L5: Functional Equations and Lagrange Inversion

Analytic Combinatorics
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The symbolic method often leads to a functional equation in which the unknown generating function appears on both sides. Recursive tree specifications are canonical examples: the root is attached to subtrees drawn from the same class. In this lecture, we introduce the *Lagrange Inversion Formula*, an algebraic tool for extracting coefficients from implicitly defined generating functions without first solving for the functions explicitly.

The Lagrange Inversion Formula

Suppose that $y(z) \in z\mathbb{C}[[z]]$ satisfies $y(z) = z\phi(y(z))$, where $\phi(0) \neq 0$. Define $f(t) = t/\phi(t)$. Since $\phi(t)$ is invertible as a formal power series, $f(t)$ has a non-zero linear coefficient, and the functional equation is equivalent to $f(y(z)) = z$. Write $\phi(t) = \sum_{j=0}^{\infty} a_j t^j$ and $y(z) = \sum_{k=1}^{\infty} y_k z^k$. Substitution into the functional equation gives

$$\sum_{k=1}^{\infty} y_k z^k \;=\; z\phi(y(z)) \;=\; \sum_{j=0}^{\infty} a_j z \cdot y(z)^j.$$

By comparing coefficients of z on both sides, $y_1 = a_0 = \phi(0) \neq 0$, so the lowest-degree nonzero term of $y(z)$ is $y_1 z$. Consequently, the lowest-degree term of $zy(z)^j$ has degree $j+1$. Hence, only the terms with $0 \leq j \leq k-1$ can contribute to the coefficient of z^k. Moreover, $[z^k]z\phi(y(z))$ depends only on $y_1, \ldots, y_{k-1}$, so coefficient comparison determines y_k recursively. For instance, the first four coefficients satisfy

$$y_1 \;=\; a_0, \qquad y_2 \;=\; a_1 y_1, \qquad y_3 \;=\; a_1 y_2 + a_2 y_1^2, \qquad y_4 \;=\; a_1 y_3 + 2a_2 y_1 y_2 + a_3 y_1^3.$$

This recurrence determines $y(z)$ uniquely coefficient by coefficient. We have already seen an example of such recurrence in Lecture 4 for rooted labelled trees, where $\phi(t) = \exp(t)$. However, the recurrence does not yield a transparent formula for y_k in general. Lagrange inversion instead expresses each coefficient directly in terms of a power of ϕ.

Theorem 1. Let $\phi(y) \in \mathbb{C}[[y]]$ satisfy $\phi(0) \neq 0$. There is a unique series $y(z) \in z\mathbb{C}[[z]]$ satisfying

$$y(z) \;=\; z\phi(y(z)).$$

For every integer $n \geq 1$,

$$[z^n]y(z) \;=\; \frac{1}{n}[y^{n-1}]\phi(y)^n.$$

We first state the formal residue substitution rule in the lemma below.

Lemma 2. Let $f(t) \in t\mathbb{C}[[t]]$ have a non-zero linear coefficient. For every formal Laurent series $H(z) \in \mathbb{C}((z))$, the following two residues are equal:

$$[z^{-1}]H(z) \;=\; [t^{-1}]H(f(t))f'(t). \tag{1}$$

Proof: We first note that the residue of a formal derivative is zero. Indeed, if $A(t) = \sum_m a_m t^m$, then $A'(t) = \sum_m m a_m t^{m-1}$. A t^{-1} term could only come from $m = 0$, but that term has coefficient $0 \cdot a_0 = 0$.

Write $H(z) = \sum_{r \geq r_0} h_r z^r$. Since $f(t)^r$ has order r, the coefficient of t^m in $H(f(t))$ receives contributions only from $r_0 \leq r \leq m$. Thus, the substitution is well-defined. Moreover, terms with $r \geq 0$ have zero residue, so only finitely many negative indices need be considered. By linearity, it therefore suffices to take $H(z) = z^r$. Write $f(t) = ct \cdot u(t)$, where $c \neq 0$ and $u(0) = 1$. When $r \geq 0$, $[z^{-1}]z^r = 0$, while $f(t)^r f'(t) \in \mathbb{C}[[t]]$ has no t^{-1} term and hence zero residue. When $r < -1$, $[z^{-1}]z^r = 0$, while $f(t)^r f'(t)$ is the formal derivative of $f(t)^{r+1}/(r+1)$ and hence has zero residue. Thus, Equation (1) holds when $r \geq 0$ or $r < -1$.

