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. Our 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:

$$\det\left(\sum_{\nu_1 \in T_1} \nu_1 \mid \cdots \mid \sum_{\nu_n \in T_n} \nu_n\right) = \sum_{\nu_1 \in T_1} \cdots \sum_{\nu_n \in T_n} \det(\nu_1 | \cdots | \nu_n)$$

Where $\det(v_1|...|v_n)$ is the determinant of a matrix with those columns. We shall see that Kirchoff's theorem can be obtained from this identity, but we first need some definitions and a lemma.

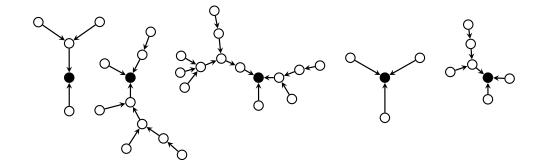


Figure 1: A forest with 5 roots.

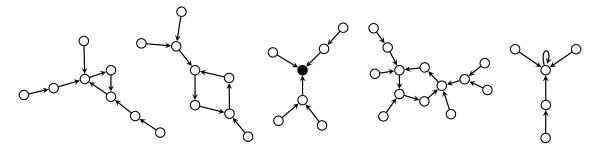


Figure 2: A 01-graph with one root. If we delete the third component, we obtain a 1-graph.

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 v 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 give us an indicator function for forests.

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

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

Proof. If *G* is empty, we have a 0×0 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 2.3 (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 the lemma.

The classic form of Kirchoff's matrix tree theorem gives us a way to count the number of spanning trees of an *undirected* and *unweighted* graph *G*. It is a special case of Theorem 2.3, as follows.

We interpret the undirected unweighted graph as a directed weighted graph where we insert two edges $i \to j$ and $j \to i$ 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 2.3.1 (Classic form of Kirchoff's theorem). Let L' be the Laplician 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, $\det(D+L) = \det(L')$, and on the other hand, $\det(D+L)$ is the number of directed trees with 1 as the root, by theorem 2.3. 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 2.3 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 2.3 gives that the (slightly modified) characteristic polynomial $\det(xI + A)$ of the adjacency matrix A 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 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 3.1. 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 3.1. (Cramer's rule) Let A be an invertible matrix and let $A_{[i,j]}$ be the same 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 3.2. Given a matrix A, provided both sides are defined,

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

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

Proof. Cramer's rule implies:

$$\det(A)^{-1} = A_{1,1}^{-1} \cdot \det(A_{\lceil 1,1 \rceil})^{-1}$$

Continuing this by induction, we get:

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

Lemma 3.3. 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 3.4. 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 3.4.1. 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 3.4.2. 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 3.4.2, then modulo sign conventions we obtain precisely Theorems 1&2 from [Rot01] about clow sequences (clow sequences are equivalent to strictly upward routes). Corollary 3.4.2 is equivalent to Theorem 2 from [Rot01], but is stated directly in terms of the polynomials, rather than in terms of their coefficients.

The main lemma follows as a corollary, which gives us a third proof of the lemma:

Corollary 3.4.3. 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 $\det(I - A_G) = 0$.

4 The matrix-tree-cycle theorem

We shall now generalize the matrix-tree theorem about det(D + L) to the *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

Definition 4.1. A TC-labeled 1-graph is called *tree-cyclic* if:

- 1. Each cycle has at least one C-edge, and
- 2. Each C-edge lies on a cycle

In other words: the T-edges form a forest, and each C-edge is part of a cycle. 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 TC graph 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 4.2. The sign of a TC-labeled 1-graph *G* is:

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

where #cycles is the number of cycles of G and #C-edges is the total number of C-labeled edges in G.

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 4.3. The matrix M_G is defined as having columns:

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

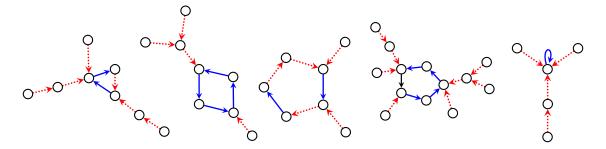


Figure 3: A tree-cyclic 1-graph. T-edges are red dotted edges, and C-edges are solid blue edges.

The following lemma generalizes the main lemma of the matrix-tree theorem.

Lemma 4.1. 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 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 $L_i = \sum_j A_{ij} (e_i e_j)$.

Definition 4.4. The weight of a tree-cyclic 1-graph *G* is:

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

Were ready to state the matrix-tree-cycle theorem.

Theorem 4.2. 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

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

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 the lemma.

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

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.

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.

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References

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