The Lagrange Inversion Formula (LIF)

Following Wilf we consider the following functional equation

$$z = x\phi(z) \tag{1}$$

Can we solve for z as an explicit function of x? Can we find a closed formula for the sequence of coefficients, $[x^n]z(x)$? *Note:* The functional equation (1) implies $z(0) = 0$.

Theorem 1. The Lagrange Inversion Formula Suppose that $W(z)$ and $\phi(z)$ are formal power series in z with $\phi(0) = 1$. Then there is a unique formal power series $z = z(x) = \sum_n z_n x^n$, satisfying (1). In addition, the value of $W(z(x))$ when expanded in a power series in x about $x = 0$ satisfies

$$n[x^n]W(z(x)) = [z^{n-1}]\{W'(z)\phi^n(z)\} \tag{2}$$

The simplest version of the theorem occurs when we take $W(z) = z$. In that case, (2) reduces to

$$n[x^n]z(x) = [z^{n-1}]\phi^n(z) \tag{3}$$

At first glance, it may look as if we are trading one problem, coefficient extraction on $W(z(x))$, for another perhaps more difficult task, coefficient extraction on the more complicated expression $W'(z)\phi^n(z)$. However, in practice this is not the case. In fact, we will see that LIF can still be quite useful even when an explicit solution (1) is known.

Our first example is a familiar one. In Math 481 we saw that the Catalan numbers $c_n := |C([n])|$ counted the number of legal strings of n pairs of matching parentheses. For example, $c_3 = 5$ since

$$C([3]) = \{()()(), (())(), ()(()), ((())), (()())\} \tag{4}$$

are the only legal strings with 3 pairs of matching parentheses. If we define $c_0 = 1$ then the first 10 Catalan numbers are

$$1, 1, 2, 5, 14, 42, 132, 429, 1430, 4862, \ldots \tag{5}$$

Now let $C(x) = \sum_n c_n x^n$ be the ordinary power series generating function of the Catalan numbers. We showed that $C(x)$ satisfied the functional equation

$$C(x) = 1 + xC^2(x) \tag{6}$$

This yielded explicit closed form

$$C(x) = \frac{1 - \sqrt{1-4x}}{2x} \tag{7}$$

It takes quite a bit more effort to conclude that

$$c_n = [x^n]C(x) = \frac{1}{n+1}\binom{2n}{n} \tag{8}$$

We now illustrate how to derive (8) using LIF.

Example 2. Let $C(x)$ be as given above. Now let $z = C(x) - 1$ and $\phi(z) = (1+z)^2$. Then $\phi(0) = 1$ and (6) becomes

$$z = C(x) - 1 = xC^2(x) = x\phi(z)$$

Now by (3), we have

$$\begin{aligned}
[x^n]z(x) &= \frac{1}{n}[z^{n-1}](1+z)^{2n} \\
&= \frac{1}{n}[z^{n-1}]\sum_k \binom{2n}{k} z^k \\
&= \frac{1}{n}\binom{2n}{n-1} \\
&= \frac{1}{n+1}\binom{2n}{n}
\end{aligned}$$

and we have recovered an explicit formula for the Catalan numbers with a lot less work. Notice also that in this example, we have an explicit solution to $z = x\phi(z)$, namely

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

The next example illustrates how to use LIF to reprove Binomial Inversion. *Warning:* This is used to illustrate another aspect of LIF only. It is certainly not the preferred proof in this case.

Example 3. Suppose that

$$f_n = \sum_{k=0}^{n} \binom{n}{k} g_k$$

and let $f(x) = \sum_n f_n\, x^n$ and $g(x) = \sum_n g_n\, x^n$. We leave it as an exercise to show that

$$f(x) = \frac{1}{1-x}\, g\left(\frac{x}{1-x}\right) \tag{9}$$

Now let $y = x/(1-x)$. Then $x = y/(1+y)$ and it's easy to see that

$$g(y) = \frac{1}{1+y} f\left(\frac{y}{1+y}\right) \tag{10}$$

It is now a simple matter to mimic the proof of Theorem 2 (Stirling Inversion) to quickly conclude that

$$g_n = \sum_k f_k \binom{n}{k} (-1)^{n-k}$$

Instead we focus on (9) and rewrite the substitution that preceded it as $x = y(1-x)$. In other words,

$$x(y) = y(1-x) = y\phi(x) \tag{11}$$

where $\phi(x) := 1 - x$. Now (10) becomes

$$\begin{aligned} g(y) &= (1 - x(y))f(x(y)) \\ &= f(x(y)) - x(y)f(x(y)) \\ &= \sum_k f_k\, x^k(y) - x(y) \sum_k f_k\, x^k(y) \\ &= \sum_k f_k\, x^k(y) - \sum_k f_k\, x^{k+1}(y) \end{aligned}$$

so that

$$g_n = [y^n]g(y) = \sum_k f_k\, [y^n]x^k(y) - \sum_k f_k\, [y^n]x^{k+1}(y) \tag{12}$$

