REU 2007 · Apprentice Program · Lecture 3

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For basic definitions and facts about graphs and digraphs (directed graphs), see Chapter 6 of the instructor's online Discrete Math Lecture Notes (DMLN) posted on the class website.

A3.1 Laplace Expansion of Determinant and Permanent

Definition A3.1.1. Let $[n] = \{1, \ldots, n\}$, $I = \{i_1, \ldots, i_k\} \subseteq [n]$ and $J = \{j_1, \ldots, j_k\} \subseteq [n]$. If A is an $n \times n$ matrix, define the $k \times k$ matrix $A(I; J) = (\tilde{a}_{rs})$ of A to be the matrix with entries $\tilde{a}_{rs} = a_{i_r j_s}$. Also define the $(n-k) \times (n-k)$ complementary matrix $A(\overline{I}; \overline{J})$, where $\overline{I}$ and $\overline{J}$ are the complements of I and J respectively. Instead of $A(\overline{\{i\}}, \overline{\{j\}})$ we shall simply write $A(\bar{i}, \bar{j})$.

Exercise A3.1.2. (Determinant expansion by a row) Suppose A is an $n \times n$ matrix and fix $i \in [n]$. Show that the following formulas hold.

$$\det A = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} \det A(\bar{i}; \bar{j})$$

$$\operatorname{per} A = \sum_{j=1}^{n} a_{ij} \operatorname{per} A(\bar{i}; \bar{j})$$

Given a subset $S \subseteq [n]$, we will write $\sum S$ as shorthand for $\sum_{s \in S} s$.

The Laplace expansion generalizes this to "expansion by a set of rows." Here is the precise statement.

Exercise A3.1.3. (Laplace Exapansion) Let A be an $n \times n$ matrix and $k \in [n]$. Fixing any $I \subseteq [n]$ with $|I| = k$ the permanent and determinant can be expanded as follows.

$$\det A = \sum_{J \subseteq [n], |J|=k} (-1)^{\sum I + \sum J} \det A(I; J) \det A(\overline{I}; \overline{J})$$

$$\operatorname{per} A = \sum_{J \subseteq [n], |J|=k} \operatorname{per} A(I; J) \operatorname{per} A(\overline{I}; \overline{J})$$

Note that these sums have $\binom{n}{k}$ terms.

A3.2 A Problem in Extremal Combinatorics

Let $A_1, \ldots, A_m$ be sets of r elements and $B_1, \ldots, B_m$ sets of s elements. Suppose further that $A_i \cap B_i = \emptyset$ and $A_i \cap B_j \neq \emptyset$ for $i \neq j$. We call such a collection of sets a **Bollobás system**. We are interested in the maximum value of m, given r and s. This is a typical problem of *extremal set theory*, a branch of combinatorics.

Notation A3.2.1. Given r and s, let $m(r, s)$ denote the maximum value m for which a Bollobás system with the given values of r and s exists.

Remark A3.2.2. Our goal is to determine $m(r, s)$. However, the "universe" of which all the A_i and B_i are subsets can be arbitrarily large (can be infinite), so it is not *a priori* evident that a maximum value of m exists at all. We shall prove it does and find its exact value.

We start with "data collection," examining small cases.

Claim A3.2.3. (Case $r = 1$) $m(1, s) = 1 + s$.

Proof. First we prove that $m(1, s) \leq 1 + s$. Since $r = 1$, each A_i consists of a single element, say a_i. As $B_1 \cap A_i \neq$ for all $i \neq 1$ we have that $\{a_2, \ldots, a_m\} \subseteq B_1$. Thus $m - 1 \leq s$ implying $m \leq 1 + s$.

To prove that $m = 1+s$ is feasible, take a set of $1+s$ elements, say $[1+s] = \{1, 2, \ldots, 1+s]$; let $A_i = \{i\}$ and $B_i = [1 + s] \setminus \{i\}$. $\square$

Claim A3.2.4. (Case $r = s = 2$) $m(2, 2) = 6$.

Proof. We first prove $m \leq 6$.
Case 1: Two of the A_i are disjoint.
WLOG $A_1 \cap A_2 = \emptyset$. Now $B_j \cap A_1 \neq \emptyset$ and $B_j \cap A_2 \neq \emptyset$ for all $j \geq 3$. As there are only 4 subsets of $A_1 \cup A_2$ with 2 elements that satisfy this condition, we see that $m \leq 6$ for this case.

