Notes on Generating Functions

Stat 703 Spring 2006

Generating functions are packages. A sequence lies in a messy pile on the floor, pieces sharp and irregular jutting out in all directions. We pick up the pieces one by one and pack them together just so ... until suddenly we have what seems another object entirely. When we find such an object, we can carry it, weigh it, discern its shape, find its center. We can combine it with others like it to make new ones. And if we look at it just right, we can discern the pieces that comprise it.

Generating functions are tools. They give an indirect representation of the sequence but one that is easy to manipulate in many respects. Some of the uses to which we can use generating functions include the following:

1. Calculate sums.
2. Solve recurrences.
3. Characterize the asymptotic behavior of sequences.
4. Prove useful properties of sequences.
5. Find expected values, variances, and other moments and cumulants of distributions.
6. Establish relationships between distributions.

We will see examples of all of these this semester.

Generating functions are fun. The feeling of cracking a tough sum or recurrence is better than ... well, no, but it's pretty darn good. The mathematics is beautiful and connects diverse areas, including algebra, number theory, complex analysis, combinatorics, and probability. And the knowledge will come in handy in surprising ways.

1. Definitions and Operations

There are different flavors of generating function, but for the moment, we'll deal with what we might call "ordinary" generating functions.

Definition 1. Let $(g_n)_{n\geq 0}$ be a sequence. The (ordinary) *generating function* for the sequence is the the function defined by

$$G(z) = \sum_{n\geq 0} g_n z^n. \tag{1}$$

A generating function like this has two modes of existence depending on how we use it. First, we can view it as a function of a complex variable. Second, we can view it as a formal power series. We will exploit both perspectives.

But first, a word about boundaries. It is most common to deal with sequences g_n defined for $n \geq 0$ – let's call them *one-sided* sequences for lack of a better name. Even with a one-sided sequence (g_n), it is convenient to extend the sequence to all integers by defining $g_n = 0$ for $n < 0$. This leads to the following conventions.

Convention 2. If a sequence g_n is defined for $n \geq n_0$ for some fixed integer n_0 (e.g., 0), then we will assume – unless otherwise indicated – that $g_n = 0$ for $n < n_0$.

Convention 3. If a sum is written with no limits specified for the summation variable (as in $\sum_n$), the summation is taken to be over all integers.

Hence, we will prefer to write our generating functions in the following form

$$G(z) = \sum_n g_n z^n \tag{2}$$

because it eliminates worrying about the boundary at $n = 0$.

We do occasionally encounter *two-sided* sequences as well, sequences defined for positive and negative integers, and the above expression of $G(z)$ works in that case just fine. The rigorous definition of two-sided generating functios entails a few additional complications, whether from the complex-functions or formal-power-series perspectives, but it can be done – and works just as you would expect – for sequences with only a finite number of non-zero terms for negative indices. (The more general case is thornier.) Most of the properties and manipulations of generating functions work with both kinds of sequences, but I'll try to make it clear when they don't. Nonetheless, one-sided sequences are the leading case to keep in mind.

It is also worth noting that we can write power series in several variables for sequences with multiple indices, such as

$$G(y, z) = \sum_{m,n} g_{m,n} y^m z^n. \tag{3}$$

This is often useful, and all the theory is a direct generalization. I'll freely use the multivariable form when needed.

1.1. Generating Functions As Functions of a Complex Variable

If we view $G(z)$ as a function of a complex variable, we must consider the question of convergence. For what values of $z \in \mathbb{C}$ does the power series in (1) converge and produce a well-defined function on the complex plane. This raises all the related issues that are familiar from analysis. For these purposes, we will consider one-sided sequences, many of the results can be extended to the two-sided cases using (??eq:twosided-decomp??).

Theorem 4. *Given a power series $\sum_{n\geq 0} g_n z^n$ in a complex variable z, there exists an extended-real number $0 \leq R \leq \infty$ such that*

1. *If $|z| < R$, the series converges.*
2. *If $|z| > R$, the series diverges.*

This number R is called the radius of convergence *of the power series, and can be expressed as*

$$R = \frac{1}{\limsup_{n\to\infty} |g_n|^{1/n}}, \tag{4}$$

where we hold to the usual conventions $1/\infty = 0$ and $1/0 = \infty$.

Example 5. The series $\sum_{n\geq 0} z^n$ has $R = 1$ because the coefficients are constant.

Example 6. The series $\sum_{n\geq 0} z^n/n!$ has $R=\infty$, which can be seen for example via Stirling's approximation.

Given a power series $G(z)=\sum_{n\geq 0} g_n z^n$ expressed as a function of a complex variable, the radius of convergence of the series determines properties of the function.

Theorem 7. If $G(z)=\sum_{n\geq 0} g_n z^n$ is a power series with radius of convergence R, then $G(z)$ is an analytic (a.k.a. holomorphic, which I tend to prefer) function on the disk $|z|<R$ and has at least one singularity on the circle $|z|=R$.

(Note: An analytic or holomorphic function on a region A in the complex plane is a function that is complex differentiable at every point in the region or equivalently that it has a convergent power series expansion in an open disk around every point of A. These conditions have profound consequences for the behavior of the function.)

Example 8. If $G(z)=\sum_{n\geq 0} z^n$, then on the disk $|z|<1$, we can write $G(z)=1/(1-z)$, which is analytic function there. This function has a pole (a simple singularity) at $z=1$.

It follows that the identification of a power series with a closed-form expression for the function – as a function of a complex variable – only holds within the region of analyticity. Consider $1/(1-z)$ evaluated at $z=2$, for example.

