Generating Functions

Generating Functions are a powerful tool in combinatorics. Wilf describes them, quite appropriately, as "a clothesline on which we hang up a sequence of numbers for display." What does he mean by that? Let's consider the well known recurrence for Fibonacci numbers: $F_{n+1} = F_n + F_{n-1}$, where F_n denotes the nth Fibonacci number. How do we find a nice formula for F_n? None of the approaches that we had learnt earlier (Domain/Range Transformations, Master method) work in this setting. But GFs come to our rescue. Formally speaking, a generating function for a sequence of numbers $(a_n)_{n\geq 0}$ is the power series $\sum_{n\geq 0} a_n x^n$, or as Wilf puts it "the clothesline". The most *fundamental generating function*: the sequence $1, 1, 1, , \ldots,$ has the power series $\sum_{n\geq 0} x^n = 1/(1-x)$ (for the moment, we do not focus on the restriction $|x| < 1$). Similarly, the generating function of the sequence $(\alpha^n)_{n\geq 0}$ is $1/(1-\alpha x)$.

1 From Recurrences to Closed Form

Let's try the generatingfunctionologist approach to get a closed form for the Fibonacci numbers. Define

$$F(x) := \sum_{n\geq 0} F_n x^n = x + F_2 x^2 + F_3 x^3 + \cdots ,$$

since $F_0 = 0$ and $F_1 = 1$. Then multiplying both sides of the recurrence $F_{n+1} = F_n + F_{n-1}$ by x^n and summing for all $n \geq 1$ we get

$$\begin{aligned} \sum_{n\geq 1} F_{n+1} x^n &= F(x) + \sum_{n\geq 1} F_{n-1} x^n \\ F_2 x + F_3 x^2 + \cdots &= F(x) + F_0 x + F_1 x^2 + F_2 x^3 + \cdots \\ \frac{F(x) - x}{x} &= F(x) + xF(x). \end{aligned}$$

After "solving" for $F(x)$ we obtain

$$F(x) = \frac{x}{1 - x - x^2} = \frac{x}{(1 - x\phi_+)(1 - x\phi_-)},$$

where $\phi_\pm = (1 \pm \sqrt{5})/2$. Using the partial fraction expansion on the RHS we further get

$$F(x) = \frac{1}{(\phi_+ - \phi_-)} \left(\frac{1}{1 - x\phi_+} - \frac{1}{1 - x\phi_-} \right) = \frac{1}{\sqrt{5}} \left(\sum_{n\geq 0} (\phi_+^n - \phi_-^n) x^n \right),$$

where in the last equality we use the expansion of the fundamental geometric function. By equating the coefficients of x^n on both sides we obtain

$$F_n = \frac{1}{\sqrt{5}} (\phi_+^n - \phi_-^n).$$

From this formula we also get the asymptotics.

Solving recurrences is but one application of GFs. There are many other applications: to prove identities; find a new recurrence formula from the gf; finding an asymptotic estimate where exact formula may not be possible; prove unimodality, convexity and other such properties. We explore some of these applications here.

Let's try to get a closed form for a more familiar sequence: let $f(n,k)$ be the number of subsets of size k of an n element set. We know $f(n,k) = \binom{n}{k}$ but nevertheless let's derive a generating function for $f(n,k)$. We have the following recurrence:

$$f(n,k) = f(n-1,k-1) + f(n-1,k).$$

An interpretation of this recurrence is as follows: fix an element, say n, in the set $[n]$; then all the k-sized subsets of the set $[n]$ can be partitioned into two classes: those that contain n, of which there are $f(n-1,k-1)$ sets, and those that do not contain n, of which there are $f(n-1,k)$ sets. Let's define $B_n(x) := \sum_{k\geq 0} f(n,k)x^k$. Then multiplying the recurrence above by x^k and summing both from $k \geq 0$ we get

$$B_n(x) = xB_{n-1}(x) + B_{n-1}(x) = (1+x)B_{n-1}(x) = (1+x)^n B_0(x).$$

Note $B_0(x) = 1$, as there is exactly one subset of the empty set, namely itself. Thus we are interested in the coefficient of x^k in $(1+x)^n$. To get hold of it, we do the following standard trick: coeff. of x^k is equal to the kth derivative of $(1+x)^n/k!$ evaluated at $x = 0$; also, evident by Taylor expansion at $x = 0$. The term so obtained is $n(n-1)\dots(n-k+1)/k! = \binom{n}{k}$, as expected.

Let's try to answer another very similar question: How many partitions are there of an n-element set? Or, in other words, how many equivalence relations can we have on an n element set? We first try to answer a simpler question: In how many ways can we partition an n-element set into k boxes such that no box remains empty, and every element goes into some box? Let $\left\{ {n \atop k} \right\}$ be this number (called the Stirling number of second kind). So, for instance, $\left\{ {n \atop 1} \right\} = 1$, since there is only one way to partition the set $[n]$ into a single partition, namely itself; with some effort we can verify that $\left\{ {n \atop 2} \right\} = 2^{n-1} - 1$. Given, the definition of $\left\{ {n \atop k} \right\}$, the answer to our first question is $\sum_{k=0}^{n} \left\{ {n \atop k} \right\}$. Can we get a recurrence, similar to $f(n,k)$? Let's proceed with the interpretation we had given earlier: consider the element n; the partitions of $[n]$ into k boxes are of two types: partitions of the first type are those in which n is the *only* member in its box, or n shares a box with other elements. In the first case, the remaining $k-1$ boxes are filled with the elements of the set $[n-1]$, which can be done in $\left\{ {n-1 \atop k-1} \right\}$ way. in the second case, there are $\left\{ {n-1 \atop k} \right\}$ ways to distribute $n-1$ elements into k boxes; but for each such partition of $[n-1]$ into k boxes, we can put n into one of the k boxes to get a partition of $[n]$ into k boxes. Thus we have the recurrence:

$$\left\{ {n \atop k} \right\} = \left\{ {n-1 \atop k-1} \right\} + k\left\{ {n-1 \atop k} \right\}.$$

It is natural to define $\left\{ {n \atop k} \right\} = 0$, if $k > n$, and $\left\{ {n \atop 0} \right\} = 0$, for all n.

