Generating Functions

Franklin

Outline

Section 1

Overview

Introduction

Suppose we have a sequence $a_0, a_1, a_2, \ldots$.

The **generating function** for this sequence is

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots ,$$

a polynomial or power series whose coefficients are the elements of the sequence.

Generating functions enable us to use manipulations to learn more about the sequence.

Examples

$1, 6, 15, 20, 15, 6, 1$	$1 + 6x + 15x^2 + 20x^3 + 15x^4 + 6x^5 + x^6 = (1+x)^6$
$1, 1, 1, 1, \ldots$	$1 + x + x^2 + x^3 + \cdots = \frac{1}{1-x}$
$0, 1, 1, 2, 3, 5, 8, 13, \ldots$	$x + x^2 + 2x^3 + 3x^4 + 5x^5 + 8x^6 + 13x^7 + \cdots$

Size

Often, the terms x^k of a generating function correspond to something of *size k*.

Consider the generating function from the Binomial Theorem:

$$\binom{n}{0} + \binom{n}{1}x + \binom{n}{2}x^2 + \cdots + \binom{n}{n}x^n = (1+x)^n.$$

The x^k term has coefficient $\binom{n}{k}$. Given a set with n elements, this coefficient is the number of ways to choose a subset of size k.

Section 2

Counting

Coin Tosses

Q: Flip 4 coins. How many ways are there to get 2 heads?

The answer is $\binom{4}{2} = 6$, but let's see how generating functions can be used.

Consider a single coin – it either gives us 1 tail (no heads), or 1 head. There's only one way each of these can occur, so the generating function for a single coin is $1 \cdot x^0 + 1 \cdot x^1 = 1 + x$.

Here x represents a head – the coefficient of x^1 is the number of ways to get 1 head with a single coin. The "size" in this problem is the total number of heads – the x^k term will correspond to getting k heads.

Combining Generating Functions

Now let's combine 2 coins by multiplying their generating functions:

$$(1+x)(1+x) = 1 \cdot 1 + 1 \cdot x + x \cdot 1 + x \cdot x = 1 + 2x + x^2.$$

What does multiplying mean here?

- $1 \cdot 1 = x^0$ corresponds to TT (no heads)
- $1 \cdot x = x^1$ corresponds to TH (1 head)
- $x \cdot 1 = x^1$ corresponds to HT (1 head)
- $x \cdot x = x^2$ corresponds to HH (2 heads)

Each way to get k heads contributes a term of x^k to the product. So the coefficient of x^k in the product is the total number of ways to get k heads!

For 2 coins, there are 2 ways to get 1 head (coefficient of x in $1 + 2x + x^2$).

More Coins

If we have 4 coins, simply multiply the generating functions for each:

$$(1+x)(1+x)(1+x)(1+x) = (1+x)^4 = 1 + 4x + 6x^2 + 4x^3 + 1.$$

The coefficient of x^2 (6) is our answer – the number of ways to get 2 heads.

More generally, if we flip n coins, the number of ways to get k heads is the coefficient of x^k in $(1+x)^n$, which is $\binom{n}{k}$.

Changemaking

Q: How many ways can we make a dollar with (unlimited) pennies, nickels, and dimes?

The generating function for the amounts we can make in pennies is

$$1 + x + x^2 + x^3 + \cdots .$$

Here our "size" is the total money – the coefficient of x^k is the number of ways to make k cents.

For pennies, the coefficients are all 1, because we can make k cents in exactly one way: use k pennies.

Changemaking

For nickels and dimes, the generating functions are

$$1 + x^5 + x^{10} + \cdots, \qquad 1 + x^{10} + x^{20} + \cdots.$$

Putting it all together, our generating function using pennies, nickels, and dimes is

$$\begin{aligned} F(x) &= (1 + x + x^2 + \cdots)(1 + x^5 + x^{10} + \cdots)(1 + x^{10} + x^{20} + \cdots) \\ &= \frac{1}{1-x} \cdot \frac{1}{1-x^5} \cdot \frac{1}{1-x^{10}}. \end{aligned}$$

The answer for making a dollar is the coefficient of x^{100}. This is nontrivial to find, but there are ways [Gas14], which we won't go into here.