Given a power series $G(z)$ as above that is analytic within $|z|<R$ for some $R>0$, we can recover the coefficients by taking derivatives. For example, $G(0)=g_0$, $G'(0)=g_1$, $G''(0)/2=g_2$, and $G^{(k)}(0)/k!=g_k$. Using Cauchy's formla from complex analysis, we can expresss this same relationship as a contour integral – an integral of a function along a closed curve $\gamma\colon[0,1]\to\mathbb{C}$ in the complex plane. Cauchy's formula states

$$g_k=\frac{1}{2\pi i}\int_\gamma \frac{G(z)}{z^{k+1}}\,dz, \tag{5}$$

for any closed curve γ around the origin that is contained in the open disk $|z|<R$. (For example, $\gamma(t)=(R/2)e^{2\pi i t}$.)

This contour integation approach has several other uses. For example, consider a power series $G(z)=\sum_{n\in\mathbb{Z}} g_n(z-z_0)^n$, then a contour integral around z_0 (say with $\gamma(t)=z_0+e^{2\pi i t}$) gives

$$g_{-1}=\frac{1}{2\pi i}\int_\gamma G(z)\,dz \tag{6}$$

the so-called *residue* of G at z_0, and for $n>0$,

$$g_{-n}=\frac{1}{2\pi i}\int_\gamma G(z)(z-z_0)^{n-1}\,dz \tag{7}$$

by the same argument.

We'll see later on how these kind of arguments can help us determine the asymptotic behavior of the sequence g_n by the behavior of $G(z)$ around singularities.

Finally, many of the same considerations apply to power series written in multiple variables, such $G(y,z)=\sum_{m,n} g_{mn}y^m z^n$, which can be viewed as a function $\mathbb{C}^2\to\mathbb{C}$.

1.2. Generating Functions As Formal Power Series

The second perspective on generating functions is to view them as *formal* power series. That is, we view the generating function as an algebraic expression for manipulating the sequence of numbers – not as a function of a complex variable.

Definition 9. A *formal power series* (over $\mathbb{C}$) is an algebraic "symbol"

$$G(z) = \sum_n g_n z^n, \tag{8}$$

for complex-valued coefficients g_n. The sum above ranges over all integers, but we will assume here that g_n is eventually zero as $n \to -\infty$. Two formal power series are equal if and only all of their coefficients are equal.

We also need a way to refer to a particular coefficient given a formal power series that is expressed as a function rather than as a sequence.

Notation 10. If $G(z)$ is a formal power series, then we write $[z^n]G(z)$ to denote the coefficient of z^n in the series. That is, if $G(z) = \sum_n g_n z^n$, $[z^n]G(z) = g_n$. Of course, the z in these expressions is a dummy variable. It's also true that $[u^n]G(u) = g_n$, for example.

This notation is standard and quite convenient in the end, though rather clunky. It also does take some getting used to. As you get comfortable with it, try expressing the coefficients in terms of a specific sequence (as we did with "g_n" above) and make the mapping. Eventually, this notation will become familiar.

To make sense of the definition, let's consider formal power series as algebraic objects and some of the operations we can perform on them. Let $G(z) = \sum_n g_n z^n$, $H(z) = \sum_n h_n z^n$, and $F(z) = \sum_n f_n z^n$.

First, we can add formal power series to produce a new formal power series:

$$G(z) + H(z) = \sum_n (g_n + h_n) z^n, \tag{9}$$

and this addition is commutative ($G(z) + H(z) = H(z) + G(z)$) and associative ($(G(z) + H(z)) + F(z) = G(z) + (H(z) + F(z))$ by the commutativity and associativity of addition for the coefficients.. Note that the set of one-sided series is closed under this operation (that is, the sum of two one-sided series is itself one-sided.)

Second, we can multiply formal power series to produce a new formal power series:

$$G(z)H(z) = \sum_n \left(\sum_k g_k h_{n-k} \right) z^n, \tag{10}$$

and again, this multiplication is commutative ($G(z)H(z) = H(z)G(z)$) and associative ($(G(z)H(z))F(z) = G(z)(H(z)F(z))$) as you can demonstrate to yourself. The term in parentheses $\sum_k g_k h_{n-k}$ is called the *convolution* of the sequences a and b. The product of formal power series thus corresponds to the convolution of the associated sequences. Note that the set of one-sided series is closed under this operation (that is, the product of two one-sided series is itself one-sided.)

Third, multiplication distributes over addition:

$$G(z)(H(z)+F(z)) = \sum_n \sum_k g_k(h_{n-k}+f_{n-k})z^n \tag{11}$$

$$= \sum_n \left(\sum_k g_k h_{n-k}\right) z^n + \left(\sum_k g_k f_{n-k}\right) z^n \tag{12}$$

$$= G(z)H(z) + G(z)F(z), \tag{13}$$

and similarly for multiplication in the other order.

Fourth, we have an identity element for both addition and multiplication. The function $G(z) = 0$ corresponding to the zero sequence acts as an identity under addition of formal power series. The function $G(z) = 1$, corresponding to the sequence $1_{(n=0)}$, acts as an identity under multiplication of formal power series.

These facts tell us that the collection of univariate formal power series over $\mathbb{C}$ has some familiar (and useful) algebraic properties. In particular, it is an Abelian (i.e., commutative) group under addition, with $G(z) \equiv 0$ as the identity, and it is an Abelian group under multiplication with $G(z) \equiv 1$ as the identity. Therefore, the collection of formal power series is an algebraic object known as a *commutative ring (with unit element)*.