How do we define the GF for $\left\{ {n \atop k} \right\}$? We had overlooked this matter earlier, or were rather lucky in our choice, since there are at least two ways of defining the GF:

$$A_n(x) := \sum_{k\geq 0} \left\{ {n \atop k} \right\} x^k \text{ and } B_k(x) := \sum_{n\geq 0} \left\{ {n \atop k} \right\} x^n.$$

Which of the two shall we choose? If we pick the first one, as we did for the binomial coefficients, then we see that to do the sum $\sum_k k\left\{ {n-1 \atop k} \right\} x^k$ we need to do a differentiation, which would make it more complicated (we need to solve a differential equation). If, however, we choose the second one then we don't face this problem. Thus taking the GF-approach, we multiply the recurrence by x^n and sum on both sides to get

$$B_k(x) = \sum_{n\geq 0} \left\{ {n-1 \atop k-1} \right\} x^n + k \sum_{n\geq 0} \left\{ {n-1 \atop k} \right\} x^n = xB_{k-1}(x) + kxB_k(x).$$

Thus

$$B_k(x) = \frac{x}{1-kx} B_{k-1}(x) = \frac{x^k}{(1-x)(1-2x)\dots(1-kx)}.$$

We are interested in knowing the coefficient of x^n on the RHS, which is the same as the coefficient of x^{n-k} in

$$\frac{1}{(1-x)(1-2x)\dots(1-kx)}.$$

Unfortunately, our Taylor's formula approach doesn't work here (differentiating the fractions, only gives more fractions). What we need is to consider the partial fraction expansion of

$$\frac{1}{(1-x)(1-2x)\dots(1-kx)} = \sum_{j=1}^{k} \frac{a_j}{1-jx}.$$

Multiplying both sides by $(1-jx)$, and plugging $x = 1/j$ we get

$$a_j = (-1)^{k-j} \frac{j^{k-1}}{(j-1)!(k-j)!}.$$

Thus the coefficient of x^{n-k} in

$$\sum_{j=1}^{k} \frac{a_j}{1-jx} = \sum_{j=1}^{k} a_j(1 + (jx) + (jx)^2 + \cdots)$$

is our expression for

$$\left\{ n \atop k \right\} = \sum_{j=1}^{k} a_j j^{n-k} = \sum_{j=1}^{k} (-1)^{k-j} \frac{j^{k-1}}{(j-1)!(k-j)!} j^{n-k} = \sum_{j=1}^{k} (-1)^{k-j} \frac{j^n}{j!(k-j)!}. \tag{1}$$

That gives us an expression for the number of partitions of $[n]$ into k boxes. What about our original question of the total number of partitions of $[n]$. As we had mentioned earlier, this number, called the nth Bell number, is

$$B_n := \sum_{k=0}^{n} \left\{ n \atop k \right\}.$$

But we observe one nice fact about the formula in (1). Recall that we had defined $\left\{ n \atop k \right\} = 0$, for $k > n$. The formula in (1) automatically encodes this definition. To prove this consider the following reformulation of (1):

$$\left\{ n \atop k \right\} = \sum_{j=1}^{k} (-1)^{k-j} \frac{j^n}{j!(k-j)!} = \frac{1}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} j^n.$$

Note that the RHS can be derived from $(x-1)^k = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} x^j$ as follows: apply n times the operator xd/dx to $(x-1)^k$, divide by $k!$, and plug $x = 1$ to get the term on the RHS. However, if $k > n$, then $(x-1)$ will *always divide* $(xd/dx)^n (x-1)^k$. Thus (1) vanishes for $k > n$. We can cleverly use this fact in getting a closed form for B_n. Let $m > n$ then the observation we just made implies

$$B_n = \sum_{k=0}^{m} \left\{ n \atop k \right\} = \sum_{k=0}^{m} \sum_{j=0}^{k} (-1)^{k-j} \frac{j^n}{j!(k-j)!} = \sum_{j=0}^{m} \frac{j^n}{j!} \sum_{k=j}^{m} (-1)^{k-j} \frac{1}{(k-j)!} = \sum_{j=0}^{m} \frac{j^n}{j!} \sum_{k=0}^{m-j} (-1)^k \frac{1}{k!}.$$

