Graph Topics

Notes for Math 447

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1 Graphs, connected graphs, trees

A *graph* on a set V is a given by specifying V and a set E of two-element subsets. An element of V is called a vertex, and an element of E is called an *edge*. Each vertex in an edge is an *end point* of the edge. A vertex and edge are *incident* if the vertex belongs to the edge. Two vertices incident to the same edge are *adjacent*.

Suppose V has n elements. The number of graphs on V is $g_n = 2^{\binom{n}{2}}$. It follows that the exponential generating function is

$$G(x) = \sum_{n=0}^{\infty} 2^{\binom{n}{2}} \frac{x^n}{n!}. \tag{1}$$

Unfortunately, there is no simple formula for $G(x)$.

A graph on a non-empty vertex set is a *connected graph* if there is no partition of V into two or more blocks such with the property that no edge has endpoints in different blocks. In general, given an arbitrary graph, there is a partition of the vertex set into blocks with a connected graph on each block. Each such block is called a *connected component*. This is true even for the graph on the empty set of vertices. The set of blocks in the corresponding partition is empty.

This last observation gives a way of counting connected graphs. Let $C(x)$ be the exponential generating function for connected graphs. Then every graph is obtained by giving a partition and a connected graph on each block. Thus

$$G(x) = e^{C(x)}. \tag{2}$$

It follows that

$$C(x) = \sum_{m=1}^{\infty} c_m \frac{x^m}{m!} = \log(G(x)). \tag{3}$$

Unfortunately, computing the logarithm is a nuisance. Therefore, this formula is awkward to use to find the number c_m of connected graphs on an m element set.

A *tree* on a vertex set is a minimal connected graph. That is, it is a connected graph with the property that removing an edge automatically disconnects it. If the vertex set has n elements, then a tree on this vertex set has $n-1$ edges. There is a famous theorem of Cayley that says that the number of trees on a set with n elements is n^{n-2} for each $n \geq 1$. This theorem has many proofs; one is given below.

Sometimes it is useful to consider a graph with a particular vertex that may be used as a starting point. A *rooted graph* is a pair consisting of a graph on a vertex set and a particular vertex. The number of rooted graphs is $g_n^\bullet = ng_n$. The number of rooted connected graphs is $c_n^\bullet = nc_n$. The number of rooted trees is $t_n^\bullet = nt_n$.

Rooted graphs give another approach to counting connected graphs. Every rooted graph defines an ordered pair consisting of a subset of the vertex set with a rooted connected graph, together with another complementary subset of the vertex set with a graph. This proves that

$$G^\bullet(x) = C^\bullet(x)G(x). \tag{4}$$

We conclude that

$$C^\bullet(x) = \sum_{m=1}^{\infty} mc_m \frac{x^m}{m!} = \frac{G^\bullet(x)}{G(x)}. \tag{5}$$

Now the problem is to compute the quotient. Finding the number c_m of connected graphs on an m element set is not easy.

2 Rooted trees

Let $w = f(z) = T^\bullet(z)$ be the exponential generating function for rooted trees. Then w satisfies the equation

$$w = ze^w. \tag{6}$$

This says that a rooted tree consists of a pair consisting of a root point and a partition of the rest of the points into blocks, each of which has a rooted tree. This recursive construction underlies the utility of rooted trees.

This equation has inverse

$$z = g(w) = we^{-w}. \tag{7}$$

The Lagrange inversion theorem applies to exactly such a situation. It says that if w is defined by $w = z\phi(w)$, where $\phi(0) \neq 0$, then the nth coefficient of the expansion of w in terms of z is $1/n$ times the $n-1$th coefficient of $\phi(w)^n$ in terms of w. In this case $\phi(w) = e^w$, so $\phi(w)^n = e^{nw}$. The $n-1$th coefficient of the expansion of e^{nw} is $\frac{1}{(n-1)!}n^{n-1}$. It follows that

$$w = f(z) = T^\bullet(z) = \sum_{n=1}^{\infty} n^{n-1}\frac{x^n}{n!}. \tag{8}$$

This proves that the number of rooted trees on a set with n elements is $t_n^\bullet = n^{n-1}$ for $n \geq 1$. As a consequence we get Cayley's theorem that says that the number of trees on a set with n elements is $t_n = n^{n-2}$ for $n \geq 1$.

3 Functions

The exponential generating functions for permutations is

$$S(x) = \frac{1}{1-x}. \tag{9}$$

According to Cayley's theorem the exponential generating function for rooted trees is

$$T^{\bullet}(z) = \sum_{n=1}^{\infty} n^{n-1} \frac{z^n}{n!}. \tag{10}$$

The generating function for endofunctions is

$$F(z) = \sum_{n=0}^{\infty} n^n \frac{z^n}{n!}. \tag{11}$$

Write it in a more interesting way as

$$F(z) = \frac{1}{1 - T^{\bullet}(z)}. \tag{12}$$

This says for each endofunction on a set there is a partition of the set into blocks with rooted trees, together with a permutation of the blocks. The permutation of the blocks may be thought of as a permutation of the roots of the trees. The corresponding function maps each vertex that is not a root to the next vertex closer to the root, and it maps each root vertex to another root vertex given by the permutation.