The sub-collection of one-sided series (of which we are most interested) has these same properties and so is also a commutative ring (with unit element), and a sub-ring of the larger collection. In addition, for one-sided series, we can often find reciprocals as well. The *reciprocal* of a (one-sided) formal power series $G(z)$ is a (one-sided) formal power series $H(z)$ such that $G(z)H(z) = 1$. In fact, a one-sided power series $G(z) = \sum_{n\geq 0} g_n z^n$ has a reciprocal $H(z)$ if and only if $g_0 \neq 0$. To see this, note first, that $G(z)H(z) = 1$ implies that $h_0 = 1/g_0$ which is well-defined only when $g_0 \neq 0$. Also, $G(z)H(z) = 1$ implies that $\sum_{k\geq 0} g_k h_{n-k} = 0$. Taking out the $k = 0$ term and solving for h_n yields:

$$h_n = \frac{-\sum_{k=1}^{n} g_k h_{n-k}}{g_0}, \tag{14}$$

which is a function of $g_0, \ldots, g_n$ and $h_0, \ldots, h_{n-1}$. Thus, the $(h_n)_{n\geq 0}$ are uniquely determined by sequential construction, so the formal power series $H(z)$ is a unique reciprocal of $G(z)$ within the sub-ring if and only if $g_0 \neq 0$.

Aside for the algebraists among you. This means that the set of one-sided formal power series with reciprocals forms an Abelian group under multiplication. The complementary set of such series without reciprocal (i.e., with $g_0 = 0$) forms an Abelian group under addition and is a unique maximal ideal of the ring. The ring of one-sided formal power series is consequently a *local ring*; it is also a unique factorization domain. Enough about that, though.

There are other operations we can perform on formal power series. Although they will look much like the typical operations on functions of a complex variable, these are all operations within the ring of power series: they are defined "axiomatically" on the symbols without the need to take any limits. Start with a formal power series $G(z) = \sum_n g_n z^n$.

1. *Right-shifting.*

$$[z^n]z^k G(z) = [z^{n-k}]G(z). \tag{15}$$

That is, if $H(z) = z^k G(z) = \sum_n h_n z^n$, then $h_n = g_{n-k}$, the shifted sequence. Try to explain each of the correspondences below in terms of sequences like (g_n) and (h_n) until you get comfortable with the $[z^n]G(z)$ notatino.

2. *Left-shifting.* For one-sided series, we can create a new series by

$$H(z) = \frac{G(z) - \sum_{n=0}^{m-1} g_n z^n}{z^m} = \sum_{n \geq 0} g_{n+m} z^n. \tag{16}$$

   That is, $[z^n]H(z) = [z^{n+m}]G(z)$ for $n \geq 0$. This is a truncated left shift, and the sum above cannot in general be extended over all integeers. A two-sided left-shift is obtained by $[z^n]G(z)/z^m = [z^{n+m}]G(z)$; this is valid for all m but usually less useful.

3. *Derivatives.* We define the derivative operator on formal power series by $G'(z) = \sum_n n g_n z^{n-1}$. Hence,

$$[z^{n-1}]G'(z) = n[z^n]G(z) \tag{17}$$

$$[z^{n-k}]G^{(k)}(z) = n^{\underline{k}}[z^n]G(z). \tag{18}$$

4. *Shift-Derivative Combinations.* Even more useful is when we combine shift and derivative operations. Let S be the right-shift operator $\mathsf{S}G(z) = zG(z)$ and D be the derivative operator $\mathsf{D}G(z) = G'(z)$. Then, we find that

$$[z^n]S^k D^k G(z) = n^{\underline{k}}[z^n]G(z) \tag{19}$$

$$[z^n](SD)^k G(z) = n^k [z^n]G(z). \tag{20}$$

   (Try this out for yourself.) Both of these are useful operators in their own right. The second identity generalizes easily to a useful form. If $Q(z)$ is some polynomial, then $Q(SD)$ is an operator consisting of a linear combination of $(SD)^k$s. Using linearity, the second equality above thus shows that

$$[z^n]Q(SD)G(z) = Q(n)[z^n]G(z). \tag{21}$$

5. *Partial Summation.* By convolution and the fact that $[z^n]1/(1-z) = 1_{(n \geq 0)}$,

$$\frac{G(z)}{1-z} = \sum_n (\sum_{k \leq n} g_k) z^n. \tag{22}$$

   Multiplying by $1/(1-z)$ converts a sequence to the sequence of partial sums.

6. *Integration.* We can define cumulative definite integrals along the real line as follows:

$$\int_0^z G(t)dt = \sum_{n \geq 1} \frac{1}{n} g_{n-1} z^n. \tag{23}$$

   Hence, $[z^n] \int_0^z G(t)dt = (1/n)[z^{n-1}]G(z)$, for $n \geq 1$.