Since our choice of m was an arbitrary number greater than n, we can let $m \to \infty$, which gives us

$$B_n = \frac{1}{e} \sum_{j \geq 0} \frac{j^n}{j!}. \tag{2}$$

Though the above equation has its usefulness and simplicity, it does not lend itself to computation as we have an indefinite sum on the RHS (it is good for estimating). Can we derive a recurrence for B_n? We next see how GFs can lead to recurrences, thus bringing us a complete circle. If we proceed along familiar lines to derive a GF for B_n we get

$$\sum_{n\geq 0} B_n x^n = \sum_n \sum_j \frac{(jx)^n}{j!} = \sum_j \frac{1}{j!(1-jx)}$$

which doesn't lend itself to further manipulation. However, there is no hard and fast rule on choosing the "clothesline". Given the similarity between B_n and the series for e^x, we should instead try

$$\begin{aligned}\sum_{n\geq 0} B_n \frac{x^n}{n!} &= \frac{1}{e}\sum_n \sum_j \frac{(xj)^n}{n!}\frac{1}{j!} \\ &= \frac{1}{e}\sum_j \frac{e^{xj}}{j!} \\ &= \frac{1}{e}\sum_j \frac{(e^x)^j}{j!} \\ &= e^{e^x-1}.\end{aligned}$$

The generating function just derived is called an exponential generating function; the earlier ones are called ordinary generating functions. Continuing further, we can *use the generating function to derive a recurrence* for B_n as follows. Taking logarithm on both sides of

$$\sum_{n\geq 0} B_n \frac{x^n}{n!} = e^{e^x-1}$$

we obtain

$$\ln \sum_{n\geq 0} B_n \frac{x^n}{n!} = e^x - 1.$$

Differentiating both sides and multiplying by x we get

$$\sum_{n\geq 1} B_n \frac{x^n}{(n-1)!} = xe^x \sum_{n\geq 0} B_n \frac{x^n}{n!} = e^x \sum_{n\geq 1} B_{n-1}\frac{x^n}{n!}$$

Comparing the coefficients of x^n on both sides we get

$$B_n = \sum_{j=0}^{n-1} B_j \binom{n-1}{j},$$

a formula that lends itself to computation.

2 Formal Power Series

Formal power series can be imagined as polynomials with infinite terms. More precisely, they are defined as $f := \sum_{n\geq 0} a_n x^n$.[1] We will often use the notation $\{a_n\}$ to denote the formal power series, and switch between the functional form f and the coefficient form $\{a_n\}$. In this section we treat them purely as algebraic objects. It is not hard to show that the set of formal power series is a ring, denoted by $R[[x]]$, where R is the underlying ring (e.g., integers) from which the coefficients are chosen; addition and subtraction are done coefficient wise, and multiplication is defined naturally as

$$\sum_n a_n x^n \sum_n b_n x^n = \sum_n (\sum_k a_k b_{n-k}) x^n. \tag{3}$$

The **reciprocal** of a formal power series f is another series g if $f \times g = 1$; the coefficients of g come from the rational field corresponding to R and are uniquely defined. The following lemma characterizes the existence of inverses.

[1] A distinction is made from power series, where the notion of convergence plays an important role.

Lemma 1 *A formal power series $\sum_n a_n x^n$ has a reciprocal iff $a_0 \neq 0$.*

Proof. Let $\{b_n\}$ be the inverse of $\{a_n\}$. Then we must have $b_0 a_0 = 1$, which implies $a_0 \neq 0$. Moreover, from the multiplication rule (3) it follows that

$$a_0 b_n = -\sum_{k \geq 1} a_k b_{n-k}.$$

Conversely, if $a_0 \neq 0$ then we can use the relation above to solve for b_k's. **Q.E.D.**

Analogous to functional calculus, we define one more notion: the **derivative** of a formal power series $f = \sum_n a_n x^n$ is the series $f' := \sum_n n a_n x^{n-1}$. The derivative is defined to be as such; we do not define it by a limiting process as is usually done. Nevertheless, we carry over the standard rules of differentiating sums, products, quotients, and compositions. The following two results will be of consequence:

- If $f' = 0$ then f is a constant.
- If $f' = f$ then $f = ce^x$, for some constant c. Let's see why. The equality states that $a_{n-1} = n a_n$. Thus, inductively, $a_n = a_0/n!$, for all $n \geq 1$, which implies that $A = a_0 e^x$.

Based upon the formalization above, we now proceed to give the details of rules for manipulating formal power series to obtain generating functions for various coefficient sequences.

By the symbol $f \overset{o}{\sim} \{a_n\}$ we mean that f is the ordinary power series generating function for the sequence $\{a_n\}$, i.e., $f = \sum_n a_n x^n$. Similarly define $f \overset{e}{\sim} \{a_n\}$ to mean that f is the exponential power series generating function for $\{a_n\}$, i.e., $f = \sum_n a_n x^n/n!$. To demonstrate the difference between the two types of gf, we see

