SPANNING TREES AND KIRCHHOFF'S MATRIX TREE THEOREM

OLGA RADKO MATH CIRCLE

ADVANCED 2

JANUARY 9, 2022

1. IF A TREE FALLS IN THE FOREST

In this worksheet, we will deal with undirected graphs where there are no edges from a vertex to itself. A *path* in a graph is a sequence of edges connecting two vertices. A *tree* is a graph in which any two vertices are connected by exactly one path. For example, the graph on the reader's left (not my left) is a tree while the graph on the reader's right (not my right) is not. A *labeled tree* is one in which each vertex has a unique label.

In the next few problems, we will outline an equivalent definition and properties of trees. A graph is *connected* if there is a path between any two vertices. A *cycle* in a graph is a path with more than one edge in which the only repeated vertex is the start and end vertex.

Problem 1. Show that a graph is a tree if and only if it is connected and does not contain cycles.

Define the *degree* of a vertex to be the number of edges connecting it.

Problem 2. Show that a tree T will have at least one vertex of degree one. A vertex of degree one is known as a *leaf*.

Problem 3.   (a) What is the least number of edges in a connected graph of n vertices?
   (b) Prove by induction that a tree of n vertices will have $n-1$ edges. (Hint: Problem 2)
   (c) Prove that a graph of n vertices is a tree if it is connected and has $n-1$ edges.

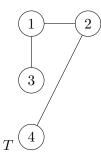**Problem 4.**   (a) How many distinct labeled trees are there on three vertices? Draw them.
   (b) How many distinct labeled trees are there with four vertices? Draw them.

Theorem (Cayley's formula)**.** The number of labeled trees with n vertices is n^{n-2}.

To prove Cayley's formula, we will find a one-to-one correspondence between the number of labeled trees on n vertices $\{1, 2, \ldots, n\}$ with sequences of length $n-2$ with elements from $\{1, 2, \ldots, n\}$. The associated sequence is known as a *Prufer code*.

Start with a tree T of labeled vertices $\{1, 2, \ldots, n\}$. By Problem 2, T will contain at least one leaf. Remove the lowest labeled leaf. What remains is another tree which will have at least one leaf by Problem 2. Continue to remove the lowest labeled leaf until two vertices remain. Each time a leaf is removed, add its neighbor to the list. The resulting length $n-2$ sequence is the Prufer code of T.

Problem 5. Find the Prufer code of the labeled tree T below.

Explain how we would construct the tree T from the resulting Prufer code.

Problem 6. (a) Prove that if a vertex appears $k - 1$ times in the Prufer code of a tree, then the vertex has degree k. (Hint: Try induction.)
   (b) How many times can a leaf appear in the Prufer code of a tree?

Problem 7. Let $N = \{1, 2, \ldots, n\}$.
   (a) Given a sequence $S = (t_1, t_2, \ldots, t_{n-2})$ from N, construct a tree T of n vertices labeled with N.
   (b) What is the number of sequences from $\{1, 2, \ldots, n\}$ of length $n - 2$?
   (c) Explain how performing the Prufer algorithm on a tree T followed by the process in part (a) will produce T. What about if we perform the process in part (a) on a Prufer code P followed by the Prufer algorithm.
   (d) Explain how the above steps prove the bijectivity between trees of length n and sequences of length $n - 2$. How does this prove Cayley's formula?

Notice that Cayley's formula refers to labeled trees. How would the situation change if we no longer label the trees? Two graphs G_1 and G_2 are *isomorphic* if there is a bijective map f from the vertices of the first to the vertices of the second for which i and j are connected by an edge in G_1 if and only if $f(i)$ and $f(j)$ are connected by an edge in G_2.

Problem 8. In this problem, think of isomorphic trees as the same.
   (a) Count the number of distinct unlabeled trees with three vertices.
   (b) Count the number of distinct unlabeled trees with four vertices.

There is no nice formula for the number of non-isomorphic unlabeled graphs of n vertices. The following problem is all we will prove for now.
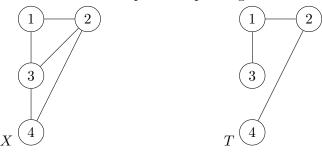
Problem 9. Let T represent the number of distinct unlabeled trees of n vertices up to isomorphism.
   (a) Show that the number of labeled trees of n vertices is at most $n! \cdot T$.
   (b) Find a lower bound for T.

2. Spanning Trees

Let G be a connected graph. A *spanning tree* of G is a tree with the same vertices as G but only some of the edges of G. We can produce a spanning tree of a graph by removing one edge at a time as long as the new graph remains connected. Once we are down to $n - 1$ edges, the resulting will be a spanning tree of the original by Problem 3.
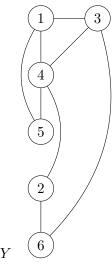
For example, the graph X is not a tree. One possible spanning tree of X is given by T on the right.