7. *Scaling.* If c is a constant,

$$[z^n]G(cz) = c^n [z^n]G(z). \tag{24}$$

8. *Extraction of Sub-sequences* (one-sided only). Let m be a positive integer. Consider the roots of unity $e^{2\pi ij/m}$ for $j = 0, \ldots, m-1$. We have the following for integer $n \geq 0$

$$\sum_{j=0}^{m-1} e^{2\pi inj/m} = \begin{cases} m & \text{if } n = dm \text{ for positive integer } d, \\ \dfrac{e^{2\pi in} - 1}{e^{2\pi in/m} - 1} = 0 & \text{otherwise.} \end{cases} \tag{25}$$

where the second case is just an ordinary finite geometric sum. Given a one-sided formal power series, consider the average over the roots of unity:

$$H(z) = \frac{1}{m} \sum_{j=0}^{m-1} G(ze^{2\pi ij/m}) \tag{26}$$

$$= \sum_{n \geq 0} g_n z^n \frac{1}{m} \sum_{j=0}^{m-1} e^{2\pi inj/m} \tag{27}$$

$$= \sum_{n \geq 0} g_{m \cdot n} z^{mn} \tag{28}$$

$$= F(z^m), \tag{29}$$

for a power series $F(z)$ with $[z^n]F(z) = [z^{mn}]G(z)$. Denote the mapping from G to F by the operator M_m.
The simplest example is the case $m = 2$, where the roots of unity are 1 and -1. In this case, $\mathsf{M}_2 G(z)$ consists of only the even terms in the series $G(z)$. To get the odd terms, we apply the same trick but with shifts: $(\mathsf{M}_2 zG(z))/z$ does the job.
Thus, we can extract all subseequences with $n \bmod m = k$ for $k = 0, \ldots, m-1$ by

$$F_k(z) = \frac{\mathsf{M}_m z^{m-k} G(z)}{z} \qquad \Longrightarrow \qquad [z^n]F_k(z) = [z^{mn+k}]G(z) \tag{30}$$

It looks worse than it is. Try it for $m = 3$.

9. *Composition.* If $G(z)$ and $F(z)$ are two generating functions, we might wish to compute the composition of the two functions. Is this well defined? Write

$$G(F(z)) = \sum_{n \geq 0} g_n F^n(z) = \sum_{n \geq 0} g_n \left(\sum_m f_m z^m \right)^n. \tag{31}$$

Notice that if $f_0 \neq 0$, then the contribution of each term in the sum to $[z^n]G(F(z))$ could be non-zero if $f_n \neq 0$ infinitely often. The algebraic construction of formal power series does not support this infinite sum (no limits, remember), so the composition is not well-defined as a formal power series in this case.. If $f_0 = 0$, however, then $[z^n]G(F(z))$ depend on at most n terms in the sum, which is well defined. The composition operation is thus well defined for two formal power series only if $f_0 = 0$ or if $G(z)$ has only finitely many non-zero coefficients (i.e., it is a polynomial).

These are the most commonly used manipulations, though by no means the only ones.

Example 11. Compute $\sum_{k=1}^{n} k^2$.

We can do this in two ways. First, $[z^n](SD)^2(1-z)^{-1} = n^2$ and by partial summation

$$\sum_{k=1}^{n} k^2 = [z^n]\frac{1}{1-z}(SD)^2\frac{1}{1-z} = [z^n]\frac{z^2+z}{(1-z)^4} = [z^n]\left(S^2(1-z)^{-4} + S(1-z)^{-4}\right). \tag{32}$$

By the binomial theorem, negating the upper index, and symmetry – as we saw in class and on homework – we have

$$(1-z)^{-4} = \sum_{n\geq 0}\binom{-4}{n}(-1)^n z^n = \sum_{n\geq 0}\binom{n+3}{n}z^n = \sum_{n\geq 0}\binom{n+3}{3}z^n. \tag{33}$$

Hence,

$$\sum_{k=1}^{n} k^2 = \binom{n+1}{3} + \binom{n+2}{3} = \frac{n\,(1+n)(1+2n)}{6}. \tag{34}$$

For another approach, begin with the polynomial

$$\sum_{k=0}^{n} z^k = \frac{1-z^{n+1}}{1-z}. \tag{35}$$

Note that $(SD)^2\sum_{k=0}^{n} z^k = \sum_{k=0}^{n} k^2 z^k$, and evaluating this polynomial at $z=1$ gives us the first sum we seek. Hence

$$\sum_{k=0}^{n} k^2 = (SD)^2\frac{1-z^{n+1}}{1-z}\bigg|_{z=1}. \tag{36}$$

Carrying out the algebra and evaluating (by taking limits via L'Hopital) yields:

$$\sum_{k=0}^{n} k^2 = \frac{n\,(1+n)(1+2n)}{6}. \tag{37}$$

1.3. Commonly Used Generating Functions

Now that we have the basic definitions in place, it's time to get to work. But first, it's useful to have a library of common generating functions at our disposal. To this end, the following brief list.

$$1 = \sum_{n} 1_{(n=0)} z^n \tag{38}$$

$$z^m = \sum_{n} 1_{(n=m)} z^n \tag{39}$$

$$\frac{1}{1-z} = \sum_{n\geq 0} z^n \tag{40}$$

$$\frac{1}{1+z} = \sum_{n\geq 0} (-1)^n z^n \tag{41}$$

$$\frac{1}{1-z^m} = \sum_{n\geq 0} 1_{(m\backslash n)} z^n \tag{42}$$

$$e^z = \sum_{n\geq 0} \frac{1}{n!} z^n \tag{43}$$

$$\sin z = \sum_{n\geq 0} \frac{(-1)^n}{(2n+1)!} z^{2n+1} \tag{44}$$

$$\cos z = \sum_{n\geq 0} \frac{(-1)^n}{(2n)!} z^{2n} \tag{45}$$

$$\log \frac{1}{1-z} = \sum_{n\geq 1} \frac{1}{n} z^n \tag{46}$$

$$\log(1+z) = \sum_{n\geq 1} \frac{(-1)^{n+1}}{n} z^n \tag{47}$$

$$(1+z)^r = \sum_n \binom{r}{n} z^n \tag{48}$$

$$\frac{1}{(1-z)^{m+1}} = \sum_n \binom{n+m}{n} z^n = \sum_n \binom{m+n}{m} z^n \tag{49}$$

You can devise many others.