When $r = -1$, $[z^{-1}]z^{-1} = 1$, while

$$\frac{f'(t)}{f(t)} \;=\; \frac{c \cdot u(t) + ct \cdot u'(t)}{ct \cdot u(t)} \;=\; \frac{1}{t} + \frac{u'(t)}{u(t)},$$

and $u'(t)/u(t) \in \mathbb{C}[[t]]$ since $u(0) = 1$ [1]. Thus, $[t^{-1}]f'(t)/f(t) = 1$, confirming Equation (1) for the case $r = -1$. $\square$

Proof of Theorem 1: We first prove existence and uniqueness. Write $y(z) = \sum_{k \geq 1} y_k z^k$. Once $y_1, \ldots, y_{k-1}$ have been determined, comparison of the coefficients of z^k requires

$$y_k \;=\; [z^{k-1}]\phi\left(\sum_{j=1}^{k-1} y_j z^j\right).$$

The coefficient on the right does not depend on y_k or any later coefficient. Starting with $y_1 = \phi(0)$, this recurrence constructs exactly one series in $z\mathbb{C}[[z]]$, and the resulting series satisfies the functional equation coefficient by coefficient.

We now extract its coefficients. Put

$$f(y) \;=\; \frac{y}{\phi(y)}.$$

The functional equation gives $f(y(z)) = z$. Moreover, composition on the left by f is injective on $z\mathbb{C}[[z]]$: if $A(z) - B(z)$ has a first non-zero term of degree d, then the first non-zero term of $f(A(z)) - f(B(z))$ is c times that term, where $c = [y]f(y) \neq 0$. Substituting $z = f(t)$ into $f(y(z)) = z$ therefore gives $f(y(f(t))) = f(t)$, and injectivity yields $y(f(t)) = t$. Applying Lemma 2 to $H(z) = y(z)/z^{n+1}$ gives

$$[z^n]y(z) \;=\; [z^{-1}]\frac{y(z)}{z^{n+1}} \;=\; [t^{-1}]\frac{y(f(t))}{f(t)^{n+1}}f'(t) \;=\; [t^{-1}]\frac{t}{f(t)^{n+1}}f'(t) \;=\; [t^{-1}]\frac{\phi(t)^{n+1}}{t^n}f'(t).$$

Differentiating $f(t) = t/\phi(t)$ gives

$$f'(t) \;=\; \phi(t)^{-1} - t\phi(t)^{-2}\phi'(t).$$

Consequently,

$$[z^n]y(z) \;=\; [t^{-1}]\left(\frac{\phi(t)^n}{t^n} - \frac{\phi(t)^{n-1}\phi'(t)}{t^{n-1}}\right).$$

The second term satisfies

$$\frac{\phi(t)^{n-1}\phi'(t)}{t^{n-1}} \;=\; \frac{1}{n}\frac{\mathsf{d}}{\mathsf{dt}}\left(\frac{\phi(t)^n}{t^{n-1}}\right) + \frac{n-1}{n}\frac{\phi(t)^n}{t^n}.$$

The derivative term on the right has zero residue, as observed in the proof of Lemma 2. Therefore,

$$[z^n]y(z) \;=\; \frac{1}{n}[t^{-1}]\frac{\phi(t)^n}{t^n} \;=\; \frac{1}{n}[t^{n-1}]\phi(t)^n \;=\; \frac{1}{n}[y^{n-1}]\phi(y)^n.$$ $\square$

[1] Since $u(0) = 1$, we can write $u(t) = 1 + v(t)$ with $v(t) \in t\mathbb{C}[[t]]$. Then $u(t)^{-1} = \left(\sum_{k \geq 0}(-v(t))^k\right) \in \mathbb{C}[[t]]$. Hence $u'(t)/u(t) = u'(t)u(t)^{-1} \in \mathbb{C}[[t]]$.