The geometric series may be expanded as

$$F(z) = \sum_{k=0}^{\infty} T^{\bullet}(z)^k. \tag{13}$$

Now $T^{\bullet}(z)^k$ is the exponential generating function for forests of k rooted trees together with an ordering of the trees. This number may be computed by a slightly more general form of Lagrange inversion. It says that if w is defined by $w = z\phi(w)$, where $\phi(0) \neq 0$, then the nth coefficient of the expansion of w^k in terms of z is k/n times the $n-k$th coefficient of $\phi(w)^n$ in terms of w. In this case $\phi(w) = e^w$, so $\phi(w)^n = e^{nw}$. The $n-k$th coefficient of the expansion of e^{nw} is $\frac{1}{(n-k)!} n^{n-k}$. We can also write this as $\binom{n-1}{k-1} n^{n-k} k!/n!$. So the number of forests of k rooted trees, together with an ordering of the trees, is $\binom{n-1}{k-1} n^{n-k} k!$. This is the same as the number of forests of k rooted trees together with a permutation of the roots. So we have

$$T^{\bullet}(z)^k = \sum_{n=k}^{\infty} \binom{n-1}{k-1} n^{n-k} k! \frac{z^n}{n!}. \tag{14}$$

Hence

$$F(z) = \sum_{n=0}^{\infty} \sum_{k=0}^{n} \binom{n-1}{k-1} n^{n-k} k! \frac{z^n}{n} \tag{15}$$

It follows that

$$n^n = \sum_{k=0}^{n} \binom{n-1}{k-1} n^{n-k} k!. \tag{16}$$

4 Appendix: Laurent series and residues

Consider a formal Laurent series

$$H(z) = \sum_{k=-\infty}^{\infty} A_k z^k. \tag{17}$$

This has formal derivative

$$dH(z)/dz = H'(z) = \sum_{k=-\infty}^{\infty} kA_k z^{k-1} = \sum_{m=-\infty}^{\infty} (m+1)A_{m+1} z^m. \tag{18}$$

Notice that the term in z^{-1} has coefficient zero.

Consider a function

$$h(z) = \sum_{k=-\infty}^{\infty} a_k z^k \tag{19}$$

expanded in a Laurent series with a possible singularity at $z = 0$. The *residue* of this form is the coefficient a_{-1} of $1/z$. We have seen that if $h(z) = dH(z)/dz = H'(z)$, where $H(z)$ has a similar Laurent series, then the residue is automatically zero. Conversely, if the residue is zero, then the antiderivative is a Laurent series

$$H(z) = \sum_{k \neq -1} \frac{1}{k+1} a_k z^{k+1} = \sum_{m \neq 0} \frac{1}{m} a_{m-1} z^m. \tag{20}$$

Say that $h(z)$ is an arbitrary Laurent series. Let

$$g(w) = \sum_{n=1}^{\infty} b_n w^n \tag{21}$$

be a change of coordinates with $g(0) = 0$ and $g'(0) = b_1 \neq 0$. Consider the new function

$$h(g(w))g'(w) = \sum_{m=-\infty}^{\infty} c_m w^n. \tag{22}$$

The residue theorem says that the residue is the same: $c_{-1} = a_{-1}$.

Here is the proof. First, note that

$$g'(w) = b_1 + \sum_{n=2}^{\infty} nb_n w^{n-1} = b_1 + \sum_{m=1}^{\infty} (m+1)b_{m+1} w^m \tag{23}$$

starts with constant term b_1. Furthermore,

$$\frac{g(w)}{w} = b_1 + \sum_{n=2}^{\infty} b_n w^{n-1} = b_1 \left[1 + \sum_{m=1}^{\infty} \frac{b_{m+1}}{b_1} w^m\right] \tag{24}$$

has the same b_1 as a factor. Consider

$$h(g(w))g'(w) = \sum_{k=-\infty}^{\infty} a_k g(w)^k g'(w). \tag{25}$$

If $k \neq -1$, then the term

$$g(w)^k g'(w) = \frac{1}{k+1} \frac{d}{dw} g(w)^{k+1} \tag{26}$$

has no residue. So the only problem is with $k = -1$. Write

$$\frac{g'(w)}{g(w)} = g'(w) \frac{w}{g(w)} \frac{1}{w}. \tag{27}$$

This has residue $b_{-1}/b_{-1} = 1$. So the residue c_{-1} of $h(g(w))g'(w)$ is the residue of $a_{-1}g'(w)/g(w)$ which is a_{-1}.

5 Appendix: Lagrange inversion

Say that $z = g(w)$ with $g(0) = 0$ and $g'(0) \neq 0$ is a known function. Consider the inverse function $w = f(z)$ with $f(0) = 0$. We want to find the Taylor expansion

$$w = f(z) = \sum_{n=1}^{\infty} b_n z^n. \tag{28}$$

This is a problem about substitution, since the relation between the two functions is

$$f(g(w)) = w. \tag{29}$$

The idea of Lagrange inversion is that this substitution problem can be reduced to a division problem.