Ordinary Power Series GF Let $f \overset{o}{\sim} \{a_n\}$	Exponential Power Series GF Let $f \overset{e}{\sim} \{a_n\}$
1) $(f - a_0)/x \overset{o}{\sim} \{a_{n+1}\}$. In general, $\frac{f - \sum_{j=0}^{k-1} a_j x^j}{x^k} \overset{o}{\sim} \{a_{n+k}\}$. E.g., $F_{n+2} = F_{n+1} + F_n$, we get $(f - x)/x^2 = f/x + f$	$Df \overset{e}{\sim} \{a_{n+1}\}$. $D^k f \overset{e}{\sim} \{a_{n+k}\}$ We get $f'' = f' + f$; solution $f = \frac{(e^{\phi_+ x} - e^{\phi_- x})}{\sqrt{5}}$.
2) $xDf \overset{o}{\sim} \{na_n\}$, D is derivative operator. What generates $\{n^2 a_n\}$? It is $(xD)^2 f$. In general, $(xD)^k f \overset{o}{\sim} \{n^k a_n\}$. Thus, $A(x) \in \mathbb{R}[x]$ then we have $A(xD)f \overset{o}{\sim} \{A(n)a_n\}$. Q:) Ogf for $\{(n^2+1)/n!\}$? We know $e^x \overset{o}{\sim} \{1/n!\}$. Applying the rule gives us $((xD)^2 + 1)e^x$ is the desired ogf.	This rule remains the same: $A(xD)f \overset{e}{\sim} \{A(n)a_n\}$
3) Convolution: If $f \overset{o}{\sim} \{a_n\}$, $g \overset{o}{\sim} \{b_n\}$ then $fg \overset{o}{\sim} \{\sum_k a_k b_{n-k}\}$. What is the result if $g = 1/(1-x)$? $f/(1-x) \overset{o}{\sim} \{\sum_{k=0}^n a_k\}$. Also, $f^k \overset{o}{\sim} \{\sum_{i_1+i_2+\cdots+i_k=n} a_{i_1} a_{i_2} \ldots a_{i_k}\}$. Apply to get the sum of squares of first n numbers. What about H_n?	$f \overset{e}{\sim} \{a_n\}$, $g \overset{e}{\sim} \{b_n\}$ then $fg \overset{e}{\sim} \{\sum_k \binom{n}{k} a_k b_{n-k}\}$. If $g = e^x$ then $fe^x \overset{e}{\sim} \{\sum_k \binom{n}{k} b_{n-k}\}$. $f^k \overset{e}{\sim} \{\sum_{i_1+i_2+\cdots+i_k=n} n! i_1! \cdots i_k! a_{i_1} a_{i_2} \ldots a_{i_k}\}$. What is the egf for $\sum_{k=0}^n \binom{n}{k} k^2 (-1)^{n-k}$?

some applications.

¶1. Example 1: Given n pairs of parenthesis, let $f(n)$ be the number of ways to arrange them in a "legal" manner, i.e., when scanning a string of parenthesis from left to right the number of left parenthesis always exceed the number of right parenthesis (similar, to the role of parenthesis in programming languages); clearly, $f(0) = 1$, the empty string. So, for instance, for $n = 3$, we have the following five legal strings

$$()()(), (())(), ((())), (()()), ()(()).$$

Can we get a closed form for $f(n)$? Every legal string contains within it smaller legal strings. In particular, there is a *first legal string*, i.e., there is a smallest number k, let's call it the **minimal legal index**, such that the *first* $2k$ characters form a legal string; in the example above, the number is $1, 2, 3, 3, 1$ resp. We call a string with n pairs of parenthesis **primitive** if the minimal legal index is n; in the example above, the third and fourth strings are primitive. Let $f(n, k)$ be the number of legal strings containing a first legal string of length $2k$. Since every string has a unique minimal legal index, it follows that $f(n) = \sum_k f(n, k)$. Can we get a recursion for $f(n,k)$? Let $g(k)$ be the number of primitive strings of length $2k$. Then for every string in $f(n,k)$, the first $2k$ characters form a primitive string, and the remaning $2(n-k)$ form a legal string (not necessarily primitive). Thus $f(n,k) = g(k)f(n-k)$. But what is $g(k)$? Every primitive string in $g(k)$ is of the form "(legal string of length $2(k-1)$)", i.e., the first left parenthesis has to be matched with the last right parenthesis (it cannot be matched anywhere in between, as that would give us a contradiction). Moreover, given a legal string of length $2(k-1)$ we can construct a primitive string in $g(k)$. This bijective correspondence implies $g(k) = f(k-1)$. Hence we have the recursion

$$f(n) = \sum_{k \geq 1} f(k-1)f(n-k).$$

This equations suggests that we use the convolution rule for ogfs. Let $F \overset{o}{\sim} \{f(n)\}$. Then we have that $xF \overset{o}{\sim} \{f(n-1)\}$. Multiplying the recurrence by x^n and summing for $n \geq 1$, by the convolution rule we get xF^2 on the RHS and $F-1$ on the left, i.e., $F - 1 = xF^2$. Solving for F in this quadratic equation we get

$$F = \frac{1 \pm \sqrt{1-4x}}{2x}.$$

Which sign to choose? If we choose the positive sign then letting $x \to 0$, we get that $F(0) = f(0) = \infty$, which is not correct. If we choose the negative sign then letting $x \to 0$ we get $F(0) = 1$ as desired. Hence $F(x) = \frac{1-\sqrt{1-4x}}{2x}$, and hence we can show that $f(n) = \binom{2n}{n}/(n+1)$. These numbers are called the **Catalan numbers**.[2]

A Combinatorial Proof of Catalan Numbers: To derive this proof, we first consider a different counting problem. Consider an $n \times n$ grid. A **monotone path** from $(0,0)$ to (n,n) is a path that either goes right or up by one unit. The total number of paths from the origin to (n,n) are $\binom{2n}{n}$. Let C_n be the number of "good" monotone paths, i.e., monotone paths that do not cross the diagonal $y = x$ (but may touch it). It is not hard to see that the number of legal parentheses string is the same as the number of good monotone paths. If we can count the number of bad monotone paths, then we can subtract it from the total number of monotone paths to get C_n. A bad monotone path must cross the diagonal. Consider the first instance when this happens. The coordinates of that point must be of the form $(k, k+1)$. The rest of the path must contain $(n-k)$ right-moves and $(n-k-1)$ up-moves. Now reflect the path starting from $(k, k+1)$, i.e., whenever we go up in the original path we go right, and vice versa. The reflected path will thus take $(n-k)$ up-moves and $(n-k-1)$ right moves and end up at the point $(n-k-1+k, n-k+k+1) = (n-1, n+1)$. That is all monotone paths to $(n-1, n+1)$ correspond to bad monotone paths to (n,n). Since the number of such paths are $\binom{2n}{n-1}$, we get that