Although the theorem is stated over $\mathbb{C}$, its proof uses only field operations and division by non-zero integers. It therefore remains valid with $\mathbb{C}$ replaced by any field K of characteristic zero. In particular, rational input remains rational: if $\phi(y) \in \mathbb{Q}[[y]]$, then the recurrence above constructs $y(z) \in z\mathbb{Q}[[z]]$, and the coefficient formula also involves only rational operations.

We now look at some classical applications of Lagrange inversion in analytic combinatorics.

Example 3. Lecture 1 introduced the class $\mathcal{T}$ of complete binary trees, where the size of a tree is its number of internal nodes. The specification is $\mathcal{T} = \mathcal{E} + \mathcal{Z} \times \mathcal{T} \times \mathcal{T}$, yielding the functional equation $T(z) = 1 + zT(z)^2$. This equation is almost in Lagrange form. Put $C(z) = T(z) - 1$. Then

$$C(z) \;=\; z(1 + C(z))^2.$$

Setting $\phi(y) = (1 + y)^2$, Theorem 1 gives, for $n \geq 1$,

$$[z^n]C(z) \;=\; \frac{1}{n}[y^{n-1}](1 + y)^{2n} \;=\; \frac{1}{n}\binom{2n}{n-1} \;=\; \frac{1}{n+1}\binom{2n}{n}.$$

Since $T(z) = 1 + C(z)$, $[z^n]T(z) = \frac{1}{n+1}\binom{2n}{n}$ for $n \geq 1$, while $[z^0]T(z) = 1$.

Example 4. In Lecture 1, a rooted plane tree was specified as an unlabelled atom attached to a sequence of subtrees, i.e., $\mathcal{T} = \mathcal{Z} \times \mathrm{SEQ}(\mathcal{T})$. This yields the functional equation

$$T(z) \;=\; \frac{z}{1 - T(z)}.$$

Setting $\phi(y) = (1 - y)^{-1}$, Theorem 1 and the generalized binomial theorem give, for $n \geq 1$,

$$[z^n]T(z) \;=\; \frac{1}{n}[y^{n-1}](1 - y)^{-n} \;=\; \frac{1}{n}\binom{2n-2}{n-1}.$$

Example 5. A rooted labelled tree is an atom attached to a set of subtrees, giving the specification $\mathcal{T} = \mathcal{Z} \star \mathrm{SET}(\mathcal{T})$. Its EGF satisfies

$$T(z) \;=\; z\exp(T(z)).$$

Setting $\phi(y) = e^y$, Theorem 1 gives, for $n \geq 1$,

$$[z^n]T(z) \;=\; \frac{1}{n}[y^{n-1}]e^{ny} \;=\; \frac{1}{n}\frac{n^{n-1}}{(n-1)!} \;=\; \frac{n^{n-1}}{n!}.$$

Since $T(z)$ is an EGF, the number of rooted labelled trees on n vertices is $t_n = n![z^n]T(z) = n^{n-1}$. Dividing by the n possible choices of root gives n^{n-2} unrooted labelled trees, known as *Cayley's formula*. Lagrange inversion extracts these coefficients without an explicit expression for $T(z)$.

Exercise 6. Consider the class $\mathcal{T}_3$ of unlabelled complete ternary trees, where the size of a tree is its number of internal nodes.

(a) Use the Lagrange Inversion Formula to compute $[z^n]T_3(z)$ for $n \geq 1$.

(b) For complete m-ary trees, define $T_m(z)$ analogously. Compute $[z^n]T_m(z)$ for $n \geq 1$.

Exercise 7. Let $\mathcal{R}$ be the class of rooted labelled trees in which every internal node has exactly three unordered immediate children. Leaves have no children and are allowed. Show that the number of such trees on $n = 3k+1$ vertices is $(3k)! \cdot \binom{3k+1}{k}/6^k$.

The Generalized Lagrange Inversion Formula

Often, we are interested not only in the coefficients of $y(z)$ but also in those of a composition $F(y(z))$. For example, a sequence or set of recursively defined trees produces such a composition. The *Lagrange-Bürmann formula* extracts these coefficients directly.