The Lagrange inversion theorem starts with the fact that the nth coefficient of the unknown inverse function $f(z)$ is a residue

$$b_n = \operatorname{res} \frac{f(z)}{z^{n+1}}. \tag{30}$$

The theorem states that the coefficient is expressed in terms of the known function $g(w)$ by another residue

$$b_n = \frac{1}{n} \operatorname{res} \frac{1}{g(w)^n}. \tag{31}$$

Here is the proof. Write

$$b_n = \operatorname{res} \frac{f(z)}{z^{n+1}} = \operatorname{res} \frac{w}{g(w)^{n+1}} g'(w) = \frac{1}{n} \operatorname{res} \frac{1}{g(w)^n}. \tag{32}$$

This last equation comes from

$$\frac{1}{n} \frac{d}{dw} \left(\frac{w}{g(w)^n} \right) = \frac{1}{n} \frac{1}{g(w)^n} - \frac{w}{g(w)^{n+1}} g'(w). \tag{33}$$

An easy application is to the function $w = z(1+w)^2$ that occurs in the enumeration of isomorphism classes of binary trees. Here $z = g(w) = w/(1+w)^2$. To find the coefficient b_n in the series expansion of $w = f(z)$ we need to find the residue of $(1+w)^{2n}/w^n$. Since $(1+w)^{2n} = \sum_{k=0}^{2n} \binom{2n}{k} w^k$, the residue is $\binom{2n}{n-1}$. So $b_n = \frac{1}{n}\binom{2n}{n-1}$. This may be written in a more symmetrical way as follows. First note that $(n+1)\binom{2n}{n-1} = n\binom{2n}{n}$. This is because we can either choose a subset with $n-1$ elements and a point in the complement, or, equivalently, a subset with n elements and a point inside. It follows that $b_n = \frac{1}{n+1}\binom{2n}{n}$. This is called a Catalan number.

The most obvious application is to the equation $w = ze^w$ for the exponential generating function for rooted trees. We have $z = g(w) = we^{-w}$. The desired inverse function is $w = f(z)$. So we see that the coefficient is

$$b_n = \frac{1}{n} \operatorname{res} \frac{1}{g(w)^n} = \frac{1}{n} \operatorname{res} w^{-n} e^{nw}. \tag{34}$$

This residue comes from the $n-1$ term in the expansion of e^{nw}, which is $(nw)^{n-1}$ divided by $(n-1)!$. Thus

$$b_n = \frac{1}{n} \frac{1}{(n-1)!} n^{n-1} = \frac{1}{n!} n^{n-1}. \tag{35}$$

It is worth noting that the Lagrange inversion theorem is sometimes formulated in terms of the function $w^n/g(w)^n$ with no singularity at $w = 0$. The theorem then states that the coefficient b_n is $1/n$ times the $n-1$th coefficient in the expansion of $w^n/g(w)^n$.

A more general form of Lagrange inversion gives the Taylor expansion of

$$H(w) = H(f(z)) = \sum_{n=1}^{\infty} B_n z^n. \tag{36}$$

The result is the improved Lagrange inversion theorem

$$B_n = \frac{1}{n} \operatorname{res} \frac{H'(w)}{g(w)^n}. \tag{37}$$

Here is the proof. Write

$$B_n = \operatorname{res} \frac{H(f(z))}{z^{n+1}} = \operatorname{res} \frac{H(w)}{g(w)^{n+1}} g'(w) = \frac{1}{n} \operatorname{res} \frac{H'(w)}{g(w)^n}. \tag{38}$$

This last equation comes from

$$\frac{1}{n}\frac{d}{dw}\left(\frac{H(w)}{g(w)^n}\right) = \frac{1}{n}\frac{H'(w)}{g(w)^n} - \frac{H(w)}{g(w)^{n+1}}g'(w). \tag{39}$$

Consider again the equation $w = ze^w$ for the exponential generating function for rooted trees. We have $z = g(w) = we^{-w}$. The inverse function is $w = f(z)$. Let us take $H(w) = w^k = g(z)^k$, which is the exponential generating function for forests consisting of k rooted trees together with an ordering of the trees. The coefficient is

$$B_n = \frac{k}{n}\operatorname{res}\frac{w^{k-1}}{g(w)^n} = \frac{k}{n}\operatorname{res} w^{k-1-n}e^{nw}. \tag{40}$$

This residue comes from the $n-k$ power term in the exponential function and is

$$B_n = \frac{k}{n}\frac{1}{(n-k)!}n^{n-k}. \tag{41}$$

To get the exponential generating function for forests consisting of k rooted trees (in no particular order), we need to divide by $k!$. To get the actual number we need to find the coefficient of $x^n/n!$, so we need also to multiply by $n!$. This gives the coefficient that enumerates such forests as

$$\frac{n!}{k!}\frac{k}{n}\frac{1}{(n-k)!}n^{n-k} = \binom{n-1}{k-1}n^{n-k}. \tag{42}$$