Biased Coin Tosses

Q: There are n coins $C_1, C_2, \ldots, C_n$. For each k, coin C_k is biased so that, when tossed, it has probability $\frac{1}{(2k+1)}$ of falling heads. If the n coins are tossed, what is the probability that the number of heads is odd? (Putnam 2001)

Consider coin C_1. It has a $\frac{1}{3}$ chance of being heads, and a $\frac{2}{3}$ chance of being tails.

The "size" in this problem is the total number of heads. For coin C_1, we can write the *probability* generating function $f_1(x) = \frac{1}{3}x + \frac{2}{3}$.

In other words, C_1 has a $\frac{1}{3}$ chance of contributing 1 to the total number of heads, and a $\frac{2}{3}$ chance of contributing 0.

Combining the Coins

The generating function for coin C_k is $f_k(x) = \frac{1}{2k+1}x + \frac{2k}{2k+1}$.

Then the probability generating function for all coins is the product of the individual generating functions for each coin:

$$F_n(x) = \left(\frac{1}{3}x + \frac{2}{3}\right)\left(\frac{1}{5}x + \frac{4}{5}\right)\cdots\left(\frac{1}{2n+1}x + \frac{2n}{2n+1}\right).$$

Given k, this product produces an x^k term for every possible way to choose k factors to take an x term from, corresponding to choosing k coins to land heads. The probabilities for each coin are multiplied, producing the probability that k specific coins land on heads.

The overall coefficient of x^k is then the sum of all these probabilities over all combinations of k heads. This is the probability of getting k heads!

The Generating Function

We have

$$\begin{aligned} F_n(x) &= \left(\frac{1}{3}x + \frac{2}{3}\right)\left(\frac{1}{5}x + \frac{4}{5}\right)\cdots\left(\frac{1}{2n+1}x + \frac{2n}{2n+1}\right) \\ &= \frac{(x+2)(x+4)\cdots(x+2n)}{3\cdot 5\cdots(2n+1)} \\ &= p_0 + p_1x + p_2x^2 + \cdots + p_nx^n, \end{aligned}$$

where p_k is the probability of getting k heads.

Expanding the generating function and finding each coefficient is difficult. But we actually only want the probability that the total number of heads is odd:

$$p_1 + p_3 + p_5 + \cdots .$$

The Generating Function

A generating function is still a function of a variable. So what happens if we plug things in?

If we plug in $x = 1$, we get

$$F_n(1) = p_0 + p_1 + p_2 + \cdots + p_n = \frac{(1+2)(1+4)\cdots(1+2n)}{3 \cdot 5 \cdots (2n+1)} = 1.$$

That seems useful, but we only want the sum of every other coefficient. Let's try $x = -1$:

$$\begin{aligned} F_n(-1) &= p_0 - p_1 + p_2 - \cdots \pm p_n \\ &= \frac{(-1+2)(-1+4)\cdots(-1+2n)}{3 \cdot 5 \cdots (2n-1)(2n+1)} = \frac{1}{2n+1}. \end{aligned}$$

Filtering Oddities

We have the sum and alternating sum of the coefficients. Subtracting them will cancel the terms we don't want:

$$\begin{aligned} F_n(1) - F_n(-1) &= 2p_1 + 2p_3 + 2p_5 + \cdots \\ &= 1 - \frac{1}{2n+1} = \frac{2n}{2n+1}. \end{aligned}$$

So $p_1 + p_3 + p_5 + \cdots = \frac{n}{2n+1}$. That's our answer – the probability of getting an odd number of heads upon rolling the coins $C_1, \ldots, C_n$.

Roots of Unity Filter

Plugging in 1 and -1 is a common way to filter out every 2nd term.

This technique can be extended to filter out every kth term, by plugging in the kth roots of unity (complex solutions to $x^k = 1$).

If you're interested, I highly recommend this 3Blue1Brown video: https://youtu.be/bOXCLR3Wric.