Theorem 8. Let $\phi(y) \in \mathbb{C}[[y]]$ satisfy $\phi(0) \neq 0$, and let $y(z) \in z\mathbb{C}[[z]]$ be the unique solution of $y(z) = z\phi(y(z))$. For every $F(y) \in \mathbb{C}[[y]]$ and every integer $n \geq 1$,

$$[z^n]F(y(z)) \;=\; \frac{1}{n}[y^{n-1}]F'(y)\phi(y)^n.$$

The constant term is $[z^0]F(y(z)) = F(0)$.

Proof: Define $G(z) = F(y(z))$. Formal differentiation gives

$$[z^n]G(z) \;=\; \frac{1}{n}[z^{n-1}]G'(z).$$

Put $f(t) = t/\phi(t)$. The identity $y(f(t)) = t$ established in the proof of Theorem 1 gives, after formal differentiation,

$$y'(f(t))f'(t) \;=\; 1.$$

The series $f'(t)$ has the non-zero constant term $1/\phi(0)$ and is therefore invertible. Hence the formal chain rule, evaluated at $z = f(t)$, gives

$$G'(f(t)) \;=\; F'(y(f(t)))y'(f(t)) \;=\; F'(t)f'(t)^{-1}.$$

Applying Lemma 2 to $H(z) = G'(z)/z^n$, we obtain

$$\begin{aligned}
[z^n]G(z) \;=\; \frac{1}{n}[z^{n-1}]G'(z) \;&=\; \frac{1}{n}[z^{-1}]\frac{G'(z)}{z^n} \\
&=\; \frac{1}{n}[t^{-1}]\frac{F'(t)f'(t)^{-1}}{f(t)^n}f'(t) \\
&=\; \frac{1}{n}[t^{-1}]\frac{F'(t)\phi(t)^n}{t^n} \;=\; \frac{1}{n}[t^{n-1}]F'(t)\phi(t)^n \;=\; \frac{1}{n}[y^{n-1}]F'(y)\phi(y)^n. \quad \square
\end{aligned}$$

Example 9. Fix $d \geq 1$. A *generalized Dyck path of final height* d is a sequence containing $n+d$ up-steps $U = +1$ and n down-steps $D = -1$ such that every partial sum is non-negative. Thus, the path ends at height d. For example, $UUDUDU$ is such a path for $(n,d) = (2,2)$, whereas $UDDUUU$ is not because its third partial sum is negative. We use the number n of down-steps as the size.

First consider the class $\mathcal{D}$ of ordinary Dyck paths, which end at height 0. Every non-empty path has a unique first-return decomposition $UPDQ$, where $P, Q \in \mathcal{D}$. If z marks a down-step, then $\mathcal{D} = \mathcal{E} + \mathcal{Z} \times \mathcal{D} \times \mathcal{D}$, which is the same specification as in Example 3. Hence, $D(z) = 1 + zD(z)^2$. Setting $C(z) = D(z) - 1$, we have $C(z) = z(1 + C(z))^2$, which has the Lagrange form with $\phi(y) = (1+y)^2$.

Now consider a path of final height d. For every $i \in \{0, 1, \ldots, d-1\}$, mark the last up-step from height i to height $i+1$. These marked steps decompose the path uniquely as

$$P_0 U P_1 U \cdots U P_d.$$

By construction, each segment P_i begins and ends at height i: for $i < d$, it ends immediately before the marked step from height i to height $i+1$, while P_d ends at the final height d. Each segment also stays at or above height i. For $i = 0$, this is exactly non-negativity. For $i \geq 1$, the segment P_i occurs after the marked last step from height $i-1$ to height i; if it later went below height i, the path would need another step from height $i-1$ to height i before reaching final height d, contradicting the choice of the marked step. Hence, after vertical translation, every P_i is an ordinary Dyck path. Conversely, any ordered $(d+1)$-tuple of ordinary Dyck paths yields a unique generalized Dyck path by inserting an up-step between consecutive paths. The inserted steps do not affect the size, so

$$D_d(z) \;=\; D(z)^{d+1} \;=\; (1 + C(z))^{d+1}.$$

Apply Theorem 8 with $F(y) = (1+y)^{d+1}$. For $n \geq 1$,

$$[z^n] D_d(z) \;=\; \frac{1}{n}[y^{n-1}](d+1)(1+y)^d(1+y)^{2n} \;=\; \frac{d+1}{n}\binom{2n+d}{n-1} \;=\; \frac{d+1}{n+d+1}\binom{2n+d}{n}.$$

The formula also equals 1 when $n = 0$. Therefore, the number of generalized Dyck paths with $n+d$ up-steps and n down-steps is $\frac{d+1}{n+d+1}\binom{2n+d}{n}$.