2. Solving Recurrences

One of the most powerful uses of generating functions is to solving recurrence relations. These are relations between elements of a sequence that enable us in principle to compute every element. The problem with this approach is that we often want to use and compute for arbitrary or very large index, making sequential computation either useless or infeasible. This leads to the idea of a *closed form*: an explicit expression for a sequence or function in terms of the free variable. We will actually consider two types of closed forms. The first is where we express the elements of the sequence exactly in terms of the free variable; the second, is when we find a closed-form expression for the generating function of the sequence. In many cases, the latter is the best we can do, but it is quite often good enough for what we need.

Let's start with a very simple example to make the ideas concrete.

$$T_0 = 0 \tag{50}$$

$$T_n = 2T_{n-1} + 1 \qquad \text{for } n > 0 \tag{51}$$

The sequence as defined is one-sided, so by our convention, we also take $T_n = 0$ for $n < 0$. As recurrences go, this one is fairly straigtforward because we can guess the closed form and prove it simply by induction. But let's illustrate the basic method of using generating functions for this kind of problem anyway.

Step 1. Express the recurrence relation as a single equation that is valid for all integers.

$$T_n = 2T_{n-1} + 1_{(n\geq 1)}, \tag{52}$$

Step 2. Multiply both sides of the equation by z^n and sum over $\mathbb{Z}$.

$$\sum_n T_n z^n = \sum_n 2T_{n-1}z^n + \sum_{n\geq 1} z^n. \tag{53}$$

Step 3. Solve the equation to get the generating function $T(z) = \sum_n T_n z^n$ in closed form.

$$\begin{aligned} T(z) &= \sum_n T_n z^n && (54)\\ &= \sum_n 2T_{n-1}z^n + \sum_{n\geq 1} z^n && (55)\\ &= 2z\sum_n 2T_{n-1}z^{n-1} + \frac{z}{1-z} && (56)\\ &= 2zT(z) + \frac{z}{1-z}, && (57) \end{aligned}$$

because we are summing over all integers. Hence,

$$T(z) = \frac{z}{(1-z)(1-2z)}. \tag{58}$$

Step 4. Expand the generating function into a power series and read off the coefficents.

Here, $T(z)$ is a rational function whose denominator polynomial has roots at 1 and 1/2. What we need is a partial fractions expansion:

$$\begin{aligned} T(z) &= \frac{z}{(1-z)(1-2z)} && (59)\\ &= z\left[\frac{A}{1-z} + \frac{B}{1-2z}\right]. && (60) \end{aligned}$$

Multiplying both sides by $(1-2z)$ and evaluating at $z = 1/2$ gives $B = 2$. Multiplying both (right hand) sides by $(1-z)$ and evaluating at $z = 1$ gives $A = -1$. Hence,

$$\begin{aligned} T(z) &= z\left[\frac{2}{1-2z} - \frac{1}{1-z}\right] && (61)\\ &= z\sum_{n\geq 0}(2^{n+1}-1)z^n && (62)\\ &= \sum_{n\geq 0}(2^{n+1}-1)z^{n+1} && (63)\\ &= \sum_{n\geq 1}(2^n-1)z^n && (64)\\ &= \sum_{n\geq 0}(2^n-1)z^n. && (65) \end{aligned}$$

Thus, $T_n = 2^n - 1$ for $n \geq 0$.

The process was somewhat pedantic in this case, but the key is that the same process works just so in much, much harder cases.

Let's use the tools developed in the last section on a related but slightly harder case.

$$T_0 = 1 \tag{66}$$
$$T_n = 2T_{n-1} - 1 + n \quad \text{for } n > 0 \tag{67}$$

Step 1. Express the recurrence with boundary conditions:

$$T_n = 2T_{n-1} + (n-1)1_{(n>0)} + 1_{(n=0)} \tag{68}$$

Step 2. Form power series:

$$\sum_n T_n z^n = 2\sum_n T_{n-1} z^n + \sum_{n\geq 1}(n-1)z^n + 1, \tag{69}$$

so

$$T(z) = 2zT(z) + z\sum_{n\geq 0} nz^n + 1 \tag{70}$$
$$= \frac{1 + z\sum_{n\geq 0} nz^n}{1-2z}. \tag{71}$$

What to make of that $\sum_{n\geq 0} nz^n$? If we look at it for a moment and remember the last section, we might recognize it as

$$\sum_{n\geq 0} nz^n = \mathsf{S}\left(\mathsf{D}\left(\frac{1}{1-z}\right)\right) = \frac{z}{(1-z)^2}. \tag{72}$$

Excellent!