It nicely presents a solution using generating functions and the roots of unity filter to the following problem:

> *Find the number of subsets of* $\{1, 2, 3, 4, 5, \ldots, 2000\}$, *the sum of whose elements is divisible by 5.*

Section 3

Binary Trees

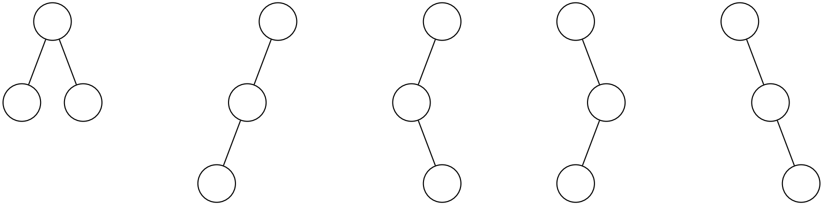
Subsection 1

Enumeration

Enumerating Binary Trees

Q: How many different binary trees have n nodes? [SF96]

- For $n = 0$, there is 1 tree – the empty tree
- For $n = 1$, there is 1 tree – a single node
- For $n = 2$, there are 2 trees – a node with a left child, or a node with a right child
- For $n = 3$, there are 5 trees:



The Generating Function

Let $\mathcal{T}$ be the set of all binary trees. Given a tree $t \in \mathcal{T}$, let $|t|$ be the number of nodes in t. We want the number of trees in $\mathcal{T}$ with n nodes (trees of "size" n).

Consider the generating function

$$T(x) = \sum_{t \in \mathcal{T}} x^{|t|}.$$

In other words, each tree contributes a single term to the sum, which is determined by the number of nodes in that tree.

For example, the 3-node trees on the previous slide would each contribute an x^3 term to $T(x)$. Since there are exactly 5 trees with 3 nodes, the coefficient of x^3 in $T(x)$ is $5x^3$.

The Generating Function

So we have the generating function

$$T(x) = \sum_{t \in \mathcal{T}} x^{|t|} = 1 + x + 2x^2 + 5x^3 + \cdots = \sum_{n \geq 0} T_n x^n.$$

The coefficients T_n represent the number of binary trees with n nodes. We want to find an expression for T_n.

To use this generating function, we exploit the recursive structure of binary trees.

Recursive Structure

A binary tree t is either:

- Empty with 0 nodes, or
- A single node with a left subtree t_L and a right subtree t_R (binary trees) – with $1 + |t_L| + |t_R|$ nodes total
  - In this case, each tree t uniquely corresponds to a pair of trees (t_L, t_R)

Using this, we can write our generating function as follows:

$$T(x) = \sum_{t \in \mathcal{T}} x^{|t|} = 1 + \sum_{t_L \in \mathcal{T}} \sum_{t_R \in \mathcal{T}} x^{|t_L| + |t_R| + 1}$$

A Functional Equation

Then,

$$\begin{aligned} T(x) &= 1 + \sum_{t_L \in \mathcal{T}} \sum_{t_R \in \mathcal{T}} x^{|t_L| + |t_R| + 1} \\ &= 1 + x \sum_{t_L \in \mathcal{T}} x^{|t_L|} \sum_{t_R \in \mathcal{T}} x^{|t_R|} \\ &= 1 + xT(x)^2. \end{aligned}$$

Solving for $T(x)$ using the quadratic formula,

$$T(x) = \frac{1 \pm \sqrt{1 - 4x}}{2x}.$$

Since $T(0) = 1$, we take the minus sign.

Binomial Expansion

We need to expand our expression for $T(x)$ to extract coefficients.

