Math 4707: Introduction to Combinatorics and Graph Theory

Lecture Addendum, November 3rd and 8th, 2010

Counting Closed Walks and Spanning Trees in Graphs via Linear Algebra and Matrices

1 Adjacency Matrices and Counting Closed Walks

The material of this section is based on Chapter 1 of Richard Stanley's notes "Topics in Algebraic Combinatorics", which can be found at `http://math.mit.edu/~rstan/algcomb.pdf`.

Recall that an m-by-n matrix is an array of numbers (m rows and n columns), and we can multiply an m-by-n matrix and an n-by-p matrix together to get an m-by-p matrix. The resulting matrix has entries obtained by taking each row of the first matrix, and each column of the second and taking their dot product.

For example,

$$\begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix} \begin{bmatrix} g & h \\ i & j \\ k & \ell \end{bmatrix} = \begin{bmatrix} ag+bi+ck & ah+bj+c\ell \\ dg+ei+fk & dh+ej+f\ell \end{bmatrix}.$$

We define the **adjacency matrix** $A(G)$ of a graph G, with $|V(G)| = n$, to be the n-by-n matrix whose entry in the ith row and the jth column is

$$a_{ij} = \#\text{ of edges between } v_i \text{ and } v_j.$$

Theorem. Letting $\left(A(G)^k\right)_{ij}$ denote the entry in the ith row and jth column of the kth power of $A(G)$, we obtain that

$$\left(A(G)^k\right)_{ij} = \#\text{ of walks of length exactly } k \text{ between } v_i \text{ and } v_j.$$

Proof. Was given in class by induction using the fact that $A(G)^k = A(G)^{k-1}A(G)$ and using the definition of matrix multiplication.

As a special case, the diagonal entry $\left(A(G)^k\right)_{ii}$ is the number of closed walks from v_i back to itself with length k. The sum of the diagonal entries of $A(G)^k$ is the total number of closed walks of length k in graph G. In linear algebra, the sum of the diagonal entries of a matrix is known as the **trace**.

Another important definition from linear algebra are **eigenvalues** and **eigenvectors** of a matrix M. We now review their definition and a few related results from linear algebra.

Definition. The vector (i.e. n-by-1 matrix) v is an **eigenvector** of M with **eigenvalue** λ if the equation

$$Mv = \lambda v$$

is satisfied. That is, multiplying the column vector v by M is equivalent to rescaling each entry of v by the same coefficient, λ.

Theorem. If an n-by-n matrix M is symmetric and has only real numbers as entries, then M has n linearly independent eigenvectors and n associated eigenvalues, although possibly with repeats.

Here, linearly independent means that one of these n eigenvectors can not be written as a scaled sum (linear combination) of the other vectors. In other words, the collection of eigenvectors looks like $\{v_1, v_2, \ldots, v_n\}$, and there does not exist numbers $c_1, c_2, \ldots, c_n$ so that

$$c_1 v_1 + \cdots + c_n v_n = 0$$

unless each of the c_i's are actually all zero themselves.

For example, the vectors $\begin{bmatrix}1\\0\\0\end{bmatrix}$, $\begin{bmatrix}2\\1\\0\end{bmatrix}$, and $\begin{bmatrix}0\\-1\\1\end{bmatrix}$ are linearly independent since the first vector has zeros in the second and third row and the second vector has a zero in the third row.

Since the adjacency matrix $A(G)$ of any graph is symmetric and has real numbers (in fact integers) as entries, any adjacency matrix has n different eigenvalues that can be found, for example by finding n linearly independent eigenvectors.

Theorem. If a matrix M has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then M can be written as the multiplication

$$M = P \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \lambda_n \end{bmatrix} P^{-1},$$

where P is some invertible n-by-n matrix. Call this diagonal matrix in the middle D.