Evidently we need to compute $[y^n]x^k(y)$ and $[y^n]x^{k+1}(y)$. So now we use (2) with $W(z) = z^k$ and $W(z) = z^{k+1}$, respectively. Thus

$$\begin{aligned} [y^n]x^k(y) &= \frac{1}{n}[x^{n-1}]kx^{k-1}(1-x)^n \\ &= \frac{k}{n}[x^{k-n}] \sum_j \binom{n}{j}(-1)^j x^j \\ &= \frac{k}{n}\binom{n}{n-k}(-1)^{n-k} = \frac{k}{n}\binom{n}{k}(-1)^{n-k} \end{aligned}$$

We leave it as an exercise to show that

$$x^{k+1}(y) = \frac{k+1}{n}\binom{n}{k+1}(-1)^{n-k-1} \tag{13}$$

Returning to (12), we have

$$\begin{aligned} g_n = [y^n]g(y) &= \sum_k f_k\, [y^n]x^{k+1}(y) - \sum_k f_k\, [y^n]x^{k+1}(y) \\ &= \sum_k f_k\, \frac{k}{n}\binom{n}{k}(-1)^{n-k} - \sum_k f_k\, \frac{k+1}{n}\binom{n}{k+1}(-1)^{n-k-1} \\ &= \sum_k f_k \left(\frac{k}{n}\binom{n}{k} + \frac{k+1}{n}\binom{n}{k+1}\right)(-1)^{n-k} \\ &= \sum_k f_k \binom{n}{k}(-1)^{n-k} \end{aligned}$$

as expected. Here the last line follows from Exercise 4 from 02/23.

If $z(x)$ is a formal power series about $x = 0$, we follow the standard convention that $[x^m]z(x) = 0$ whenever $m < 0$.

Proof (of Theorem 1): We proceed by induction on $n \geq 0$. For the base case, both sides of (2) are clearly 0 whenever $n = 0$. Now suppose that (2) is true for $0 < m < n$. As we attempted to illustrate in Example 3, it is enough to show that the following holds for all k.

$$n[x^n]z^k(x) = k[z^{n-1}]\{z^{k-1}\phi^n(z)\} \tag{14}$$

We consider a few special cases:

(i) $k = 0$: The right-hand side of (14) is clearly 0, and $n > 0$ implies that $n[x^n]z^0(x) = n[x^n]\,1 = 0$.

(ii) $k > n$: Then $n - k < 0$ so that

$$n[x^n]z^k(x) = n[x^n]x^k\phi^k(z(x)) = n[x^{n-k}]\phi^k(z(x)) = 0$$

as we remarked above. The right-hand side is 0 for the same reason.

(iii) $k = n$: We have

$$\begin{aligned} n[x^n]z^n(x) &\overset{(1)}{=} n[x^n]x^n\phi^n(z(x)) = n[x^0]\phi^n(z(x)) = n\phi^n(z(0)) \\ &= n\phi^n(0) \\ &= n[z^0]\phi^n(z) = n[z^{n-1}]\{z^{n-1}\phi^n(z)\} \end{aligned}$$

since $\phi(0) = 1$. Now suppose that $0 < k < n$. Then

$$\begin{aligned} n[x^n]z^k(x) &\overset{(1)}{=} n[x^{n-k}]\phi^k(z(x)) \\ &\overset{(*)}{=} \frac{n}{n-k}[z^{n-k-1}]\left(\phi^k(z)\right)'\phi^{n-k}(z) \\ &= \frac{n}{n-k}[z^{n-k-1}]k\phi^{k-1}(z)\phi'(z)\phi^{n-k}(z) \\ &= \frac{k}{n-k}[z^{n-k}]nz\phi^{n-1}(z)\phi'(z) \\ &= \frac{k}{n-k}[z^{n-k}]zD_z\left(\phi^n(z)\right) \\ &\overset{(**)}{=} \frac{k}{n-k}[z^{n-k}](n-k)\phi^n(z) \\ &= k[z^{n-1}]z^{k-1}\phi^n(z) \end{aligned}$$

as desired. Notice that we were able to use the induction hypothesis (14) at step (*) since $n - k < n$ and that we invoked Wilf Rule 2 at step (**). ∎