According to an extended form of the binomial theorem,

$$(1+y)^{1/2} = 1 + \binom{1/2}{1} y + \binom{1/2}{2} y^2 + \binom{1/2}{3} y^3 + \cdots = \sum_{k=0}^{\infty} \binom{1/2}{k} y^k.$$

where we can generalize the definition of $\binom{n}{k}$ to real n as follows:

$$\binom{n}{k} = \frac{n(n-1)\cdots(n-k+1)}{k!}.$$

Extracting Coefficients

Using this expansion with $y = -4x$,

$$T(x) = \frac{1 - \sqrt{1-4x}}{2x}$$

$$= \frac{1 - \left(1 + \binom{1/2}{1}(-4x) + \binom{1/2}{2}(-4x)^2 + \binom{1/2}{3}(-4x)^3 + \cdots\right)}{2x}$$

After some simplification, we find that the coefficient of x^n is

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

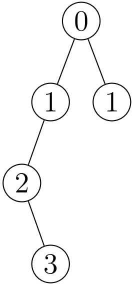
This is the number of binary trees with n nodes! Note: The numbers T_n are called the *Catalan numbers*.

Subsection 2

Path Length

Path Length

Given a binary tree t, its **path length** $\pi(t)$ is the sum of the lengths of the paths from the root to each node in the tree.



For example, this binary tree has path length $0 + 1 + 1 + 2 + 3 = 7$.

If we divide the path length by the number of nodes, we get the average distance from the root to a node in the tree. This is useful for analyzing algorithms that involve searching for nodes in a tree.

Path Length in Random Trees

Q: What is the expected path length of a random binary tree with n nodes? [SF96]

Here, "random" means that each of the T_n binary trees with n nodes has an equal probability of being selected (*random binary Catalan trees*).

- This is often used in compiler design for parse trees for expression evaluation. However, other models of random trees exist.

In other words, over all binary trees with n nodes, what is the average path length?

We'll answer this question using a similar approach to enumerating binary trees.

The Generating Function

Recall that $\mathcal{T}$ is the set of all binary trees.

Define the *cumulative* generating function

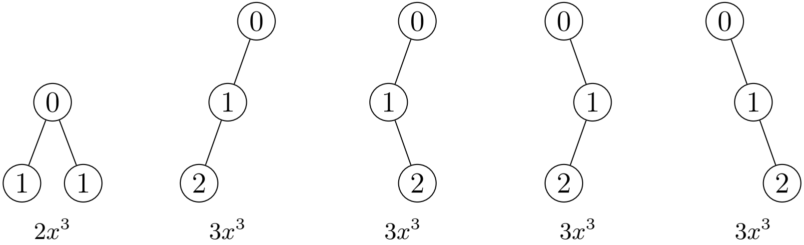
$$C_T(x) = \sum_{t \in \mathcal{T}} \pi(t) x^{|t|} = \sum_{n \geq 0} C_n x^n.$$

In the middle is the generating function written summing tree-by-tree. On the right, all the like terms are collected, and we sum over each term.

The coefficients C_n tell us the total path length over all trees with n nodes.

Example

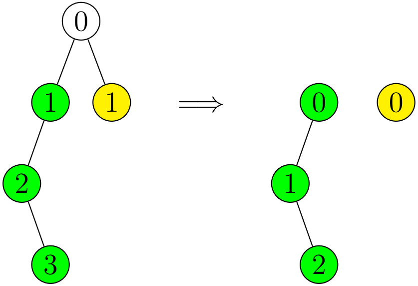
Here are the five 3-node trees from earlier, and their contribution to $C_T(x)$:



The coefficient corresponds to path length; the exponent of x corresponds to the number of nodes.

Recursive Definition of Path Length

Consider the tree t from earlier; its subtrees t_L and t_R are colored.



When t_L is split off from t, the "new root" is one level lower.

So the depths of the nodes in t_L are one less than the depths of the same nodes of in t.

The same is true for t_R.

So $\pi(t) = 0 + \pi(t_L) + |t_L| + \pi(t_R) + |t_R|$.

Using Recursion

Now,

$$\begin{aligned} C_T(x) &= \sum_{t \in \mathcal{T}} \pi(t) x^{|t|} \\ &= \sum_{t_L \in \mathcal{T}} \sum_{t_R \in \mathcal{T}} (\pi(t_L) + \pi(t_R) + |t_L| + |t_R|) x^{|t_L|+|t_R|+1} \end{aligned}$$

Note that there's no constant term $(1 + \cdots)$ since the only tree with 0 nodes (the empty tree) has path length 0, so the coefficient of x^0 is 0.