Case 2: The A_i are pairwise intersecting.
(2a) There is an element a in the intersection of all of the A_i. Then we have that $A_i = \{a, a_i\}$ for distinct a_i. Since B_1 cannot intersect A_1 we have that $a \notin B_1$ and since $B_1 \cap A_i \neq \emptyset$ for all $i \neq 1$ we have that $a_i \in B_1$ for all $i \neq 1$. But as $|B_1| = 2$, this implies that $B_1 = \{a_2, a_3\}$ an thus $m = 3 < 6$.
(2b) The only collection of 2-element sets that are pairwise intersecting do not all have a common element is the edges of a triangle. Here again $m = 3$. This completes the proof that $m(2, 2) \leq 6$.

We also see that the only case when $m = 6$ is conceivable is Case 1; and indeed, the system suggested by the proof of Case 1, the set of all pairs of a set of 4 elements, paired up in complementary pairs, realizes $m = 6$. $\square$

Let us write these results as follows:

If $r = 1$ then $m(1, s) = 1 + s = \binom{1+s}{1}$

If $r = s = 2$ then $m(2, 2) = 6 = \binom{4}{2}$

With this scant evidence, we might "conjecture" the following result which is a theorem of Bollobás.

Theorem A3.2.5. (Bollobás) $m(r, s) = \binom{r+s}{r}$.

Exercise A3.2.6. Show that $m(r, s) \geq \binom{r+s}{r}$.

The hard part of the proof of Bollobás' Theorem will be to show that $m(r, s) \leq \binom{r+s}{r}$. We shall give two proofs; one based on the linearity of expectation, the other based on the Laplace expansion.

A3.3 Counting Trees

We now consider the following classical question:

Given a set of n labeled vertices, how many distinct trees are there?

The following exercise helps in collecting data.

Exercise A3.3.1. Let X be a graph on n vertices and let $\mathrm{Aut}(X)$ denote its group of automorphisms. Prove that the number of isomorphic copies of X on the vertex set $[n]$ is $\dfrac{n!}{|\mathrm{Aut}(X)|}$.

Using this exercise one can work out the number of trees on n vertices for small values of n; the result is the following table.

n	Number of Trees
2	1
3	3
4	16
5	125

The pattern is compelling and makes us conjecture the following result, called Cayley's formula.

Theorem A3.3.2. (Cayley's formula) *The number of trees on a set of n vertices is n^{n-2}.*

Remark A3.3.3. One method used to prove Cayley's formula is the "Prüfer code." This method gives a bijection between trees and strings of length $n - 2$ over an alphabet of size n. See the *Wikipedia* for details.

A more general question than finding the number of trees on n vertices is to find the number of spanning trees of a graph.

Definition A3.3.4. Given a connected graph $X = (V, E)$, a spanning tree of X is a subgraph that is a tree whose vertices are all of V.

Question A3.3.5. Given a graph, how many spanning trees are there?

This question was solved by Kirchhoff in 1848. In order to state and prove his result, we need to establish some notation. First recall that the adjacency matrix of a graph $X = (V, E)$ with n vertices is the $n \times n$ matrix $A = (a_{ij})$ where a_{ij} is 1 if $\{i, j\} \in E$ and zero otherwise. We will also take D to be a diagonal matrix with $\deg(i)$ in the i-th diagonal position. (Recall that $\deg(i)$, the degree of vertex i, is the number of edges incident with i). Now we will introduce some novel definitions.

Definition A3.3.6. The **Laplacian** of the graph X is the $n \times n$ matrix $L = D - A$. For $i = 1, \ldots, n$, the **reduced Laplacian** of X corresponding to vertex i is the $(n-1) \times (n-1)$ matrix $\Delta_i = L(\bar{i}; \bar{i})$ (we delete the i-th row and the i-th column).

Exercise A3.3.7. Show that for any graph X, $\det(L) = 0$.

Remark A3.3.8. Although the reduced Laplacian depends on a choice $i \in [n]$, the results that follow will not depend on this choice unless otherwise stated.

The following is known as Kirchhoff's **Matrix Tree Theorem**.

Theorem A3.3.9. (Kirchhoff, 1848) *The number of spanning trees of a graph X is* $\det(\Delta_i)$.