$$C_n = \binom{2n}{n} - \binom{2n}{n-1} = \frac{1}{n+1}\binom{2n}{n}.$$

¶2. Example 2: A **derangement** of n letters is a permutation without a fixed point. We want to compute D_n, the number of derangements of n letters. Let $P(n,k)$ be the number of permutations that have exactly k fixed points; $P(n,0) = D(n)$. Then $n! = \sum_{k \geq 0} P(n,k)$. But each permutations in $P(n,k)$ is set of k fixed points, and the remaining $n-k$ letters form a derangement. Thus $P(n,k) = \binom{n}{k} D_{n-k}$, and hence

$$n! = \sum_{k \geq 0} \binom{n}{k} D_{n-k}.$$

The equation above fits the pattern of convolution of egf. Thus let $D(x) \overset{e}{\sim} \{D_n\}$. Then dividing the equation above by $n!$, multiplying it by x^n, and summing for $n \geq 0$, we get

$$\frac{1}{1-x} = e^x D(x),$$

[2] Catalan was a mathematician from Belgium, famous for his conjecture in 1844 that the only two consecutive powers of natural numbers are 8 and 9. This was proved in 2003 by Preda Mihailescu.

or $D(x) = e^{-x}/(1-x)$. Thus by the convolution rule for ogfs, we get

$$\frac{D_n}{n!} = 1 - 1 + \frac{1}{2!} - \frac{1}{3!} + \cdots + (-1)^n \frac{1}{n!}.$$

Later we will see another approach to derive the same result.

3 The Analytic Aspects of Power Series

As we have seen above, the algebraic, or formal, aspects of power series are useful when we are trying to get a precise count or closed formula for the counting function, which is the nth term of the series. Often, however, this might not be possible, and even when it is, it might be desirable to get an asymptotic understanding of the growth of the coefficients of the series. So, for instance, we know from above that the Catalan numbers $C_n = \binom{2n}{n}/(n+1)$. Using Stirling's approximation $n! \sim \sqrt{2\pi n}(n/e)^n$, we get that

$$C_n \sim \sqrt{4\pi n}(2n/e)^{2n} \left(\frac{1}{\sqrt{2\pi n}(n/e)^n}\right)^2 \frac{1}{n+1} = \frac{4^n}{\sqrt{\pi n^3}}.$$

This can be interpreted as a special case of a class of generating functions for which the asymptotics is of the form $E(n)\theta(n)$, where $E(n)$ is an exponential factor in n and $\theta(n)$ is some sub-exponential factor. Can we derive the above asymptotics directly? The analytic aspects of the GF $C(z) = (1 - \sqrt{1-4z})/2z$ help us in this regard. The crucial aspect here is the study of the *singularities* of the GF, in this case $C(z)$. Intuitively, singularities are points in the complex plane where either the function or one of its derivatives is not continuous. If we consider $C(z)$ then as $z \to 1/4$, $C(z) \to 2$, however, its first derivative tends to infinity. If ρ is the singularity with the smallest absolute value then we will see that the exponential factor $E(n) = \rho^{-n}$; that explains 4^n in C_n. The sub-exponential factor $\theta(n)$ is governed by the nature of the singularity – whether it is simple or not, algebraic, etc. These two remarks may be considered as the two fundamental principles of coefficient asymptotics. To explain these, we need some basics from complex analysis.

The approach will be modified to get better estimates, for instance, for the **Ordered Bell numbers**, $\widetilde{B}(n)$ that is the number of ways to partition a set $[n]$ where the orderings of the partition matter. We know that $\left\{{n \atop k}\right\}$ are the number of ways to partition n into k equivalence classes. If the ordering of the classes matter then we have $k!\left\{{n \atop k}\right\}$ ways of partitioning $[n]$. Thus

$$\widetilde{B}(n) = \sum_{k=0}^{n} k! \left\{{n \atop k}\right\} = \sum_{k=0}^{n}\sum_{j=0}^{k}(-1)^{k-j}\binom{k}{j} j^n.$$

Again, using the observation that the second sum on the RHS vanishes for any $k > n$, we can choose $m > n$ and rewrite

$$\begin{aligned}
\widetilde{B}(n) &= \lim_{m\to\infty} \sum_{k=0}^{m}\sum_{j=0}^{k}(-1)^{k-j}\binom{k}{j} j^n \\
&= \lim_{m\to\infty} \sum_{j=0}^{m} j^n \sum_{k=0}^{m-j}(-1)^k \binom{k+j}{j} \\
&= \sum_{j\ge 0} \frac{j^n}{2^{j+1}}.
\end{aligned}$$

What is a generating function for $\widetilde{B}(n)$? Multiplying by $z^n/n!$ and summing over $n \ge 0$, we obtain the following egf for $\widetilde{B}(n)$

$$\widetilde{B}(z) = \sum_{n\ge 0}\sum_{j\ge 0} \frac{z^n j^n}{2^{j+1} n!} = \sum_{j\ge 0}\frac{1}{2^{j+1}}\sum_{n\ge 0}\frac{(jz)^n}{n!} = \sum_{j\ge 0}\frac{e^{jz}}{2^{j+1}} = \frac{1}{2}\left(\frac{1}{1-e^z/2}\right) = \frac{1}{2-e^z}.$$

Though the idea of studying the smallest singularity works for a large class of geneerating functions, it fails when the function has no singularity, that is the function is entire on the whole complex plane; for example, the egf for the ordinary Bell numbers e^{e^z-1}. How do we derive asymptotics in this scenario? In this case, we will see an approach due to Hayman, generalized the basic bound we obtain on the coefficient using the Cauchy's integral formula:

$$a_n = \frac{1}{2\pi i}\int_\gamma \frac{f(z)}{z^{n+1}}dz,$$

where γ is some contour around the origin contained in the region of analyticity of the function.

