More on generating functions

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1 Generating functions

Recall that the (ordinary) *generating function* of a sequence $a_0, a_1, a_2, \ldots$ is the function defined by the series

$$A(x) = \sum_{n=0}^{\infty} a_n x^n.$$

Typically, we are interested in this function in case that a_n is the number of certain combinatorial objects/structures/... of size n (with n points/vertices/...). This representation is convenient, because:

- Many operations on these objects (such as disjoint union, selection of a single vertex, ...) transform the sequence in a way that corresponds to a simple arithmetic operation on the generating function.
- Consequently, if the objects are obtained by a composition of such operation, we can easily obtain the corresponding generating function.
- Once we have the generating function, we can sometimes use it to obtain an exact formula for its coefficient.
- Perhaps even more importantly, using the tools from mathematical analysis, we can estimate the speed of the growth of the elements of the sequence, thus getting (often arbitrarily precise) approximations for the number of objects of certain size.

For example:

- For $B(x) = \sum_{n=0}^{\infty} b_n x^n$, we have

$$A(x)B(x) = \sum_{n=0}^{\infty} \Big(\sum_{i=0}^{n} a_i b_{n-i} \Big) x^n,$$

and thus $A(x)B(x)$ is the generating function of the sequence whose n-th element is $\sum_{i=0}^{n} a_i b_{n-i}$; combinatorially, this is the number of ways how to combine two types of objects—one represented by A, the other one by B—to a single object of size B.

- $A(x) + B(x)$ has coefficients $a_n + b_n$, which count the number of objects that can be of two types, one represented by A and the other represented by B.

Example 1. *For $n \geq 0$, let s_n denote the number of strings of length n consisting of digits 1, 2, and 3, and not containing consecutive digits 1. Let $S(x) = \sum_{n=1}^{\infty} s_n x^n$ be the generating function of this sequence. Such a string is empty or consists of just 1 (generating function $1 + x$, corresponding to one object of size 0 and one object of size 1), or is the composition of one of '2', '3', '12', '13' (generating function $2x + 2x^2$) with another such string (generating function S). Hence, we get*

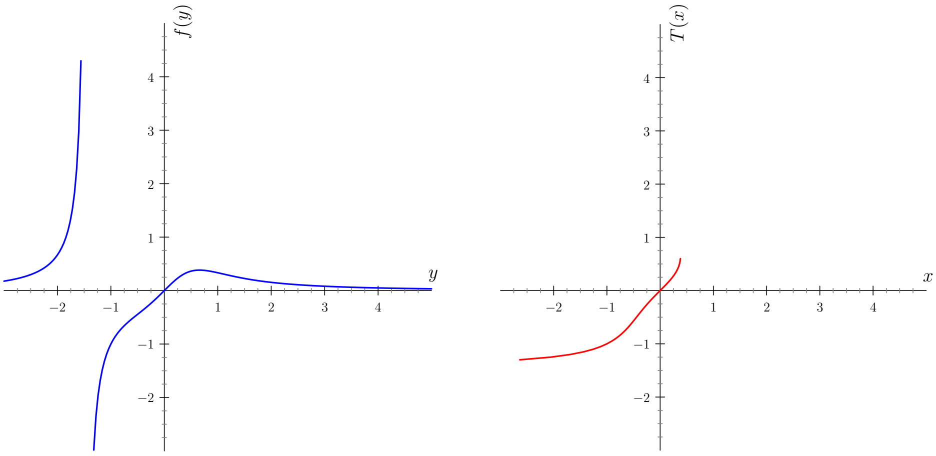
$$S = 1 + x + (2x + 2x^2)S$$
$$S = \frac{1+x}{1-2x-2x^2}$$

We could now obtain an exact formula for the coefficients of the power series expansion of S, and thus express s_n exactly.

Example 2. *For $n \geq 1$, let T_n denote the number of rooted trees with n vertices such that every non-leaf vertex has 2 or 3 children, and let $T(x) = \sum_{n=1}^{\infty} t_n x^n$ be the generating function of this sequence. Each such tree is either a single vertex, or a single vertex combined with two trees represented by T, or a single vertex combined with three trees represented by T. The generating function of a single vertex is x (there is just one such object of size 1), and thus*

$$T = x + xT^2 + xT^3$$
$$x = \frac{T}{1+T^2+T^3}$$

Hence, writing $f(y) = \frac{y}{1+y^2+y^3}$, we have $T = f^{-1}$. The graphs of the functions f and T are as follows:



It is not easy to see how to turn the expression for T (the inverse to some rational function) to an exact formula for t_n; we will see a way to do it later. We will also be able to use the generating function to approximate t_n.

