The Matrix-Tree Theorem

Connecting graphs with matrices

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Mathcamp 2019

1 Motivation

Let's start with a particularly curious fact from graph theory:

> **Proposition 1.1** (Cayley formula)
> The number of **labeled trees** on n vertices – that is, trees where the vertices are numbered from 1 to n – is n^{n-2}.

Since Mark's class isn't running, I'll give a brief sketch of the non-Prufer code proof of this. This is not directly related to the rest of class – it's just for curiosity's sake.

Proof. Assign a monomial to each tree T in the variables $x_1, \cdots, x_n$

$$m(T) = \prod_i x_i^{\text{degree}(i)-1}.$$

If we add up all such monomials, we get a degree $(n-2)$ polynomial f in $x_1, \cdots, x_n$ (because we have $(n-1)$ edges, each of which contributes 2 to the degree of the monomial, and then we subtract 1 for each vertex). **We claim that**

$$\sum_{\text{trees } T} m(T) = (x_1 + \cdots + x_n)^{n-2}.$$

Do this by induction! $n = 1$ doesn't quite work because polynomials break, but it's true for $n = 2$. In the inductive step, we claim that x_i is a factor of

$$\sum_{\text{trees } T} m(T) - (x_1 + \cdots + x_n)^{n-2}$$

for all $1 \le i \le n$. This is because plugging in $x_i = 0$, all $m(T)$ terms disappear unless the degree of i is 1: this means that all trees can be constructed by taking a tree on the remaining vertices, and then attaching vertex i to one of the remaining vertices. This means

$$\sum_{\text{trees } T} m(T)|_{x_i=0} = (x_1+\cdots+x_{i-1}+x_{i+1}+\cdots+x_n)^{n-3}\cdot(x_1+\cdots+x_{i-1}+x_{i+1}+\cdots+x_n) = (x_1+\cdots+x_{i-1}+x_{i+1}+\cdots+x_n)^{n-2}$$

by the inductive hypothesis, which cancels out exactly with the other term!

Repeating this argument for all i, we find that $x_1 \cdots x_n$ is actually a root of f. But $\sum_{\text{trees } T} m(T) - (x_1 + \cdots + x_n)^{n-2}$ has degree at most $n - 2$, so it must then be 0.

To finish, just set $x_1 = \cdots = x_n = 1$: then all trees have weight 1, and the total weight is $(1 + \cdots + 1)^{n-2} = n^{n-2}$, as desired. □

Although this does give an explicit construction for each of the n^{n-2} trees, there isn't much that we can learn about the mathematics behind generalizations: notably, what if we want other constraints on our vertices (for example, we can't connect two even-labeled vertices to each other)? This motivates trying to find a more computational approach to our question, and to start on that, let's rephrase our initial question.

Definition 1.2

A **spanning tree** of a graph G is a tree whose edges are all edges of G.

We want to find the number of **spanning trees** by picking edges from a graph G. There is exactly 1 spanning tree of G if G is a tree, and there are n^{n-2} spanning trees if G is K_n: what's in between?

2 Representing graphs as matrices: the matrix-tree theorem

We assume our graphs do not have loops: we can't use loops in a spanning tree anyway (which does not contain cycles). However, multiple edges are indeed allowed: it's important to note that picking different edges between two vertices does count as picking a different spanning tree.

These two objects both describe a graph completely under these situations: they may be familiar from computer science.

Definition 2.1

The **adjacency matrix** A of a graph G is an $n \times n$ matrix, where A_{ij} is the number of edges connecting i to j.

We'll refine this a little more:

Definition 2.2

The **Laplacian matrix** of a graph G is an $n \times n$ matrix

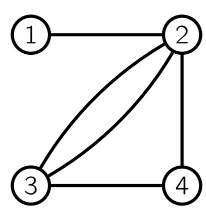
$$L = D - A,$$

where D is a diagonal matrix with $d_i = \deg(i)$. In other words,

$$L_{ij} = \begin{cases} \text{degree}(i) & i = j \\ \text{number of edges } i \iff j & i \neq j. \end{cases}$$

Example 2.3

Consider the graph below:



Here is the Laplacian for this matrix:

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 4 & -2 & -1 \\ 0 & -2 & 3 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$$

Notice that by definition, we are currently dealing with undirected graphs, so both the Laplacian and adjacency matrices are symmetric.

Fact 2.4

All row sums of L are 0, and this means that the determinant of L is 0.

Now we're ready to formulate the main result.

Theorem 2.5 (Matrix Tree Theorem)

The determinant of the matrix

$$L^i = L \text{ with the } i\text{th row and column removed},$$

for any $1 \leq i \leq n$, is the number of spanning trees of G.

In particular, all of those determinants are the same! This is actually a general fact about matrices:

Fact 2.6

For any square $n \times n$ matrix B with row and column sums 0, the determinants of B^i and B^j are always equal. In fact, all **cofactors** are equal: delete the ith row and jth column and multiply the determinant of the remaining matrix by $(-1)^{i+j}$.

Proof. Search "matrices with zero row and column sum" on Google. This is one of my favorite examples of why row-reduction is actually useful! □

Example 2.7

There are

$$L^2 = \det \begin{bmatrix} -1 & 0 & 0 \\ 0 & -3 & 1 \\ 0 & 1 & -2 \end{bmatrix} = 5$$

spanning trees of the above diagram. It can be checked that (possibly magically), all other cofactors are also equal to 5.

With that, let's return to our initial question.

Example 2.8

Let's come up with another proof of the Cayley formula! The Laplacian matrix for K_n is

$$L = \begin{bmatrix} (n-1) & -1 & \cdots & -1 \\ -1 & (n-1) & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & (n-1) \end{bmatrix},$$

and regardless of what row and column we remove, L^i will also take this form, but as an $(n-1)\times(n-1)$ matrix.