Exercise 10. Fix integers $m \geq 2$ and $r \geq 1$. Let $D_m(z)$ be the OGF of complete m-ary trees, where the size is the number of internal nodes, and put $C_m(z) = D_m(z) - 1$. Thus,

$$C_m(z) \;=\; z(1 + C_m(z))^m.$$

(a) Explain why $D_m(z)^r$ is the OGF of ordered forests consisting of exactly r complete m-ary trees.

(b) Prove that, for $n \geq 0$,

$$[z^n] D_m(z)^r \;=\; \frac{r}{mn+r}\binom{mn+r}{n}.$$

(c) Recover the enumeration of generalized Dyck paths in Example 9 by taking $m = 2$ and $r = d+1$.

Example 11. A *rooted labelled forest* is a set of rooted labelled trees, so every component has a distinguished root. Fix integers $1 \leq k \leq n$. The class of rooted labelled forests with exactly k components on n vertices is $\mathcal{F}_k = \mathrm{SET}_k(\mathcal{T})$, with EGF

$$F_k(z) \;=\; \frac{T(z)^k}{k!}.$$

Here $T(z) = z\exp(T(z))$. Apply Theorem 8 with $\phi(y) = e^y$ and $F(y) = y^k$:

$$[z^n] T(z)^k \;=\; \frac{1}{n}[y^{n-1}] k y^{k-1} e^{ny} \;=\; \frac{k}{n}[y^{n-k}] e^{ny} \;=\; \frac{k}{n}\frac{n^{n-k}}{(n-k)!}.$$

Therefore, the number of such rooted labelled forests is

$$f_{n,k} \;=\; n![z^n]\frac{T(z)^k}{k!} \;=\; \binom{n-1}{k-1} n^{n-k}.$$

Further Applications

Example 12. In Lecture 1, $\mathcal{U}$ denoted the class of unary-binary trees, or Motzkin trees, in which each node has 0, 1 or 2 ordered children. Its OGF satisfies

$$U(z) \;=\; z + zU(z) + zU(z)^2 \;=\; z(1 + U(z) + U(z)^2).$$

Thus, Theorem 1 with $\phi(y) = 1 + y + y^2$ gives, for $n \geq 1$,

$$[z^n]U(z) \;=\; \frac{1}{n}[y^{n-1}](1 + y + y^2)^n.$$

Writing $1 + y + y^2 = 1 + y(1 + y)$ and expanding twice yields

$$(1 + y + y^2)^n \;=\; \sum_{k=0}^{n}\sum_{j=0}^{k}\binom{n}{k}\binom{k}{j} y^{k+j}.$$

The relation $k + j = n - 1$, together with $0 \leq j \leq k$, gives

$$[z^n]U(z) \;=\; \frac{1}{n}\sum_{k=\lceil (n-1)/2\rceil}^{n-1}\binom{n}{k}\binom{k}{n-1-k}.$$

Lecture 1 calls $[z^{m+1}]U(z)$ the m-th Motzkin number. Thus, the displayed formula gives the $(n-1)$-st Motzkin number directly, without expanding the radical in the quadratic solution.