Before we show how we can analyze the behavior of the coefficients, let us remark that in some circumstances, it may be useful to consider different kinds of generating functions. The most common are exponential generating functions; the *exponential generating functions* of a sequence $a_0, a_1, \dots$ is defined as the power series

$$A(x) = \sum_{n=0}^{\infty} a_n \frac{x^n}{n!}.$$

The operations with different kinds of generating functions have different semantics. For example, if

$$B(x) = \sum_{n=0}^{\infty} b_n \frac{x^n}{n!}$$

is the exponential generating function of another series $b_0, b_1, \dots$, then

$$A(x)B(x) = \sum_{n=0}^{\infty} \Big(\sum_{i=0}^{n} \frac{a_i b_{n-i}}{i!(n-i)!} \Big) x^n = \sum_{n=0}^{\infty} \Big(\sum_{i=0}^{n} \binom{n}{i} a_i b_{n-i} \Big) \frac{x^n}{n!}$$

is the exponential generating function of the series whose n-th element

$$\sum_{i=0}^{n} \binom{n}{i} a_i b_{n-i}$$

counts the number of ways how, among n points, select i and put an object represented by A on the selected points, and put an object represented by B on the remaining $n-i$ points (in contrast with ordinary generating functions, where we are putting the object next to one another).

Example 3. *Let s_n denote the number of spanning trees of K_n with one vertex selected as a root, and let $S(x) = \sum_{n\ge 0} s_n \frac{x^n}{n!}$ be the corresponding exponential generating function. We can obtain a spanning tree of K_n by partitioning $\{1,\ldots,n-1\}$ into a single-vertex part (exponential generating function x) and any number k of other parts containing a rooted spanning tree, and joining the selected single vertex by edges to the roots of the spanning trees of the parts. By the interpretation of the product of exponential generating functions, the coefficient at x^n in xS^k is the number of such choices where the order of the parts matters (we specify which part is the first one, the second one, ...). To compensate for this overcounting, we need to divide by $k!$. Hence, we have*

$$S(x) = \sum_{k=0}^{\infty} x\frac{S^k}{k!} = xe^{S(x)}.$$

Similarly to Example 2, we conclude that S is the inverse to the function $\frac{y}{e^y}$.

2 Asymptotic behavior of coefficients

The *radius of convergence* of a power series $\sum_{n=0}^{\infty} a_n x^n$ is

$$R = \sup\{c > 0 : |a_n| \le (1/c)^n \text{ for all but finitely many } n\}.$$

Lemma 4. *Let $A = \sum_{n=0}^{\infty} a_n x^n$ be a power series with radius of convergence R. Then*

- *A diverges for every $x \in \mathbb{C}$ such that $|x| > R$, and*
- *A converges for every $x \in \mathbb{C}$ such that $|x| < R$.*

Proof. A necessary condition for a series to converge is that the limit of its terms is 0. However, by the definition of the radius of convergence, if $|x| > R$, then there exist infinitely many n such that $|a_n| \ge (1/|x|)^n$, and thus $|a_n x^n| \ge 1$. Hence, A diverges at x.

If $|x| < R$, then choose y such that $|x| < y < R$. By the definition of the radius of convergence, there exists n_0 such that for every $n \ge n_0$, we have

$|a_n| < (1/y)^n$. Hence, for $m \geq n_0$, we have

$$\begin{aligned}\Bigl|\sum_{n=m}^{\infty} a_n x^n\Bigr| &\leq \sum_{n=m}^{\infty} |a_n| \cdot |x|^n = \sum_{n=m}^{\infty} |a_n| y^n (|x|/y)^n \\ &\leq \sum_{n=m}^{\infty} (|x|/y)^n = \tfrac{1}{1-|x|/y} \cdot (|x|/y)^m.\end{aligned}$$

Since $|x|/y < 1$, we have

$$\lim_{m\to\infty} \sum_{n=m}^{\infty} a_n x^n = 0,$$

and thus the series A converges at x. □

Hence, considering the function $A(x)$ defined as the sum of the power series at any point $x \in \mathbb{C}$ where the series converges, we conclude that $A(x)$ is defined everywhere in the open circle $|x| < R$ and undefined outside of the closure of this circle, with no information about the behavior for $|x| = R$. Actually, the following is true.

Lemma 5. *Let* $A = \sum_{n=0}^{\infty} a_n x^n$ *be a power series with radius of convergence* R *such that* $0 < R < \infty$. *Then there exists* $x \in \mathbb{C}$ *such that* $|x| = R$ *and* A *diverges at* x. *Moreover, if* $a_n \geq 0$ *for all* n, *this is the case for* $x = R$.