In Section 1, we found a count for the number of trees of n vertices. We will likewise want to count the number of spanning trees of an arbitrary graph G, denoted $t(G)$. The difficulty of this problem will become clear with some examples.

Problem 10. Find $t(X)$. (Hint: The degree of vertex 2 is three. Break into cases based on the degree of vertex 2 in the spanning tree.)

Problem 11. (Challenge) Find $t(Y)$. (Hint: Break up $t(Y)$ based on the degree of vertex 4 in the corresponding spanning tree.)

Problem 12. The cycle graph on n vertices, C_n, is a graph with vertices $\{1, 2, \ldots, n\}$, an edge between 1 and n, and edges between i and $i+1$ for $1 \leq i < n$.

    (a) Draw the cycle graph C_4.
    (b) What is $t(C_n)$?

Problem 13. The complete graph on n vertices, K_n, is a graph with vertices $\{1, 2, \ldots, n\}$ with edges between i and j for each $1 \leq i, j \leq n$.

    (a) Draw the complete graph K_4.
    (b) What is $t(K_n)$?

Problem 14. The complete bipartite graph, $K_{m,n}$, has vertices $\{1, 2, \ldots, m+n\}$ broken up into two sets $S_1 = \{1, 2, \ldots, m\}$ and $S_2 = \{m+1, m+2, \ldots, m+n\}$. There is an edge between each element of S_1 and each element of S_2 but no edges between vertices of the same set.

    (a) Draw the complete bipartite graph $K_{2,2}$.
    (b) What is $t(K_{2,2})$?
    (c) Draw the complete bipartite graph $K_{2,3}$.
    (d) What is $t(K_{2,3})$?
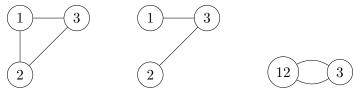   (e) (Challenge) What is $t(K_{2,n})$? We will find $t(K_{m,n})$ at the end of the worksheet.

Even for the small examples above, computing the number of spanning trees in a given graph can be a difficult task. Deletion-contraction and Kirchhoff's Matrix Tree Theorem will provide algorithmic ways to compute $t(G)$ for all graphs.

3. Deletion-Contraction

Let G be a graph with vertices V and edges E. Let e be an edge between vertices v and w. The *deletion* denoted $G - e$ is the graph with vertices V and edges $E \setminus \{e\}$. In other words, the deletion of G along e is the graph where we remove the edge e. The contraction denoted G/e is the graph given by identifying vertices v and w of $G - e$ as a single vertex.

Problem 15. What happens if we define G/e as the identification of vertices v and w in G as opposed to $G - e$?

As an example, the graph below on the left is G. Let e be the edge between vertices 1 and 2. The graph in the middle is $G - e$ and the graph on the right is G/e.

Some of you may have seen these concepts before when we computed the chromatic polynomial of a graph. The recursive technique in Problem 16 also mimics that of the chromatic polynomial.

Problem 16.   (a) Prove that there is a bijection between the set of spanning trees of G that do not contain e and the set of spanning trees of $G - e$.
   (b) Prove that there is a bijection between the set of spanning trees that do contain e and the set of spanning trees of G/e.
   (c) Explain how these bijections can be used to compute the number of spanning trees of a graph G.

Problem 17. Verify the formula for $t(C_n)$ from Problem 12 using the deletion-contraction technique.

Problem 18. Verify the formula for $t(K_4)$ from Problem 13 using the deletion-contraction technique.

Problem 19. Verify the formula for $t(K_{2,3})$ from Problem 14 using the deletion-contraction technique.

Problem 20. What are some limitations of the deletion-contraction algorithm for finding the number of spanning trees of a graph?

Kirchhoff's Matrix Tree Theorem will be a more efficient algebraic way of finding the number of spanning trees in a graph. First, however, we need to figure out operations on matrices.

4. THE MATRIX RELOADED

A *matrix* is a rectangular array of numbers arranged in rows and columns. The matrices in this worksheet will have as many rows as columns. For example,

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 3 \end{pmatrix}$$

is a 2×2 matrix where the first 2 refers to the number of rows and the second 2 refers to the number of columns. We will often write a_{ij} to represent the number in the ith row and jth column of A. In the above example, $a_{12} = -1$ and $a_{21} = 1$.

We can add two $n \times n$ matrices A and B by adding $a_{ij} + b_{ij}$ for each $1 \leq i, j \leq n$ and placing this in the ith row and jth column of the result.
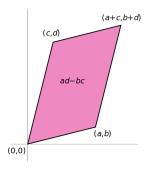
Problem 21. Find $A + B$ where $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & -1 \\ 2 & 1 \end{pmatrix}$.