4 Asymptotics for Entire Functions

Consider the egf for the Bell numbers e^{e^z-1}. There are no singularities for this function and it is holomorphic everywhere in the plane, or in other words, an **entire function**. How do we find asymptotics for the Bell numbers B_n? One can in fact start with the simpler functions $(1+z)^{2n}$ and e^z, which are again entire functions, and ask the asunptotics for their coefficients. The method of singularities doesn't work in this setting. What can we do?

We start with an explicit expression for the coefficients of a power series: Cauchy's integral formula states that if $f(z) = \sum_n a_n z^n$ is an analytic function then

$$a_n = \frac{1}{2\pi i}\oint_\gamma \frac{f(z)}{z^{n+1}}dz,$$

where γ is a closed simple path contained in the domain of analyticity of f that encircles around the origin. Since we treat f to be anlaytic if it has a convergent power series expansion, the result above follows with a combination of the following fundamental integral over the boundary of a disc and the claim that the integral doesn't change under deformation of paths from γ to the boundary of the disc.

Claim:

$$\oint_{\partial D(0,r)} z^n = \begin{cases} 0 & \text{if } n \neq -1 \\ 2\pi i & \text{if } n = -1. \end{cases} \tag{4}$$

Note that the integral is independent of the choice of r.

Let's see how we can use Cauchy's formula to get an estimate for $n!$: Taking absolute values, we get that

$$\frac{1}{n!} \leq \frac{1}{2\pi}\max_{z\in D(0,r)} \frac{|e^z|}{r^{n+1}}\cdot(2\pi r) = \frac{e^r}{r^n}. \tag{5}$$

We want to choose a disc that minimizes the RHS. This is precisely attained at $r = n$, which yields

$$\frac{1}{n!} \leq \frac{e^n}{n^n}$$

a not-so-bad estimate compared to Stirling's estimate.

4.1 Landscape of holomorphic functions

Saddle points. Maximum modulus principle. Fundamental theorem of algebra.

4.2 Stirling's approximation: A case study

Stirling's approximation is that $n! \sim (n/e)^n\sqrt{2\pi n}$. How do we go from the bound above to a tighter estimate? The quantity $\sqrt{2\pi}$ suggests something to do with the Gaussian integral $\int_{-\infty}^{\infty} e^{\frac{-x^2}{2}}\mathrm{dx}$. The problem with our approach in deriving the bound in (5) is that we have taken the maximum growth of the exponential along the real axis and applied that upper bound on the whole contour. Note that the growth of the exponential drops pretty fast along the imaginary axis (since it's periodic in that direction). Therefore, this suggests that not only we should choose our contour carefully, namely, crossing at the point where the supremum of the function is the least, that is a saddle point, but also expanding the contour integral of the absolute value in a carefully chosen neighbourhood around the saddle point, which would capture the dominating behavior. This is what we do next.

We first express the integral in the polar coordinates: $z = re^{i\theta}$, in which case $\mathrm{d}z = \mathrm{i}re^{\mathrm{i}\theta}\mathrm{d}\theta$. Since the saddle point is at $r = n$, substituting $r = n$, we obtain,

$$a_n = \frac{1}{2\pi}\left(\frac{e}{n}\right)^n \int_{-\pi}^{\pi} e^{n(e^{i\theta}-1-i\theta)}\mathrm{d}\theta.$$

The integral on the RHS will be broken into two portions

$$C := \int_{-\theta_0}^{\theta_0} e^{n(e^{i\theta}-1-i\theta)}\mathrm{d}\theta$$

and

$$T := \int_{\theta_0}^{2\pi-\theta_0} e^{n(e^{i\theta}-1-i\theta)}\mathrm{d}\theta$$

for some appropriate choice of θ_0 such that the following holds:

1. First, **Central Approximation**: $e^{ng(\theta)}$ is well approximated by a simple function like e^{-nx^2}, and
2. Second, **Tails Pruning**: $|T| = o(C)$.

The third step is **Tails completion** by approximating the definite integral C with the Gaussian integral $\int_{-\infty}^{\infty} e^{-x^2/2}dx$.

We start with the getting a central approximation. Let $g(\theta) := e^{i\theta} - 1 - i\theta$. Then for small values of θ we have

$$\begin{aligned} e^{ng(\theta)} &= e^{n(\cos\theta-1)+in(\sin\theta-\theta)} \\ &= e^{n(\cos\theta-1)}e^{in(\sin\theta-\theta)} \\ &\sim e^{-n\theta^2/2}e^{-in\theta^3/6} \\ &= e^{-n\theta^2/2}\left(\cos\left(n\theta^3/6\right) - i\sin\left(n\theta^3/6\right)\right). \end{aligned}$$

where $\theta \in [-\theta_0, \theta_0]$. For θ small, the real part of the function above dominates the imaginary part. Therefore, $e^{ng(\theta)} \sim e^{-n\theta^2/2}(1 - O(n\theta^3))$. For the error term to be meaningul, we want $n\theta_0^3 \to 0$ as $n \to \infty$, that is $\theta_0 = o(n^{-1/3})$. If this happens then, we have $e^{ng(\theta)} \sim e^{-n\theta^2/2}$ in the range $[-\theta_0, \theta_0]$. Note that there is no lower bound as of now, and at this stage we could choose $\theta_0 = 0$.