As a consequence, the kth power of M can be written as

$$M^k = PDP^{-1}\ PDP^{-1}\ \ldots PDP^{-1} = PD^kP^{-1}.$$

The kth power of D is again a diagonal matrix, with $(D^k)_{ij} = 0$ if $i \neq j$, and $(D^k)_{ii} = \lambda_i^k$.

The trace of D^k is thus simply the sum of powers,

$$Tr(D^k) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k.$$

One last important theorem from linear algebra is that

Theorem. The trace of a matrix M is the same as the trace of the matrix multiplication PMP^{-1}.

Consequently, the trace of $A(G)^k$ is simply the sum of the powers of $A(G)$'s eigenvalues. Putting all of this together, we come to the following result.

Main Theorem. The number of total closed walks, of length k, in a graph G, from any vertex back to itself, is given by the formula

$$\lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k,$$

where the λ_i's are the eigenvalues of $A(G)$, graph G's adjacency matrix.

Example 1. Let $G = C_3 = K_3$, so $A(C_3) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$.

Let $v_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$, $v_2 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$, and $v_3 = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}$. Note that these three vectors are linearly independent, and

$$A(C_3)v_1 = 2v_1, \quad A(C_3)v_2 = -v_2, \quad \text{and} \quad A(C_3)v_3 = -v_3.$$

Thus the three eigenvalues of $A(C_3)$ are 2, -1, and -1, and

$$\#\text{ closed walks in } C_3 \text{ of length } k \text{ is } 2^k + (-1)^k + (-1)^k = \begin{cases} 2^k + 2 \text{ if } k \text{ is even,} \\ 2^k - 2 \text{ if } k \text{ is odd.} \end{cases}$$

We can also prove this formula combinatorially. For i and $j \in \{1, 2, 3\}$, let $W_{ij}(k)$ denote the number of walks of length k from v_i to v_j. Notice that by symmetry,

$$W_{11}(k) = W_{22}(k) = W_{33}(k), \quad \text{and}$$

$$W_{12}(k) = W_{13}(k) = W_{23}(k) = W_{21}(k) = W_{31}(k) = W_{32}(k),$$

thus it suffices to compute $W_{11}(k)$ and $W_{12}(k)$, noting that the quantity $3W_{11}(k)$ equals the total number of closed walks in C_3. Considering the last possible edge of a closed walk from v_1 to v_1, and the last possible edge of a walk from v_1 to v_2, we obtain the equations

$$W_{11}(k) = W_{12}(k-1) + W_{13}(k-1) = 2W_{12}(k-1), \text{ and}$$

$$W_{12}(k-1) = W_{11}(k-2) + W_{13}(k-2) = 2W_{12}(k-3) + W_{12}(k-2).$$

Thus, letting $G_k = W_{12}(k)$, we see that G_k satisfies the recurrence

$$G_{k-1} = G_{k-2} + 2G_{k-3}.$$

It is easy to verify that the formula

$$G_k = \begin{cases} \frac{1}{6}\left(2^{k+1} - 2\right) & \text{if } k \text{ is even,} \\ \frac{1}{6}\left(2^{k+1} + 2\right) & \text{if } k \text{ is odd} \end{cases}$$

satisfies this recurrence and equals $W_{12}(k)$ in the base case when $k = 1$ or 2. Consequently,

$$W_{12}(k) = \begin{cases} \frac{1}{6}\left(2^{k+1} - 2\right) & \text{if } k \text{ is even,} \\ \frac{1}{6}\left(2^{k+1} + 2\right) & \text{if } k \text{ is odd,} \end{cases}$$

and we conclude that the total number of closed walks, $3W_{11}(k)$, which equals $3 \cdot 2W_{12}(k-1)$, has the desired expression.

Example 2. Let $G = C_5$, so $A(C_5) = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$. **Exercise:** The value 2 is an eigenvalue again.