Step 3. Solve for $T(z)$: It follows that

$$T(z) = \frac{1 + z^2/(1-z)^2}{1-2z} \tag{73}$$
$$= \frac{(1-z)^2 + z^2}{(1-2z)(1-z)^2} \tag{74}$$
$$= \frac{1-2z+2z^2}{(1-2z)(1-z)^2}. \tag{75}$$

Step 4. Expand and find coefficients. Since neither 1 nor 1/2 is a root of $1-2z+2z^2$, we need to solve

$$\frac{1-2z+2z^2}{(1-2z)(1-z)^2} = \frac{A}{1-2z} + \frac{B}{(1-z)^2} + \frac{C}{1-z}. \tag{76}$$

Multiplying both sides by $(1-2z)$ and evaluating at $z = 1/2$ yields $A = 2$. Multiplying both sides by $(1-z)^2$ and evaluating at $z = 1$ yields $B = -1$. Evaluating at $z = 0$ then yields $C = 1 - A - B = 0$. Thus, using the common generating functions given earlier:

$$T(z) = \frac{2}{1-2z} - \frac{1}{(1-z)^2} \tag{77}$$

$$= \sum_{n\geq 0} 2^{n+1} z^n - \sum_{n\geq 0} (n+1) z^n \tag{78}$$

$$= \sum_{n\geq 0} (2^{n+1} - (n+1)) z^n, \tag{79}$$

and $T_n = 2^{n+1} - (n+1)$ for $n \geq 0$.

A few comments on the steps. For Step 1, while it's most convenient to express the recurrence in a single equation, but it's not strictly necessary. If there are odd boundary conditions, we can form the generating function by considering several equations. We took one approach in class on the Gambler's Ruin problem by summing only over the indices for which the main recurrence held true, but we could equivalently have summed over all indices with the same result, though on the boundary the right-hand side would have the boundary values not the recurrence value. For Step 2, we can often express the generating function in closed form, but occasionally we get a functional equation for the generating function, not quite as good but often sufficient.

For Step 4, a common situation is to have $G(z) = P(z)/Q(z)$ for polynomials P and $Q \neq 0$. We can assume that degree$(P) <$ degree(Q). If not, then there are unique polynomials $S(z)$ and $R(z)$ with degree$(R) <$ degree(Q) such that $P(z)/Q(z) = R(z)/Q(z) + S(z)$, and we work with $R(z)/Q(z)$. Assume that Q is non-zero and, for the moment, that it has distinct roots. Then, we can write $Q(z) = c(1-\rho_1 z)(1-\rho_2 z)\cdots(1-\rho_d z)$, and we want to represent

$$\frac{P(z)}{Q(z)} = \sum_{k=1}^{d} \frac{A_k}{1-\rho_k z}. \tag{80}$$

If we multiply both sizes by $(1-\rho_j z)$ and evaluate at $z = 1/\rho_j$, we get

$$A_j = \frac{P(1/\rho_j)}{c\prod_{k\neq j}(1-\rho_d/\rho_j)} = -\frac{P(1/\rho_j)}{\rho_j Q'(1/\rho_j)}. \tag{81}$$

The generating function thus satisfies:

$$[z^n]G(z) = \sum_{k=1}^{d} A_k \rho_k^n. \tag{82}$$

If $Q(z)$ has roots with multiplicity, it's not quite as easy, be we can often use this basic approach to reduce the unknowns. For example, suppose $Q(z) = (1-\rho_1 z)^2(1-\rho_2 z)\cdots(1-\rho_d z)$. Then, the partial fractions expansion looks like

$$\frac{P(z)}{Q(z)} = \frac{B_1}{(1-\rho_1 z)^2} + \sum_{k=1}^{d} \frac{A_k}{1-\rho_k z}. \tag{83}$$

If we multiply both sides by $(1-\rho_1 z)^2$ and evaluate at $z = 1/\rho_1$, we find B_1 but not A_1. Assuming that zero is not a root of Q, however, then once we have B_1 and $A_2, \ldots, A_d$, we can find A_1 by evaluating at $z = 0$ to get:

$$A_1 = \frac{P(0)}{Q(0)} - B_1 - \sum_{k=2}^{d} A_k. \tag{84}$$

Another variation on the basic procedure comes when we have more than one generating function to solve for simultaneously. This comes up, for instance, with coupled recurrences. We saw this in the Pentagon Mole problem on homework and in solving for the random walk return times and on this week's homework as well. As this shows, introducing coupled recurrences can sometimes make a problem easier.

Yet another variation is a recurrence in more than one variable. The ideas here are the same, it's just that we use multiple summations. Consider the following example.

$$C_{n,0} = 1 \tag{85}$$

$$C_{n,m} = C_{n-1,m} + C_{n-1,m-1}, \quad m > 0. \tag{86}$$

Define $C_n(z) = \sum_m C_{n,m} z^m$. Note that by our one-sided condition, $C_{-1,m} = 0$ for all $m > 0$, so $C_0(z) = 1$.

Step 1. Here the boundary condition has to be dealt with.

$$C_{n,m} = (C_{n-1,m} + C_{n-1,m-1}) 1_{(m>0)} + 1_{(m=0)}. \tag{87}$$

Step 2. We're summing over all m, be careful.

$$C_n(z) = \sum_m C_{n,m} z^m \tag{88}$$

$$= 1 + \sum_{m \geq 1} C_{n-1,m} z^m + \sum_{m \geq 1} C_{n-1,m-1} z^m \tag{89}$$

Step 3. Solve for $C_n(z)$:

$$C_n(z) = C_{n-1}(z) + z C_{n-1}(z) \tag{90}$$

$$= (1+z) C_{n-1}(z), \tag{91}$$

with $C_0(z) = 1$. Thus, $C_n(z) = (1+z)^n$.