As for pruning the tails, note from above that $|e^{g(\theta)}| = e^{n(\cos\theta-1)}$. The function $(\cos\theta - 1)$ attains its maximum for small values of θ, then drops as θ increases till π and then increases to its initial value. Therefore, in the interval $[\theta_0, 2\pi - \theta_0]$, we have $|T| \le 2\pi\left|e^{ng(\theta_0)}\right| \sim 2\pi e^{-n\theta_0^2/2}$. We will later see that $C = O(1/\sqrt{n})$. So if we want $T = o(C)$, it suffices that $e^{-n\theta_0^2} \to 0$, or $\theta_0 = \omega(n^{-1/2})$.

The two conditions

$$\theta_0 = \omega(n^{-1/2}) \text{ and } \theta_0 = o(n^{-1/3})$$

yield us that $\theta_0 \in (n^{-1/2}, n^{-1/3})$ a convenient choice is $\theta_0 = n^{-2/5}$. With this choice, we have

$$C \sim \int_{-n^{-2/5}}^{n^{-2/5}} e^{-n\theta^2/2}d\theta.$$

Taking $x := \sqrt{n}\theta$ we get that

$$C \sim \frac{1}{\sqrt{n}}\int_{-\sqrt{n}\theta_0}^{\sqrt{n}\theta_0} e^{-x^2/2}dx = \frac{1}{\sqrt{n}}\int_{-n^{1/10}}^{n^{1/10}} e^{-x^2/2}dx.$$

Now

$$\int_{-n^{1/10}}^{n^{1/10}} e^{-x^2/2}dx = \int_{-\infty}^{\infty} e^{-x^2/2}dx - 2\int_{n^{1/10}}^{\infty} e^{-x^2/2}dx.$$

But observe that for any $a > 0$

$$\int_a^{\infty} e^{-x^2/2}dx = \int_0^{\infty} e^{-(x+a)^2/2}dx \leq e^{-a^2/2}\int_0^{\infty} e^{-x^2/2}dx = O(e^{-a^2/2}).$$

Plugging this estimate in the bound above,

$$C \sim \sqrt{\frac{2\pi}{n}}(1 + O(e^{-n^{1/5}})).$$

Let's verify that

$$T = O(e^{-n\theta_0^2/2}) = O(e^{-n^{1/5}}) = o(C)$$

as desired. Hence

$$\frac{1}{n!} \sim \left(\frac{e}{n}\right)^n \sqrt{2\pi n}.$$

5 Unimodality of Sequences

A sequence $\{a_n\}$ is said to be unimodal if there exists an index j such that

$$a_0 \leq a_1 \leq \cdots \leq a_{j-1} \leq a_j \geq a_{j+1} \geq \cdots \geq a_n \geq \cdots .$$

Binomial coefficients $\binom{n}{k}$, $k = 0, \ldots, n$, are a typical example of a unimodal sequence, where the maximum is obtained at $k = \lfloor n/2 \rfloor$. In this section, we see how generating functions can be used to decided unimodality of a sequence.

A stronger notion than unimodality is **log-concavity**: A sequence $\{a_n\}$ is said to be log-concave, if for all $n \geq 1$

$$\log a_n \geq \frac{\log a_{n-1} + \log a_{n+1}}{2},$$

or equivalently $a_n^2 \geq a_{n-1}a_{n+1}$. Unlike unimodality, log-concavity is a "local" condition. Why is it a stronger notion? Because, if a sequence is not unimodal then it is not log-concave as well, since there must be an index j such that $a_{j-1} > a_j < a_{j+1}$, which implies $a_j^2 < a_{j-1}a_{j+1}$. Thus, if we can detect log-concavity then we can show that the sequence is unimodal.

Theorem 2 *If all the roots of the polynomial $f(x) := \sum_{k=0}^n a_k x^k$ are non-positive, then its coefficient sequence is a log-concave sequence.*

Proof. Prove by induction that the coeffecients of $(x + \alpha)f$ are also log-concave, given f is log-concave. The base case $(x + \alpha)$ is trivial, the quadratic case follows from $(a + b)^2 \geq 4ab > ab$. **Q.E.D.**

The proof hints that in fact something stronger holds true:

Theorem 3 (Newton) *If all the roots of the polynomial $f(x) := \sum_{k=0}^n a_k x^k$ are real, then the sequence $(a_j/\binom{n}{j})_{j=0,\ldots,n}$ is (ultra) log-concave sequence.*

Note that

$$(a_j/\binom{n}{j})^2 \geq (a_{j-1}/\binom{n}{j-1})(a_{j+1}/\binom{n}{j+1})$$

is equivalent to

$$a_j^2 \geq a_{j-1}a_{j+1}\left(1 + \frac{1}{n-j}\right)(1 + 1/j)$$

which is stronger than $a_j^2 \geq a_{j-1}a_{j+1}$. Also, observe that the coefficients can be negative. however, that doesn't affect the result: since the sign of a_j doesn't matter in the inequality, the claim states that the inequality holds even when a_{j-1} and a_{j+1} have the same sign (if their signs are opposite then the inequality is trivially true). So, for instance, we will use the claim for polynomials such as $\sum_k a_k(-x)^k$.