Example 13. Let $\mathcal{M}$ be the class of mappings. Its decomposition and EGF are

$$\mathcal{M} \;=\; \mathrm{SET}(\mathrm{CYC}(\mathcal{T})), \qquad M(z) \;=\; \frac{1}{1 - T(z)},$$

where $T(z) = ze^{T(z)}$. Apply Theorem 8 with $F(y) = (1 - y)^{-1}$:

$$[z^n]M(z) \;=\; \frac{1}{n}[y^{n-1}](1 - y)^{-2}e^{ny}.$$

Since $(1 - y)^{-2} = \sum_{k\geq 0}(k + 1)y^k$, we obtain, for $n \geq 1$,

$$[z^n]M(z) \;=\; \frac{1}{n}\sum_{k=0}^{n-1}(k + 1)\frac{n^{n-1-k}}{(n - 1 - k)!}.$$

A mapping on an n-element labelled set is just a function from the set to itself, so there are n^n such mappings and $[z^n]M(z) = n^n/n!$. Equating the two expressions yields the identity

$$\sum_{k=0}^{n-1}(k + 1)\frac{n^{n-1-k}}{(n - 1 - k)!} \;=\; \frac{n^{n+1}}{n!}.$$

Example 14. We can also enumerate *connected mappings*. A mapping is connected precisely when its functional graph consists of one directed cycle of rooted labelled trees. Thus,

$$\mathcal{C} \;=\; \mathrm{CYC}(\mathcal{T}), \qquad C(z) \;=\; \log \frac{1}{1-T(z)}.$$

Apply Theorem 8 with $F(y) = \log(1/(1-y))$, so $F'(y) = (1-y)^{-1}$. For $n \geq 1$,

$$[z^n]C(z) \;=\; \frac{1}{n}[y^{n-1}]\frac{e^{ny}}{1-y} \;=\; \frac{1}{n}\sum_{k=0}^{n-1}\frac{n^k}{k!}.$$

Therefore, the number of connected mappings on n vertices is

$$c_n \;=\; n![z^n]C(z) \;=\; (n-1)!\sum_{k=0}^{n-1}\frac{n^k}{k!}.$$

Exercise 15. Let $\mathcal{G}_0$ be the class of connected simple unicyclic graphs. Recall from Lecture 4 that, with $T(z) = ze^{T(z)}$, its EGF is

$$G_0(z) \;=\; \frac{1}{2}\left(\log\frac{1}{1-T(z)} - T(z) - \frac{T(z)^2}{2}\right).$$

Use Examples 5, 11 and 14 to show that, for $n \geq 3$, the number of connected unicyclic graphs on n labelled vertices is

$$g_{0,n} \;=\; n![z^n]G_0(z) \;=\; \frac{1}{2}\left((n-1)!\sum_{k=0}^{n-1}\frac{n^k}{k!} - n^{n-1} - (n-1)n^{n-2}\right).$$

Example 16. Let $T(z,u)$ be the bivariate OGF of rooted plane trees, where z marks vertices and u marks leaves. Thus, $[z^n u^\ell]T(z,u)$ counts trees with n vertices and ℓ leaves. A plane tree is either a leaf or a root followed by a non-empty sequence of subtrees, so

$$T(z,u) \;=\; z\left(u + \frac{T(z,u)}{1-T(z,u)}\right).$$

To apply Lagrange inversion, work over the characteristic-zero coefficient field $\mathbb{C}(u)$, treating u as independent of z and y. Set $\phi_u(y) = u + y/(1-y)$. Since $\phi_u(0) = u \neq 0$ in $\mathbb{C}(u)$, Theorem 1 gives

$$[z^n]T(z,u) \;=\; \frac{1}{n}[y^{n-1}]\left(u + \frac{y}{1-y}\right)^n.$$

For each fixed n, this is a polynomial identity in u, so we may now extract $[u^\ell]$. Exactly ℓ of the n factors must contribute u, and hence

$$[u^\ell]\left(u + \frac{y}{1-y}\right)^n \;=\; \binom{n}{\ell}\left(\frac{y}{1-y}\right)^{n-\ell}.$$

Therefore, for $n \geq 2$ and $1 \leq \ell \leq n-1$, the generalized binomial theorem yields

$$[z^n u^\ell]T(z,u) \;=\; \frac{1}{n}\binom{n}{\ell}[y^{\ell-1}](1-y)^{-(n-\ell)} \;=\; \frac{1}{n}\binom{n}{\ell}\binom{n-2}{\ell-1}.$$

The exceptional one-vertex tree contributes $[zu]T(z,u) = 1$.