Step 4. Find the coefficients. By the binomial theorem,

$$[z^m] C_n(z) = C_{n,m} = \binom{n}{m}. \tag{92}$$

That all worked out quite tidily, but notice that we treated the two variables asymmetrically. What happens if we do the full two-variable funtion. We have $[y^n z^m] C(y,z) = \binom{n}{m}$, so:

$$C(y,z) = \sum_n \sum_m \binom{n}{m} y^n z^m \tag{93}$$

$$= \sum_n (1+z)^n y^n \tag{94}$$

$$= \frac{1}{1-(1+z)y}. \tag{95}$$

Abusing notation just a bit, we can write $[y^n]\frac{1}{1-(1+z)y} = (1+z)^n$. But by interchanging the order of summation, we also get

$$C(y,z) = \sum_m \left(\sum_n \binom{n}{m} y^n \right) z^m \tag{96}$$

$$= \frac{1}{1-y-yz} \tag{97}$$

$$= \frac{1}{1-y} \frac{1}{1-\frac{y}{1-y}z} \tag{98}$$

$$= \frac{1}{1-y} \sum_{m \geq 0} \left(\frac{y}{1-y} \right)^m z^m. \tag{99}$$

By a similar stretch of the notation $[z^m]\frac{1}{1-(1+z)y} = \frac{y^m}{(1-y)^{m+1}}$. This gives us immediately two useful sums:

$$\sum_m \binom{n}{m} z^m = (1+z)^n \tag{100}$$

$$\sum_n \binom{n}{m} y^n = \frac{y^m}{(1-y)^{m+1}}. \tag{101}$$

Nice.

Double summation like this can be a useful technique for calculating sums. Our sum – like $\sum_m \binom{n}{m} z^m$ or $\sum_n \binom{n}{m} y^n$ – is really a parameterized family of sums. We do the power series trick – multiply by y^n or z^m, respectively, and sum – to get a two dimensional generating function. By interchanging the order of the sums and other tricks, we can often reduce the sum to simpler form. Just as above.

3. Twists and Turns

There are many places we could go from here, and many nifty techniques based on generting functions. But this document is getting too long as it is, so I'll hold off on some of these until later and defer the rest to the references.

One I will mention is one we've seen briefly in class – The Lagrange Inversion formula.

Theorem 12. (The Lagrange Inversion Formula). Let $F(u)$ and $G(u)$ be generating functions with $G(0) = 1$. Then there is a unique formal power series $U = U(z)$ that satisfies the functional equation

$$U(z) = zG(U(z)). \tag{102}$$

In addition, if $F(U(z))$ is expanded in a power series in z, the coefficients satisfy

$$[z^n]F(U(z)) = \frac{1}{n}[u^{n-1}](F'(u)G^n(u)). \tag{103}$$

This is a variant (see References) of a traditional theorem on formal power series known variously as the Lagrange Inversion Theorem or Lagrange Inversion Theorem. The idea is that it shows how to compute the power series expansion of a function that is defined implicitly in terms of a holomorphic function. As it's traditionally written: Let u be defined implicitly by $u = c + zG(u)$. Then, we can expand $F(u)$ in a power series about $z = 0$ ($u = c$) as

$$F(u) = F(c) + \sum_{n=1}^{\infty} \frac{z^n}{n!} \mathsf{D}^{n-1}(G^n \cdot F')(c). \tag{104}$$

In our case, we are taking $c = 0$, and notice that by our rules above

$$[u^0]\frac{1}{n!}\mathsf{D}^{n-1}(G^n \cdot F') = \frac{(n-1)!}{n!}[u^{n-1}](G^n(u)F'(u)), \tag{105}$$

and so,

$$[z^n]F(u) = \frac{1}{n}[u^{n-1}](G^n(u)F'(u)). \tag{106}$$

This isn't a proof but it does connect it to the traditional form of the Lagrange theorem. This theorem is applied in Statistics in developing Cornish-Fisher expansions and their generalizations.

Exercise 13. Let t_n represent the number of labeled, rooted trees on n vertices. Let $T(z)$ be the generating function for this sequence. Then, $T(z)$ satisfies

$$T(z) = ze^{T(z)}. \tag{107}$$

Use the LIF to find t_n. (This is a fairly standard example for applying the theorem but is good practice, cf. Homework 3.)

4. Other Kinds of Generating Functions

The generating functions we've seen so far are power series, but it turns out to be useful to consider alternative forms.

A critical feature of power series is that $G(z) = 0$ if and only that $[z^n]G(z) = 0$ for all n. In principle, if we identify component functions $\phi_n(z)$ such that

$$A(z) = \sum_n a_n \phi_n(z) = 0 \iff a_n = 0 \quad \text{for all } n, \tag{108}$$

then we can consider generating functions based on the ϕ_n. The ordinary generating functions are based on $\phi_n(z) = z^n$.

Two other important examples are $\phi_n(z) = z^n/n!$, which give *exponential generating functions* and $\phi_n(z) = n^{-z}$ $(n > 0)$ which give *Dirichlet generating functions.* There are others as well, but these are the most important.

In each case, we can develop a formal theory and a set of manipulations that help us solve problems, much as we did above. Depending on the situation, one or the other form of generating functions might be more convenient. For our purposes now, the key thing is to be aware of this as an option.

5. Asymptotics

In many applications, we will are interested in (or are willing to accept) an approximation to a sequence g_n for large n. The asymptotic behavior of the sequence is closely tied to the location and nature of the singularities in $G(z)$ and to the behavior of the function there.