Proof. The proof relies on the closure properties of real rootedness under differentiation and inverse, that is, the j-th derivative of f is also real rooted, and so is the polynomial $x^n f(1/x)$. First consider the $(j-1)$th derivative of f and let $g(x)$ be its reciprocal (of degree $(n-j+1)$). Then consider the $(n-j-1)$th derivative of g, that is,

$$\frac{n!}{2}\left(\frac{a_{j-1}}{\binom{n}{j-1}}x^2 + 2\frac{a_j}{\binom{n}{j}} + \frac{a_{j+1}}{\binom{n}{j+1}}\right).$$

This quadratic polynomial is real rooted iff the discriminant is non-negative, i.e.,

$$\left(\frac{a_j}{\binom{n}{j}}\right)^2 \geq \frac{a_{j-1}}{\binom{n}{j-1}}\frac{a_{j+1}}{\binom{n}{j+1}}.$$

Q.E.D.

Binomial coefficients: $\sum_{k=0}^n \binom{n}{k} x^k = (1 + x)^n$ has -1 as a root of multiplicity n.

Sterling number of second kind: $A_n(x) := \sum_{k=0}^{n} \left\{ {n \atop k} \right\} x^k$. Define $A_n(x) := \sum_{k=0}^{n} \left\{ {n \atop k} \right\} x^k$; note the difference from the generating function we had earlier. Using the recurrence relation for $\left\{ {n \atop k} \right\}$ we can show that

$$e^x A_n(x) = x(e^x A_{n-1}(x))'.$$

Assume inductively that the roots of $A_{n-1}(x)$ are all non-positive; then so are the roots of $e^x A_{n-1}(x)$. Now, we want to account for n roots of $A_n(x)$. From Rolle's theorem we know that there are $n-2$ non-positive roots of $(e_x A_{n-1}(x))'$; to these add zero as a root, to get $n-1$ roots. To find the last missing root, we observe that as $x \to -\infty$, $e^x A_{n-1}(x)$ goes to zero; so the derivative $(e_x A_{n-1}(x))'$ must have one more root smaller than all the roots of $e_x A_{n-1}(x)$. Thus we have accounted all the n real non-positive roots of $A_n(x)$. A sequence of polynomials that have this interlacing of their real roots is called a Sturm sequence.

5.1 Unimodality of the Matching Polynomial – Heilmann-Lieb'72

Given an undirected graph G over n vertices, let m_k denote the number of matchings of G with exactly k edges. So m_1 is the number of edges, $m_{n/2}$ the number of perfect matchings (if n is even), and so on. Is the sequence m_k unimodal? In particular, consider the **matching polynomial**

$$\mu_G(x) := \sum_{k=0}^{n/2} m_k (-1)^k x^{n-2k}. \tag{6}$$

It was shown by HL that the polynomial is indeed real rooted. The proof relies on the following observation that a vertex v either doesn't contribute to m_k in G (so it can be deleted) or it contributes exactly one edge (in which case the remaining $(k-1)$ edges come from $G \setminus u, v$. More precisely, we have

$$m_k(G) = m_k(G \setminus v) + \sum_{u \in N(v)} m_k(G \setminus u, v).$$

Multiplying by $(-1)^k x^{n-2k}$ and summing over k we get

$$\sum_k m_k(G) x^{n-2k} (-1)^k = \sum_k m_k(G \setminus v) x^{n-2k} (-1)^k + \sum_{u \in N(v)} \sum_k m_k(G \setminus u, v) x^{n-2k} (-1)^k.$$

Pulling out x from the first summation on the right side and a (-1) from the second to match the summation indices, along with the observation that $x^{n-2k} = x^{n-2-2(k-1)}$, we get

$$\mu_G(x) = x\mu_{G \setminus v}(x) - \sum_{u \in N(v)} \mu_{G \setminus u,v}(x).$$

The proof shows that the subgraphs of G form a Sturm sequence (or interlacing family) of simple real roots. Let's first assume that G is a complete graph. We will show the real rootedness in this case. Then we will put a weight $1/K$ on non-edges and consider the sequence of graphs G_K, as K increases. In the limit G_K approach G coefficient wise and so the real-rootedness should be preserved.

Let $\lambda_{n-1} < \lambda_{n-2} < \cdots < \lambda_1$ be the $(n-1)$ roots of $\mu_{G \setminus v}$. By induction hypothesis roots of $\mu_{G \setminus u,v}$ interlace with these $(n-1)$ roots. At λ_i, the polynomial
$mu_{G \setminus u,v}(\lambda_i)$ has sign $(-1)^{i+1}$. Therefore, $\mu_G(\lambda_i) = (-1)^i$. This accounts for $n-2$ roots in each of the open intervals $(-\lambda_{i+1}, \lambda_i)$, $i = 1, \ldots, n-1$. In particular, at λ_1 the poly $\mu_G(\lambda_1) < 0$ but as $x \to \infty$ it is positive since it is monic. Therefore, there is a $\lambda_0 > \lambda_1$ that is a root of $\mu_G(x)$. Similarly, at λ_{n-1} the sign of $\mu_G(x)$ is $(-1)^{n+1}$, which has the opposite parity of x^n as $x \to -\infty$. Therefore, there must be a root $\lambda_n < \lambda_{n-1}$. Thus we have accounted for all the n roots of $\mu_G(x)$.