The other four eigenvalues are $\frac{-1-\sqrt{5}}{2}$, $\frac{-1-\sqrt{5}}{2}$, $\frac{-1+\sqrt{5}}{2}$, and $\frac{-1+\sqrt{5}}{2}$. Thus

$$\#\text{ closed walks in } C_5 \text{ of length } k \text{ is } 2^k + 2\left(\frac{-1-\sqrt{5}}{2}\right)^k + 2\left(\frac{-1+\sqrt{5}}{2}\right)^k = \begin{cases} 2^k + 2L_k & \text{if } k \text{ is even,} \\ 2^k - 2L_k & \text{if } k \text{ is odd.} \end{cases}$$

Recall that L_k is the kth Lucas number defined as $L_1 = 1$, $L_2 = 3$, $L_{k+2} = L_{k+1} + L_k$.

Interesting Challenge: Since we know a combinatorial interpretation of the Lucas numbers, it is possible to try to find a combinatorial formula for this formula as well. However, this is much more difficult than in the previous example.

2 Counting spanning trees in graphs

We next use linear algebra for a different counting problem. Recall that a **spanning tree** of a graph G is a subgraph T that is a tree that uses every vertex of G. Before we express the formula for the number of spanning trees in a graph, we need to define another type of matrix that can be associated to a graph.

The **Laplacian matrix** of a graph $L(G)$ is defined entrywise as follows:

$$L(G)_{ij} = \begin{cases} -A(G)_{ij} = -(\#\text{ edges from } v_i \text{ to } v_j) & \text{if } i \neq j, \\ \deg(v_i) & \text{if } i = j. \end{cases}$$

Notice that $\deg(v_i)$ is the sum of (# edges from v_i to v_1) + (# edges from v_i to v_2) $+ \cdots +$ (# edges from v_i to v_n), and so the sum of each row or column of $L(G)$ is zero. Consequently, $L(G)\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = \begin{bmatrix}0\\ \vdots\\ 0\end{bmatrix}$, and in particular $L(G)$ is a **singular matrix**. However, it turns out that if G is connected, whenever we cross out the kth row and kth column of $L(G)$ (will not actually matter which k we choose), we get a **nonsingular matrix**. We can for instance always cross out the last column and last row of $L(G)$, call this matrix $L(G)_0$, the **Reduced Laplacian Matrix**.

Theorem (Kirchhoff's Matrix-Tree-Theorem). The number of spanning trees of a graph G is equal to the determinant of the reduced Laplacian matrix of G:

$$\det L(G)_0 = \#\text{ spanning trees of graph } G.$$

(Further, it does not matter what k we choose when deciding which row and column to delete.)

Remark. Even though we allow multigraphs to have loop edges, adding or deleting these from our multigraph does not affect the number of spanning trees.

Recall that the determinant of an n-by-n matrix M, with entries M_{ij}, is a number we assign to it by the following formula

$$\det M = \sum_{\sigma \text{ is a permuation of } \{1,2,\ldots,n\}} \operatorname{sgn}(\sigma)\ M_{1,\sigma(1)} M_{2,\sigma(2)} \cdots M_{n,\sigma(n)}.$$

Here $M_{i,\sigma(i)}$ signifies the entry of M in the ith row and the $\sigma(i)$th column and $\operatorname{sgn}(\sigma) = \pm 1$ according to how many cycles are in the permutation σ.

Example The determinant of a 2-by-2 matrix $\begin{bmatrix}M_{11} & M_{12}\\ M_{21} & M_{22}\end{bmatrix}$ is $M_{11}M_{22} - M_{12}M_{21}$, and the determinant of $\begin{bmatrix}M_{11} & M_{12} & M_{13}\\ M_{21} & M_{22} & M_{23}\\ M_{31} & M_{32} & M_{33}\end{bmatrix}$ is $M_{11}M_{22}M_{33} - M_{11}M_{23}M_{32} + M_{12}M_{23}M_{31} - M_{12}M_{21}M_{33} + M_{13}M_{21}M_{32} - M_{13}M_{22}M_{31}$.