Before proceeding to the proof of this theorem, observe that Cayley's formula is a corollary. Indeed, take X to be the complete graph on n vertices (K_n), and we see that the number of spanning trees of X equals the number of distinct trees. One can calculate the reduced Laplacian to be the following $(n-1) \times (n-1)$ matrix.

$$\begin{bmatrix} n-1 & -1 & \cdots & -1 \\ -1 & n-1 & -1 & \vdots \\ \vdots & & \ddots & \\ -1 & \cdots & -1 & n-1 \end{bmatrix}$$

Applying a result from **A2.1** to this matrix, Cayley's formula quickly follows (remember though that this is an $(n-1) \times (n-1)$ matrix).

A3.4 Counting arborescences

Definition A3.4.1. Let $X = (V, R, r)$ be a **rooted digraph**. This means that (V, R) is a graph and a "root" $r \in V$ is specified.

Definition A3.4.2. An **arborescence** T of a rooted digraph X is a set of edges of X such that for every vertex v of X, there is a unique path along T from v to the root, and T is minimal under this constraint.

Assumption A3.4.3. We shall make the following assumption throughout this discussion except where otherwise stated:

The root $r \in V$ is accessible from every vertex of X (along directed paths).

Exercise A3.4.4. Prove that an arborescence exists in X if and only if Assumption A3.4.3 holds.

Exercise A3.4.5. Prove that in an arborescence, the root has outdegree zero and all other vertices have outdegree 1. Infer that an arborescence (a) has $n-1$ edges where $n = |V|$; (b) if we ignore the orientation of edges, an arborescence is a tree.

Now recall that the outdegree $\deg^+(i)$ of a vertex $i \in V$ is the number of edges starting at i (directed away from i). Define D_+ to be the $n \times n$ diagonal matrix with i-th entry $\deg^+(i)$. Recall that the adjacency matrix of a digraph is an $n \times n$ matrix $A = (a_{ij})$ where a_{ij} is 1 if the directed edge $(i, j) \in R$ and zero otherwise.

Definition A3.4.6. The Laplacian of a digraph is the matrix $L = D_+ - A$. The **reduced Laplacian** of a rooted digraph is the matrix $\Delta = L(\overline{r}; \overline{r})$ (we delete the row and the column corresponding to the root).

Exercise A3.4.7. Show that $\det(L) = 0$ for any directed graph X.

Theorem A3.4.8. (Matrix-Tree Theorem, rooted digraph version) *Let X be a rooted digraph. The number of arborescences of X is* $\det(\Delta)$.

Exercise A3.4.9. Show that if Assumption A3.4.3 *fails* for the rooted digraph X then $\det(\Delta) = 0$. So the Matrix-Tree Theorem holds even in this case.

Note A3.4.10. This theorem implies Theorem A3.3.9 (Kirchhoff's Matrix-Tree Theorem). Indeed, given an undirected graph, make it into a digraph by replacing each edge $\{i, j\}$ by two directed edges $(i, j), (j, i)$. Then one easily sees that every vertex is a root and, after choosing a root, every spanning tree can be oriented uniquely so it becomes an arborescence.

A3.5 The Inclusion–Exclusion Principle

We start this section by asking:

How many positive integers are there with n digits, each of which is odd, and in which all odd digits actually appear?

Let us call the number of these integers N. One observes that there are 5^n numbers in which all of the n digits are odd. So the first approximation to N is 5^n. We then proceed by subtracting the number of n-digit integers without one of the odd digits. For each odd digit, there are 4^n such n-digit numbers, so the second approximation to N is $5^n - 5 \cdot 4^n$. But we see that we have taken too many numbers away as each of the numbers that were missing exactly two odd digits were taken away twice. Continuing with this reasoning we may conjecture that N must equal:

$$5^n - \binom{5}{1}4^n + \binom{5}{2}3^n - \binom{5}{3}2^n + \binom{5}{4}1^n$$

This is indeed the case; and this result is a special case of the general formula called Inclusion–Exclusion Principle (or "Sieve Formula" or "Elimination Principle").

Theorem A3.5.1. (Inclusion-Exclusion Principle) *Let Ω be a finite set and $A_1, \ldots, A_k \subseteq \Omega$.*

$$|\overline{A_1 \cup \cdots \cup A_k}| = S_0 - S_1 + S_2 - \cdots \pm S_k$$

where $S_0 = |\Omega|$ and $S_i = \sum_{J \subseteq [k], |J|=k} |\bigcap_{j \in J} A_j|$.