Let's start with a basic relation. Suppose $G(z)$ is a power series with radius of convergence R. Then, by definition, $\limsup_{n\to\infty} |a_n|^{1/n} = 1/R$. By the definition of lim sup, this implies that for every $\epsilon > 0$ we have

$$|a_n|^{1/n} < \frac{1}{R} + \epsilon \quad \text{eventually} \tag{109}$$

$$|a_n|^{1/n} > \frac{1}{R} - \epsilon \quad \text{infinitely often,} \tag{110}$$

which tells us that

$$|a_n| < \left(\frac{1}{R} + \epsilon\right)^n \quad \text{eventually} \tag{111}$$

$$|a_n| > \left(\frac{1}{R} - \epsilon\right)^n \quad \text{infinitely often,} \tag{112}$$

The radius of convergence thus gives us a basic asymptotic bound on the sequence. But notice that R is determined by the modulus of the singularity *closest to 0.*

Suppose we can find a function $\widetilde{G}(z)$ that is easy to work with and has the same singularities as $G(z)$ on the circle $|z| = R$ in the complex plane. Then, $G(z) - \widetilde{G}(z)$ has its smallest singularities farther than R from the origin and is thus analytic on a disk $|z| < S$ for $S > R$. By the above, the coefficient $[z^n](G(z) - \widetilde{G}(z))$ are eventually smaller than $(1/S + \epsilon)^n$ for any $\epsilon > 0$. But

$$\frac{(1/S+\epsilon)^n}{(1/R+\epsilon)^n} = \left(\frac{1/S+\epsilon}{1/S+\epsilon}\right)^n \to 0. \tag{113}$$

So, $[z^n]G(z)$ should be like $[z^n]\widetilde{G}(z)$ plus terms of smaller order.

A meromorphic funtion $G(z)$ on an open subset of the complex plane is a function that can be expressed as a ratio $F(z)/H(z)$ of two holomorphic (analytic) functions on that domain, with the restriction that $H(z)$ not be identically 0. Such a $G(z)$ is analytic except at (at most countably many) isolated points called *poles* where the function behaves like $a(z-z_0)^k$ for some k.

If $G(z)$ is meromorphic and z_0 is a pole of order p, then in some neighborhood of z_0 (but excluding z_0 itself), we can expand $G(z)$ as

$$G(z) = \sum_{n=-p}^{\infty} g_n (z-z_0)^n. \tag{114}$$

This is called the Laurent expansion of G around z_0. The part of the above sum with negative indices, call it $G_-(z; z_0)$, is called the *principal part* of that expansion.

If $G(z)$ has radius of convergence R and has finitely many poles $z_1, \ldots, z_m$ on the circle $|z| = R$, then $G(z) - \sum_{k=1}^m G_-(z; z_k)$ is analytic on some disk of radius $S > R$, so by the above argument for any $\epsilon > 0$,

$$[z^n]G(z) = [z^n]\sum_{k=1}^{m} G_-(z, z_k) \, + \, O\left(\left(\frac{1}{S}+\epsilon\right)^n\right). \tag{115}$$

We could take this analysis even farther. Two famous results are Darboux's method for branch points and Hayman's method for entire functions. These are discussed very nicely in [Wilf 2005] and generalized further in [Flajolet and Odlyzko 1990]. See references below.

6. Selected References

Flajolet, P. and Odlyzko, A. (1990). Singularity Analysis of Generating Functions. *SIAM Journal of Discrete Mathematics*, **3**, 216.
[New and improved asymptotic methods for generating fucntions. Very technical overall, but the introduction gives a clear feel for the results. Generalizations of Darboux's theorem. Available on-line from Flajolet's web site, see next entry.]

Flajolet, P. and Sedgewick, R. (2006). *Analytic Combinatorics*,
[An in-depth and rigorous exploration of combinatorics using generating functions and other tools. A strong emphasis on asymptotics, which Flajolet specializes in, and analysis of problems that arise in computer science. Not yet published, but several relevant sample chapters are available on-line at `http://pauillac.inria.fr/algo/flajolet/Publications/books.html`.]

Gould, H. (1972) *Combinatorial Identities.*

* Graham, R., Knuth, D., and Patashnik, O. (1994). *Concrete Mathematics.*
[This is one of my favorite books period. Clearly written, fun, inspiring, and filled with challenging ideas and problems. I've only used the first edition, but the second edition is supposedly even better. Chapter 7 on Generating Functions is a good place to start on the topic period, but I'd suggest reading the whole thing.]

Ranjan, R. (1987). Binomial identities and Hypergeometric Series, *American Mathematical Monthly*, **94** (1987), 36.

Szpankowski, W. (2001). *Average Case Analysis of Algorithms on Sequences.*
[See Chapter 7 available on-line at `http://www.cs.purdue.edu/homes/spa/book.html` for another overview of Generating Functions.]

Wilf, H. (2005). *generatingfunctionology*, Third Edition.
[I only discovered this recently, and it looks to be very good and clearly written. Nice chapters on applications of generating functions and on asymptotic approaches (Darboux's theorem and Hayman's method). It also has some nice methodological development of the double summation technique and other methods for finding sums and identities. I adapted the form of the Lagrange Inversion Formula above from Wilf's presentation. I'll report further as I go through it more carefully, but I have high hopes. Further good news is that older editions are available for free on line at `http://www.math.upenn.edu/ wilf/DownldGF.html`.]

Wilf, H. and Zeilberger, D. (1990) Rational Functions Certify Combinatorial Identities. *Journal of the American Mathematical Society*, **3**, 147.
[The details on one method Wilf presents in his book. Quite readable; available on-line from Carnegie Mellon.]