The determinant of an n-by-n matrix will involve $n! = \#$ permutations of $\{1, 2, \ldots, n\}$ entries, so for $n \geq 4$, these formulas are not as compact. However, there are four important properties that determinants have that we remind you of, as they make it easier to compute them.

Properties of Determinants.

1) If M is a singular matrix, then $\det M = 0$. (Also, if M is nonsingular, $\det M \neq 0$.)

2) If we add a multiple of one row of M to another, the determinant is left unaffected. Recall that we can add multiples of one row to another until we get an **upper-triangular matrix**, one where $a_{ij} = 0$ for every $i > j$. This method is called **Gaussian elimination**.

3) The determinant of an upper-triangular matrix is the product of the diagonal entries.

4) Let $E[i]$ denote a square matrix which has entry $E_{ii} = 1$ and all other entries are zero. If matrix M and $E[i]$ have the same size, then $\det(M + E[i]) = \det(M) + \det M'$, where M' is obtained from M by deleting the ith row and ith column of M. This property is known as **multilinearity** of the determinant. (Note that repeated use of a slight generalization of this method results in the Laplace expansion of a matrix, but we will not need this for our purposes.)

We use these properties, in particular, multilinearity of the determinant, to prove the Matrix-Tree-Theorem described above. First, we need to prove another result about spanning trees of graphs.

Definition. Recall that the notation $G-\{e\}$ denotes the subgraph obtained by taking graph G and **deleting** edge e, but leaving all other edges and vertices as is.

We can also define the **contraction** of a graph, $G/\{e\}$ is the multigraph (not a subgraph) obtained from G by contracting the edge $e = \{v, w\}$ until the two vertices v and w coincide. Call this new vertex vw.

Remark. Note that if edge e is part of a triangle C_3 on vertices $\{u, v, w\}$ then after e is contracted and v, w coincide, there are now two edges from u to vw in $G/\{e\}$. Hence, why in general $G/\{e\}$ is not a graph, but is a multigraph.

Furthermore, if we continue the contraction procedure, so that we contract one of the two edges from u to vw, say e' then we end up with a loop in the contracted graph $(G/\{e\})/\{e'\}$. So our multigraphs are also allowed to have loops.

We define the number of spanning trees in a multigraph to be the same as our previous definition except that if there are multiple edges between two vertices to use, each choice gives rise to a different spanning tree. We cannot include two parallel edges in a spanning tree as this would be a 2-cycle. We similarly never have loop edges in a spanning tree.

Theorem. Let $\kappa(G)$ denote the number of spanning trees in a multigraph G. Then $\kappa(G)$ satisfies the following **deletion-contraction** formula: For any choice of edge e in the multigraph G,

$$\kappa(G) = \kappa(G - \{e\}) + \kappa(G/\{e\}).$$

The upshot of this theorem is that we reduce the problem to computing the number of spanning trees in a multigraph with one less edge and one less vertex and a multigraph with one less vertex. Thus inductively, we could compute the number of spanning trees in any graph this way, since for example we know that any tree has one spanning tree and a disconnected graph has no spanning trees.

Example 1: Cycle Graphs. While we can see that $\kappa(C_n) = n$ combinatorially, as explained in class, we can also prove that this family of graphs have the right number of spanning trees using the deletion-contraction technique.

If we pick any edge of C_n and delete it, the resulting $C_n - \{e\} = P_n$, a path graph on n vertices. Since this is a tree, it has only 1 spanning tree, itself.

On the other hand, if we contract the edge e, we obtain $C_n/\{e\} = C_{n-1}$. Since we know that $C_3 = K_3$ has 3^1 spanning trees by Cayley's Theorem, we can thus show by induction that $\kappa(C_n) = 1 + \kappa(C_{n-1})$, and the formula $\kappa(C_n) = n$ satisfies both this recurrence and the base case.