A more compact way of writing this formula is this:

$$|\overline{A_1 \cup \cdots \cup A_k}| = \sum_{J \subseteq [k]} (-1)^{|J|} \left| \bigcap_{j \in J} A_j \right|. \tag{A3.5.1}$$

Note that the sum on the right-had side has 2^k terms, one for each subset of $[k]$. We need to make a convention to interpret the case $J = \emptyset$: we understand the intersection of r subsets of Ω for $r \geq 2$, and the meaning is clear enough even if $r = 1$. But what if $r = 0$? What if we intersect no sets at all? The more sets we intersect, the smaller the intersection, so the only reasonable convention for the intersection of nothing at all is the largest set possible, which in our case is Ω:

$$\bigcap_{j \in \emptyset} A_j = \Omega. \tag{A3.5.2}$$

Under this convention, the definition of S_0 given in Theorem A3.5.1 can be omitted since it becomes a special case of the definition of S_i $(i = 0)$.

To prove the Inclusion–Exclusion Principle, take an element $x \in \Omega$ and examine the count that the right hand side will give for x. If $x \in \overline{A_1 \cup \cdots \cup A_k}$ then it is counted once in the term $|\Omega|$ (corresponding to $J = \emptyset$) and that is all. If not, then after relabeling the A_j, we can assume that $x \in A_j$ for $1 \leq j \leq r$ and $x \notin A_j$ otherwise. One can then check that the number of times the right hand side of the equation counts x is

$$1 - \binom{r}{1} + \binom{r}{2} - \cdots + (-1)^r \binom{r}{r}.$$

Exercise A3.5.2. Show that the above number (alternating sum of binomial coefficients) is zero for any $r \geq 1$. Use the Binomial Theorem.

Exercise A3.5.3. Show that the above number is zero by producing a (very simple) bijection between the set of all odd subsets of $[r]$ with all even subsets of $[r]$. (An AH-HA problem!)

Exercise A3.5.4. (Bonferroni's Inequalities) Show that the truncations of the Inclusion–Exclusion formula $S_0 - S_1 + S_2 - + \dots$ bound the quantity $|\overline{A_1 \cup \dots \cup A_k}|$ from alternating sides. More precisely,

$$|\overline{A_1 \cup \dots \cup A_k}| \leq S_0 - S_1 + \dots + S_{2i}$$

and

$$|\overline{A_1 \cup \dots \cup A_k}| \geq S_0 - S_1 + \dots - S_{2i+1}.$$

A3.6 Return to Counting Arborescences

We would like to use the Inclusion–Exclusion Principle to count the number of arborescences in a rooted digraph X with root $r \in V$. To achieve this we start with a definition.

Definition A3.6.1. An **arrow configuration** of a rooted digraph X is a collection of $n-1$ directed edges, one outward pointing edge for each vertex except the root.

Exercise A3.6.2. Show that every arborescence is an arrow configuration.

Exercise A3.6.3. Show that an arrow configuration is an arborescence if and only if it does not contain a directed cycle.

It is clear that the number of arrow configurations of X is precisely $\prod_{i=1}^{n-1} \deg^+(i)$. To employ the Inclusion–Exclusion Principle, we will take the set of arrow configurations as Ω and eliminate all configurations containing directed cycles.

Lemma A3.6.4. *Any two cycles in an arrow configuration are vertex-disjoint (they don't share a vertex).*

Proof. Suppose in the arrow configuration K we have two directed cycles, $\{(i_1, i_2), (i_2, i_3), \dots, (i_k, i_{k+1})\}$ where $i_{k+1} = i_1$, and $\{(j_1, j_2), (j_2, j_3), \dots, (j_\ell, j_{\ell+1})\}$, where $j_{\ell+1} = j_1$. Suppose they share a vertex; WLOG this vertex is $i_1 = j_1$. This means that both (i_1, i_2) and (i_1, j_2) are present in K. But i_1 has only one out-neighbor in K, so $i_2 = j_2$. By induction, using the same argument, we see that $i_s = j_s$ for all s, so the two cycles are identical. $\square$

Exercise A3.6.5. Let $C_1, \dots, C_k$ be k disjoint cycles and let U be the union of their vertex sets. Prove: the number of arrow configurations containing these cycles (and possibly other cycles) is

$$\prod_{i \notin U, i \neq r} \deg^+(i).$$

This is the quantity which figures in the elimination of cycles from all arrow configurations via Inclusion–Exclusion. Tomorrow we shall see that these same quantities correspond to the expansion terms of determinat of the reduced Laplacian, proving the Matrix-Tree Theorem (for digraphs).