases} 1 & \text{if } G \text{ is a forest} \\ 0 & \text{if } G \text{ has a cycle} \end{cases}$$

*Proof.* If *G* is a forest, then it has no strictly upward loops, so  $f_i(x) = 0$ , so  $\det(I - xA_G) = 1$ . If *G* has a cycle, let *i* be the lowest vertex on the cycle. Then  $f_i(x) = x^k$  where *k* is the length of the cycle. Now substitute x = 1 to obtain  $\det(I - A_G) = 0$ .

**Definition 4.2.** Let *K* be a matrix of natural numbers. Define  $A^K = \prod_{i,j} A_{ij}^{K_{ij}}$ .

**Theorem 4.3.** The coefficient of  $A^K$  in det(I - A) is given by

$$[A^K] \det(I - A) = \begin{cases} \frac{\prod_i c(K)_i!}{\prod_{ij} K_{ij}!} & \text{if } c(K) = r(K) \\ 0 & \text{otherwise} \end{cases}$$

where c(K) and r(K) are the column and row sums of K:

$$c(K)_i = \sum_j K_{ji} \qquad \qquad r(K)_i = \sum_j K_{ij}$$

**Acknowledgements.** Thanks to Darij Grinberg for pointing out mistakes and suggesting improvements, and for informing me about the relationship of Corollary 4.2.2 to Theorems 1&2 of [Rot01].

## References

[Rot01] Gunter Rote. *Division-Free Algorithms for the Determinant and the Pfaffian: Algebraic and Combinatorial Approaches*, pages 119–135. Springer Berlin Heidelberg, 2001.