The proof of this Lemma requires some (elementary) knowledge from complex analysis and we will skip it (we do not actually need this result). However, as a way of motivation, let us remark that already this gives us some useful knowledge about the rate of the growth of the coefficients. Suppose $A(x)$ is a generating function of some combinatorial objects, and thus its coefficients are nonnegative. Then the radius of convergence of A is the smallest R such that $A(R)$ is not defined, and by Lemma 4, we have $a_n \leq \left(\frac{1}{R-\varepsilon}\right)^n$ for every $\varepsilon > 0$ smaller than R and for every sufficiently large n (and also, this is the best possible bound of such form).

Example 6. *Consider the generating function* $S(x)$ *from Example 1. This function is defined everywhere except for the points* $x_{1,2} = \frac{-1\pm\sqrt{3}}{2}$ *where the denominator is* 0. *Therefore, the radius of convergence of the series is* $R = \frac{-1+\sqrt{3}}{2}$, *and since* $1/R < 2.7321$, *we conclude that* $s_n = O(2.7321^n)$.

Example 7. *Let us now consider the generating function* $T(x)$ *from Example 2. From the graphs, we see that the point where the function stops to be* *defined (and thus also the radius of convergence of T) is $R = f(y_0)$, where y_0 is the point where $f'(y_0) = 0$, that is*

$$\begin{aligned}
0 = f'(y_0) &= \frac{1}{1+y_0^2+y_0^3} - \frac{y_0(2y_0+3y_0^2)}{(1+y_0^2+y_0^3)^2}\\
0 &= 2y_0^3 + y_0^2 - 1\\
y_0 &\approx 0.657\\
R = f(y_0) &=\approx 0.383
\end{aligned}$$

Since $1/R < 2.62$, we have $t_n = O(2.62^n)$.

Exercise 8. *Perform a similar analysis for the generating function from Example 3 and show that the number of spanning trees of K_n is $O((e+\varepsilon)^n n!)$ for every $\varepsilon > 0$.*

We now describe how to improve on the bound from Example 6. Suppose $B(x) = \sum_{n\ge 0} b_n x^n$ is a power series with the same radius R of convergence as A such that

- B is some simple function, and thus we know the sequence $b_0, b_1, \ldots$ exactly, and
- B diverges at the circle of convergence in the same way as A, in the sense that the radius R' of convergence of $A - B$ is larger than R.

Then the coefficients of A and B have the same asymptotic behavior—they differ by $O(1/(R'-\varepsilon)^n)$ for any $\varepsilon > 0$ smaller than R', while the coefficients of B are roughly $1/R^n$.

Example 9. *Consider again the generating function $S(x)$ from Example 1, and recall that $x_1 = \frac{-1+\sqrt{3}}{2}$ and $x_2 = \frac{-1-\sqrt{3}}{2}$ are the points where $S(x)$ is not defined. Note that $S(x) = \frac{1}{x_1-x}\cdot\frac{1+x}{2(x-x_2)}$, and let $q(x) = \frac{1+x}{2(x_2-x)}$. We have $q(x_1) = \frac{3+\sqrt{3}}{12}$. Let $B(x) = q(x_1)/(x_1-x)$, so that*

$$\lim_{x\to x_1} S(x) - B(x) = \lim_{x\to x_1} \frac{q(x)-q(x_1)}{x_1-x} = -q'(x_1).$$

Therefore, the function $S(x) - B(x)$ is defined at x_1, and clearly also at all points other than x_2. Consequently, $S(x) - B(x)$ has radius of convergence $|x_2| = \frac{1+\sqrt{3}}{2}$.

Moreover,

$$B(x) = q(x_1)/(x_1-x) = \frac{q(x_1)/x_1}{1-x/x_1} = \sum_{n=0}^{\infty} \frac{q(x_1)/x_1}{x_1^n} x^n.$$

Since $1/x_1 = \sqrt{3}+1$, *we conclude that for any* $\varepsilon > 0$, *we have*

$$s_n = \frac{3+\sqrt{3}}{12} \cdot (\sqrt{3}+1)^{n+1} + O\big((2/(1+\sqrt{3})+\varepsilon)^n\big).$$

Similarly, we can deal with the singularity of $T(x)$ from Example 2 to obtain an exact asymptotics for t_n; however, this is a bit more involved and we will not go into the details. Instead, let us use another result from analysis to get a convenient formula for the coefficients of T.

3 Lagrange inversion formula

Lagrange inversion formula is a powerful result that enables us to deal with generating functions of the form arising in Example 2. Let us first state a more general version, which is easier to prove by induction.