Here, we use three facts:

- The determinant of a matrix is the product of its eigenvalues. (Expand out the definition of the characteristic polynomial as both $\det(\lambda I - A)$ and as $(\lambda - \lambda_1)(\lambda - \lambda_2)\cdots$. Another intuitive way to think of this is that the determinant is always the "volume scaling factor.")
- The trace of a matrix is the sum of its eigenvalues. (Diagonalization preserves the eigenvalues.)
- If λ is an eigenvalue of A, then $\lambda + c$ is an eigenvalue of $A + cI$.

With this in mind, note that $L^i - nI$ is a matrix of all -1s. Therefore, all but one of its eigenvalues must be 0 (because it has rank 1), and the last eigenvalue must be $1-n$ to make the trace $1-n$. Thus, we get the eigenvalues of L^i by adding n to each eigenvalue: L^i has eigenvalues $1, n, \cdots, n$, which means the determinant is n^{n-2}. Magic!

3 How do you prove this?

We'll actually prove this in a more general form, which is occasionally useful (but not very often) by directing our edges!

Definition 3.1

Let G be a directed graph with at least two vertices (for technical reasons which aren't very important).

- An **out-tree** rooted at a vertex v is a spanning tree of G, except that all edges point away from v (along the shortest path).
- An **in-tree** is the same, except that all edges are directed toward the root instead.

We again have two versions of our Laplacian matrix:

Definition 3.2

Define the directed Laplacian matrices L^{in} and L^{out} as follows:

$$(L^{\text{in}})_{ij} = \begin{cases} \text{indegree}(i) & i = j \\ -\text{number of directed edges } i \to j & i \neq j. \end{cases}$$

$$(L^{\text{out}})_{ij} = \begin{cases} \text{outdegree}(i) & i = j \\ -\text{number of directed edges } i \to j & i \neq j. \end{cases}$$

In an undirected graph, these are the same. Note that all row sums of L^{out} are zero, but not necessarily row sums, and vice versa for L^{in}.

With this, we'll generalize our initial theorem into something that's actually easier to prove. (The regular version of the matrix-tree theorem holds by replacing every undirected edge with a pair of edges going both ways.)

Theorem 3.3 (Directed Matrix Tree Theorem)
Let v be a vertex of a graph G, and pick any $1 \le i \le n$. Then the number of out-trees rooted at v is $(-1)^{i+v}\det(L^{\text{in}})^{iv}$ (the (i, v) cofactor), and the number of in-trees rooted at v is $(-1)^{v+i}\det(L^{\text{out}})^{vi}$.

The proofs for in- and out-trees are very similar, so we'll just do one direction (in-trees). Note that all in-trees must have all non-root outdegrees equal to 1: think about why this is true!

Proof. Induct on the **number of directed edges whose starting point is not v.** Denote $\text{In}_v(G)$ to be the number of in-trees of G rooted at v: our goal is to show that this is the cofactor $(L^{\text{out}})^{vi}$.

First, consider the base case, where all edges are out of v: then there are no in-trees because there's no way to get an edge into v. In this case, L^{out} has all zero entries except row v, and any cofactor $(L^{\text{out}})^{vi}$ is zero because it must remove the vth row.

So now for the induction step: pick any non-root-originating edge e, say from i to j, where $i \neq v$. Construct two other graphs: G_1 is the graph G with e removed, and G_2 is G from all edges from i except e removed (this is all edges with the same source as e). (In other words, we split up the edges from i into two groups, because any in-tree must use exactly one of these edges.) So now

$$\text{In}_v(G) = \text{In}_v(G_1) + \text{In}_v(G_2),$$

because any spanning tree has to use either edge e or one of the other ones through vertex i.

Fact 3.4
By the way, if there's only one edge from vertex i (to vertex j), we can just **contract it** (aka combine edges to and from i and j into a single vertex) and use the inductive hypothesis anyway! To rigorize this, note that the ith row of L^{out} has a 1 in the ith column and a -1 in the jth column, so if we are taking a cofactor that removes the ith column, our determinant has a row that only contains one nonzero entry in the jth column. But this is equivalent to also removing the jth column up to a $\pm$ sign, so we can treat i and j as the same vertex and remove them together in our cofactor calculation.

Now by induction, if we look at the Laplacian matrices, the ith row of $L^{\text{out}}(G)$ has some entries $(a_1, \cdots, a_n)$. $L^{\text{out}}(G_1)$ looks almost identical, except that one edge is removed: in particular, this means in row i, we **decrease** a_i by one and **increase** a_j by one. On the other hand, $L^{\text{out}}(G_2)$ also looks identical to $L^{\text{out}}(G)$ except in row i: then we have all 0s, except a 1 in the ith column and a -1 in the jth column.

Now we just use magic! In particular, the sum of the ith rows of $L^{\text{out}}(G_1)$ and $L^{\text{out}}(G_2)$ add up to the ith row of $L^{\text{out}}(G)$. By linearity of determinants, this just means that **whenever we don't remove the ith row**,

$$(L^{\text{out}}(G))^{vi} = (L^{\text{out}}(G_1))^{vi} + (L^{\text{out}}(G_2))^{vi},$$

and we're done by induction, since the right hand side counts the number of in-trees for graph G_1 and G_2 separately! $\square$

Fact 3.5

There's another more combinatorial proof which relies on the idea of involutions: determinants are a sum of monomials over a bunch of permutations of the vertices. We can create an involution on subgraphs of G which reverses the sign of all non-trees and keeps trees fixed: this means that all non-trees cancel out. See my notes online if you want to learn more about this!