This expands into 4 parts. The first is

$$\sum_{t_L \in \mathcal{T}} \sum_{t_R \in \mathcal{T}} \pi(t_L) x^{|t_L|+|t_R|+1} = x \sum_{t_L \in \mathcal{T}} \pi(t_L) x^{|t_L|} \sum_{t_R \in \mathcal{T}} x^{|t_R|} = x C_T(x) T(x).$$

Expansion

The second part is similarly

$$\sum_{t_L\in\mathcal{T}}\sum_{t_R\in\mathcal{T}}\pi(t_R)x^{|t_L|+|t_R|+1} = x\sum_{t_L\in\mathcal{T}}x^{|t_L|}\sum_{t_R\in\mathcal{T}}\pi(t_R)x^{|t_R|} = xT(x)C_T(x).$$

The third part is (recall $T(x) = \sum_{t\in\mathcal{T}} x^{|t|}$, so $T'(x) = \sum_{t\in\mathcal{T}} |t|x^{|t|-1}$)

$$\sum_{t_L\in\mathcal{T}}\sum_{t_R\in\mathcal{T}}|t_L|x^{|t_L|+|t_R|+1} = x^2\sum_{t_L\in\mathcal{T}}|t_L|x^{|t_L|-1}\sum_{t_R\in\mathcal{T}}x^{|t_R|} = x^2T'(x)T(x).$$

Similarly, the fourth part is

$$\sum_{t_L\in\mathcal{T}}\sum_{t_R\in\mathcal{T}}|t_R|x^{|t_L|+|t_R|+1} = x^2\sum_{t_L\in\mathcal{T}}x^{|t_L|}\sum_{t_R\in\mathcal{T}}|t_R|x^{|t_R|-1} = x^2T(x)T'(x).$$

The Functional Equation

Putting it all together,

$$\begin{aligned} C_T(x) &= \sum_{t \in \mathcal{T}} \pi(t) x^{|t|} \\ &= \sum_{t_L \in \mathcal{T}} \sum_{t_R \in \mathcal{T}} (\pi(t_L) + \pi(t_R) + |t_L| + |t_R|) x^{|t_L|+|t_R|+1} \\ &= 2x C_T(x) T(x) + 2x^2 T(x) T'(x). \end{aligned}$$

Earlier we found that $T(x) = \dfrac{1 - \sqrt{1-4x}}{2x}$. Solving for $C_T(x)$,

$$C_T(x) = \frac{2x^2 T(x) T'(x)}{1 - 2xT(x)} = \frac{1}{x}\left(\frac{x}{1-4x} - \frac{1-x}{\sqrt{1-4x}} + 1\right).$$

Coefficients

The coefficient of x^n is the total path length over all binary trees with n nodes.

We want the average path length, so we divide the coefficient by the number of trees with n nodes: T_n.

After some messy expansions, the average path length comes out as

$$\frac{(n+1)4^n}{\binom{2n}{n}} - 3n - 1 = n\sqrt{\pi n} - 3n + O(\sqrt{n}).$$

Other Applications of Generating Functions

- General trees, permutations, strings/regular expressions, many other combinatorial structures for analyzing algorithms
- Symbolic method (analytic combinatorics)
  - To get the generating function $T(x)$ for binary trees, we can actually just write this, since a tree is either empty or a node and two subtrees:

$$\mathcal{T} = \{\square\} + \{\bullet\} \times \mathcal{T} \times \mathcal{T} \implies T(x) = 1 + xT(x)^2.$$

- Snake Oil method: evaluate terrible sums like $f_n = \sum_k \binom{n+k}{2k} 2^{n-k}$ by throwing them in as coefficients of a generating function and swapping the order of summation
- Solving recurrences (e.g. finding a formula for Fibonacci numbers)

Questions?

A generating function is a device somewhat similar to a bag. Instead of carrying many little objects detachedly, which could be embarrassing, we put them all in a bag, and then we have only one object to carry, the bag.

— George Polya (1954)

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