Lemma 10. *Let* $F(x) = \sum_{n=0}^{\infty} f_n x^n$, $H(x) = \sum_{n=0}^{\infty} h_n x^n$, *and* $A(x) = \sum_{n=0}^{\infty} a_n x^n$ *be power series such that* $A(x) = xF(A(x))$. *Then*

$$[x^n]H(A(x)) = \frac{1}{n}[x^{n-1}]H'(x)F^n(x)$$

holds for every $n \geq 1$.

Proof. Note that $a_0 = 0$, since $A(x) = xF(A(x))$. We prove the claim by induction on n. We have

$$\begin{aligned}
[x^n]H(A(x)) &= [x^n]\sum_{k=0}^{\infty} h_k A^k(x) = [x^n]\sum_{k=0}^{\infty} h_k x^k F^k(A(x)) \\
&= \sum_{k=0}^{\infty} h_k [x^{n-k}]F^k(A(x)) \\
&= h_n f_0^k + \sum_{k=1}^{n-1} h_k [x^{n-k}]F^k(A(x)),
\end{aligned}$$

where the last inequality holds since

- when $k = 0$, we have $[x^{n-k}]F^k(A(x)) = [x^n]1 = 0$ (recall that $n \geq 1$),
- when $k = n$, we have $[x^{n-k}]F^k(A(x)) = [x^0]F^k(A(x)) = f_0^k$, since $a_0 = 0$, and
- when $k > n$, we trivially have $[x^{n-k}]F^k(A(x)) = 0$.

For each $k \in \{1, \dots, n-1\}$, let $G_k(x) = F^k(x)$. By the induction hypothesis (with G_k playing the role of H), we have

$$\begin{aligned}
[x^{n-k}]F^k(A(x)) = [x^{n-k}]G_k(A(x)) &= \frac{1}{n-k}[x^{n-k-1}]G_k'(x)F^{n-k}(x) \\
&= \frac{1}{n-k}[x^{n-k-1}]\big(F^k(x)\big)'F^{n-k}(x) = \frac{1}{n-k}[x^{n-k-1}]kF^{k-1}(x)F'(x)F^{n-k}(x) \\
&= \frac{k}{n-k}[x^{n-k-1}]F'(x)F^{n-1}(x) = \frac{k}{n-k}[x^{n-k-1}]\frac{1}{n}\big(F^n(x)\big)' \\
&= \frac{k}{n(n-k)}[x^{n-k-1}]\big(F^n(x)\big)' = \frac{k}{n(n-k)} \cdot (n-k)[x^{n-k}]F^n(x) \\
&= \frac{k}{n}[x^{n-k}]F^n(x).
\end{aligned}$$

Therefore,

$$\begin{aligned}
[x^n]H(A(x)) &= h_n f_0^k + \sum_{k=1}^{n-1} \frac{kh_k}{n}[x^{n-k}]F^n(x) \\
&= \sum_{k=1}^{n} \frac{kh_k}{n}[x^{n-k}]F^n(x) \\
&= \frac{1}{n}[x^{n-1}]\Big(\sum_{k=1}^{\infty} kh_k x^{k-1}\Big)F^n(x) \\
&= \frac{1}{n}[x^{n-1}]H'(x)F^n(x).
\end{aligned}$$

□

As a special case, when $H(x) = x$, we get the following corollary, which we actually need.

Corollary 11. *Let $F(x) = \sum_{n=0}^{\infty} f_n x^n$ and $A(x) = \sum_{n=0}^{\infty} a_n x^n$ be power series such that $A(x) = xF(A(x))$. Then*

$$a_n = \frac{1}{n}[x^{n-1}]F^n(x)$$

holds for every $n \geq 1$.

Let us note that the proof that we presented is a bit careless, ignoring concerns such as for which x are the considered functions defined. This can be fixed by defining all the operations that we performed purely formally, as operations on the sequences of coefficients in the power series.

Example 12. *In Example 2, we have* $T = x(1 + T^2 + T^3)$*, and thus we can apply Corollary 11 with* $F = 1 + x^2 + x^3$*. Consequently,*

$$t_n = \frac{1}{n}[x^{n-1}](1 + x^2 + x^3)^n = \frac{1}{n} \sum_{a,b \in \mathbb{Z}_0^+, 2a+3b=n-1} \binom{n}{n-a-b, a, b}.$$

Example 13. *Let us now apply Lagrange inversion formula to the generating function from Example 3; we have*

$$\frac{s_n}{n!} = [x^n]S(x) = \frac{1}{n}[x^{n-1}]e^{xn} = \frac{1}{n} \cdot \frac{n^{n-1}}{(n-1)!},$$

and thus $s_n = n^{n-1}$*. Hence,* K_n *has* n^{n-1} *rooted spanning trees, and since we can select the root in* n *ways,* K_n *has* n^{n-2} *spanning trees.*