Proof of Deletion-Contraction Theorem. Choose an edge e of graph G. We divide the set of spanning trees of G into the union of two disjoint subsets: (i) those that contain e, and (ii) those that do not contain e.

(i) A spanning tree of G not containing e is also a spanning tree of $G - \{e\}$.

(ii) A spanning tree of G that does contain e is equivalent to a spanning tree of $G/\{e\}$.

To see the equivalence of (ii), we note that $G/\{e\}$ has one less vertex and one less edge than G, but except for edge e, every edge of G corresponds to a unique edge of $G/\{e\}$, and vice-versa. Thus, let $E(T)$ denote the edges of G corresponding to a spanning tree. Then edge-set $E(T) - \{e\}$ corresponds to T', an edge-set of $G/\{e\}$. Since the subgraph corresponding to T' is connected and has the right number of edges, T' is a spanning tree of $G/\{e\}$. The correspondence also works in reverse. Thus adding up the number of spanning trees of type (i), and those of type (ii), gives us the number of spanning trees of G, and the desired formula.

Proof of Matrix Tree Theorem. The following proof appears in Section 13.2 of Godsil and Royle's "Algebraic Graph Theory":

We prove the theorem by induction on the number of edges of G. It is easy to see that $\det L(G)_0 = \kappa(G)$ when G is a graph with one edge. Either the graph has two vertices and is a two-path P_2 and the determinant is 1, or the graph has more than two vertices, is disconnected, and $L(G)_0$ is singular.

Let e be the edge $\{u, v\}$ and E be the n-by-n matrix with $E_{uu} = 1, E_{vv} = 1, E_{uv} = -1, E_{vu} = -1$, and all other entries are 0. Then by the definition of Laplacian matrices,

$$L(G) = L(G - \{e\}) + E.$$

If we delete the row and column corresponding to vertex u in all three of these matrices, we obtain the identity

$$L(G)_0 = L(G - \{e\})_0 + E[v],$$

where $E[v]$ is the $(n-1)$-by-$(n-1)$ matrix defined above, with $E_{vv} = 1$ and all other entries are zero.

By using property (4) of determinants, we deduce from the above equation that

$$\det L(G)_0 = \det L(G - \{e\})_0 + \det L(G - \{e\})_e.$$

Here, $L(G-\{e\})_e$ denotes the matrix obtained from $L(G-\{e\})$ by deleting both rows and columns corresponding to vertices u and v, the two endpoints of edge e. Note that $L(G - \{e\})_e$ also can be thought of as $L(G)_e$, but more importantly for our purposes, it can be thought of as $L(G/\{e\})_0$ as well, by reducing from $L(G/\{e\})$ by deleting the row and column corresponding to the new vertex uv. Thus

$$\det L(G)_0 = \det L(G - \{e\})_0 + \det L(G/\{e\})_0.$$

By induction, $\det L(G - \{e\})_0 = \kappa(G - \{e\})$ and $\det L(G/\{e\})_0 = \kappa(G/\{e\})$ since these both have less edges than G, and we conclude the desired determinantal formula.

Example 2: If I asked you to compute the determinant of

$$M = \begin{bmatrix} 5 & -1 & -1 & -1 & -1 \\ -1 & 5 & -1 & -1 & -1 \\ -1 & -1 & 5 & -1 & -1 \\ -1 & -1 & -1 & 5 & -1 \\ -1 & -1 & -1 & -1 & 5 \end{bmatrix},$$

you could use Gaussian elimination to reduce M to an upper-triangular matrix or compute the determinant otherwise. However, now we can instead recognize that the matrix $M = L(K_6)_0$, the reduced Laplacian matrix for complete graph K_6. Thus by the Matrix Tree Theorem, $\det M =\#$ spanning trees in K_6. Furthermore, by Cayley's theorem, this number is $6^4 = 1296$.

In general, the Matrix Tree Theorem can be helpful in both directions. Both, showing that the number of spanning trees can be computed via matrices, or using combinatorics to easily compute certain determinants.