The *determinant* of a 2×2 matrix $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ is $\det(A) = a_{11}a_{22} - a_{12}a_{21}$. We can define the determinant of an $n \times n$ matrix A inductively via a process known as cofactor expansion. Let $\widehat{A}_{ij}$ be the $(n-1) \times (n-1)$ matrix where the ith row and jth column of A has been removed. Then

$$\det(A) = a_{11} \det(\widehat{A}_{11}) - a_{12} \det(\widehat{A}_{12}) + \cdots + (-1)^{n+1} a_{1n} \det(\widehat{A}_{1n}).$$

For matrices with a lot of rows and columns, this computation is unfortunately quite tedious since each $\det(\widehat{A}_{1i})$ will then need to be reduced in a similar fashion.

One motivation for the bizarre definition of the determinant is it arises as the area formula of parallelograms. Let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. The area of the pictured parallelogram with vertices $(0,0)$, (a,b), (c,d), and $(a+c, b+d)$ will have area $\det(A) = ad - bc$.

This barely scratches the surface of the uses of the determinant in linear algebra and beyond. Feel free to go the determinant Wikipedia page (which is where I stole the beautiful picture) to learn about its various applications.

Problem 22. Compute the determinants of the following matrices:

(a) $A = \begin{pmatrix} 2 & -1 \\ 2 & 1 \end{pmatrix}$

(b) $B = \begin{pmatrix} 4 & -3 & 0 \\ 2 & -1 & 2 \\ 1 & 5 & 7 \end{pmatrix}$

(c) $C = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 3 & -1 & 1 & 0 \\ 2 & 0 & 2 & 0 \\ 5 & 4 & 1 & -1 \end{pmatrix}$

Problem 23. Let A be an $n \times n$ matrix for which $a_{ij} = 0$ for all $i > j$. We call A *upper triangular*. Show by induction $\det(A) = a_{11} \cdot a_{22} \cdots a_{nn}$ is the product of the diagonal entries.

We can show that adding a multiple of one row to another row does not change the value of the determinant. As a result, an alternative method for computing the determinant is to add multiples of one row to another until we reach upper triangular form.
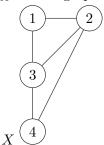
Problem 24. Redo Problem 22 by instead adding multiples of one row to another in order to obtain an upper triangular matrix.

5. Kirchhoff's Matrix Tree Theorem

Let G be a graph with n vertices. We will assign to G two different matrices. First, the *adjacency matrix* of G, denoted A_G, is the $n \times n$ matrix for which

$$a_{ij} = \begin{cases} 1 & \text{if there is an edge from } i \text{ to } j \text{ in } G \\ 0 & \text{if there is not an edge from } i \text{ to } j \text{ in } G. \end{cases}$$

Problem 25. Find the adjacency matrix A_X for the graph X from Problem 10.

Problem 26. Let G be an undirected graph on n vertices. Let A_G be the adjacency matrix of G.

(a) When would $a_{ii} = 1$ for some $1 \le i \le n$?

(b) The adjacency matrix A_G satisfies $a_{ij} = a_{ji}$ for all $1 \le i, j \le n$.

The elements a_{ii} are said to be on the diagonal of A_G. We are only looking at graphs G that do not have edges from a vertex to itself. Thus the diagonal entries of the adjacency matrix will be 0.

Recall that the degree of a vertex is the number of edges connecting it. The second matrix we want to define is the *degree matrix* of G, denoted D_G. The diagonal entry d_{ii} will be equal to the degree of vertex i in G. The non-diagonal entries will be equal to $d_{ij} = 0$ for all $i \neq j$.

Problem 27. Find the degree matrix D_X for the graph X above.

Theorem (Kirchhoff's Matrix Tree Theorem)**.** Let G be an undirected graph with n vertices. Define $L = D_G - A_G$, the difference of the degree matrix of G and the adjacency matrix of G. Then

$$t(G) = \det(\widehat{L}_{ij})$$

for any choice of $1 \leq i, j \leq n$.

It is miraculous that we can compute a graph-theoretic concept of spanning trees by doing some algebra on matrices. Further, it seems surprising that it doesn't matter which row and column we remove. The proof of Kirchhoff's Matrix Tree Theorem is too technical for this worksheet so we will try some examples to convince us of its validity.

Problem 28. Apply Kirchhoff's Matrix Tree Theorem to the graph X above. Compare the result to that of Problem 10. Try multiple choices of $\widehat{L}_{ij}$.

Problem 29. Let G be an undirected graph of n vertices. Show that the sum of each row of $L = D_G - A_G$ is 0. What is the sum of each column?

Problem 30. Compute $\det(L)$.

Problem 31. Let $G = K_{m,n}$ the complete bipartite graph.
   (a) Compute $t(K_{3,3})$ using Kirchhoff's Matrix Tree Theorem.
   (b) Find a general form for the matrix $L = D_G - A_G$.
   (c) Show that $t(G) = m^{n-1}n^{m-1}$ using Kirchhoff's Matrix Tree Theorem.