Coefficient Extraction From Multivariate Generating Functions

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Table lookup

- Applying the basic operations $(+, \cdot, d/dz, \int \dots)$ to known series such as $(1-z)^{-1} = \sum_{n\geq 0} z^n$ yields a table of known results.
- Linear combinations of these can often be used for simple problems to obtain the desired result (we do this a lot in COMPSCI 720).
- Standard example: GF for average number of comparisons of quicksort on size n permutation is

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

  Thus by lookup we have $a_n = 2(n+1)H_n - 4n$, $H_n := \sum_{j=1}^{n} 1/j$.
- Problems: table may be incomplete; decomposition of GF may be unclear; exact formulae are often too complicated to be useful anyway.

Implicit functions: Lagrange inversion

- A functional equation of the form $f(z) = z\phi(f(z))$ has a unique solution provided $\phi'(0) \neq 0$. In this case we have

$$[z^n]\psi(f(z)) = [y^n]y\psi'(y)\phi(y)^n = [x^n y^n]\frac{y\psi'(y)}{1 - x\phi(y)}.$$

  Easy proofs all use the Cauchy integral formula. Formal power series proofs exist but are not very natural.

- In particular ϕ is an automorphism of $\mathbb{C}[[z]]$ and, with $v = \phi(z)$, $\psi(z) = z^k$,

$$n[z^n]v^k = k[v^{-k}]z^{-n}.$$

- Example: degree-restricted trees.

Degree-restricted trees example

- Let $0 \in \Omega \subseteq \mathbb{N}$. We consider the combinatorial class $\mathcal{T}_\Omega$ of ordered plane trees with the outdegree of each node restricted to belong to Ω.
- Examples: $\Omega = \{0, 1\}$ gives paths; $\Omega = \{0, 2\}$ gives binary trees; $\Omega = \{0, t\}$ gives t-ary trees; $\Omega = \mathbb{N}$ gives general ordered trees.
- Let $T_\Omega(z)$ be the enumerating GF of this class. The symbolic method immediately gives the equation

$$T_\Omega(z) = z\phi(T_\Omega(z))$$

  where $\phi(x) = \sum_{\omega \in \Omega} x^\omega$.
- Lagrange inversion is tailor-made for this situation. For Ω as above, we obtain an answer involving binomial coefficients.

Basic complex-analytic method

- (Cauchy integral formula) Let D be the open disc of convergence, Γ its boundary, U a simply connected set containing D. Then
$$a_n = \frac{1}{2\pi i} \int_C z^{-n-1} F(z) \, dz$$
where C is a simple closed curve in U.
- Usually (if all $a_n \geq 0$ and (a_n) is not periodic), there is a unique singularity ρ of smallest modulus on Γ, and ρ is positive real. WLOG $\rho = 1$.
- Further progress depends on singularities of F. In one variable, not many types are possible, and there are methods for each.
  - If ρ is large (essential), use the saddle point method.
  - If ρ is a pole or algebraic/logarithmic and F can be continued past Γ, use singularity analysis.
  - If Γ is a natural boundary, use Darboux' method or circle method or . . . .

"Singularity analysis" (Flajolet-Odlyzko 1990)

- Assume F is analytic in a Camembert region.
- Choose an appropriate ("Hankel") contour approaching the singularity at distance $1/n$.
- This yields asymptotics for $[z^n]F(z)$ where F looks like $(1-z)^\alpha(\log 1/(1-z))^\beta$. "Looks like" means o, O, Θ.
- Asymptotics for $F(z)$ near $z = 1$ yields asymptotics for $[z^n]F(z)$ automatically. Very useful: singularities in applications are mostly poles, logarithmic, or square-root.
- If ρ is a pole then a simpler contour can be used, along with Cauchy residue theorem.

Darboux' method

- Assume F is of class C^k on Γ. Change variable $z = \exp(i\theta)$, integrate by parts k times. Get

$$a_n = \frac{1}{2\pi(in)^k} \int_0^{2\pi} f^{(k)}(e^{i\theta})e^{-in\theta}.$$

- Analyze the oscillating integral using Fourier techniques (Riemann-Lebesgue lemma).
- Can't be used for poles or if f has infinitely many singularities on Γ. In that case, sometimes the circle method of analytic number theory works.

Saddle point method

- Used for "large" (essential) singularities (for example, entire function at ∞). Example: Stirling's formula.
- Cauchy integral formula on a circle C_R of radius R gives $a_n \leq (2\pi)^{-1} f(R)/R^n$.
- Choosing $R = n$ minimizes this upper bound. We find that the integral over C_R has most mass near $z = n$, so that

$$\begin{aligned} a_n &= \frac{1}{2\pi n^n} \int_0^{2\pi} \exp(-in\theta + \log f(ne^{i\theta}) \, d\theta \\ &\approx \frac{1}{2\pi n^n} \int_0^{2\pi} \exp(-n\theta^2/2) \, d\theta. \end{aligned}$$

Now Laplace's method gives asymptotics of the Laplace-like integral.

Some references for this section

- Univariate GF asymptotics — Flajolet and Sedgewick, Analytic Combinatorics (book in progress, `algo.inria.fr`)
- Pemantle-Wilson mvGF project `www.cs.auckland.ac.nz/~mcw/Research/mvGF`
- M. Wilson, Asymptotics of generalized Riordan arrays, to appear in DMTCS;
- R. Pemantle and M. Wilson, Twenty combinatorial examples of asymptotics derived from multivariate generating functions, submitted to SIAM Review.
- Above two appers are CDMTCS reports and also available from my webpage.

Multivariate coefficient extraction — some quotations

- (E. Bender, SIAM Review 1974) Practically nothing is known about asymptotics for recursions in two variables even when a GF is available. Techniques for obtaining asymptotics from bivariate GFs would be quite useful.

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- (A. Odlyzko, Handbook of Combinatorics, 1995) A major difficulty in estimating the coefficients of mvGFs is that the geometry of the problem is far more difficult. . . . Even rational multivariate functions are not easy to deal with.
- (P. Flajolet/R. Sedgewick, Analytic Combinatorics Ch 9 draft, 2005) Roughly, we regard here a bivariate GF as a collection of univariate GFs . . . .

Our project

- Robin Pemantle (U. Penn.) and I have a major project on mvGF coefficient extraction.
- Thoroughly investigate coefficient extraction for meromorphic $F(\mathbf{z}) := F(z_1, \ldots, z_{d+1})$ (pole singularities). Amazingly little is known even about rational F in 2 variables.
- Goal 1: improve over all previous work in generality, ease of use, symmetry, computational effectiveness, uniformity of asymptotics. Create a theory!
- Goal 2: establish mvGFs as an area worth studying in its own right, a meeting place for many different areas, a common language. I am recruiting!

Notation and basic taxonomy

- $F(\mathbf{z}) = \sum a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}} = G(\mathbf{z})/H(\mathbf{z})$ meromorphic in nontrivial polydisc in $\mathbb{C}^d$.
- $\mathcal{V} = \{\mathbf{z} | \, H(\mathbf{z}) = 0\}$ the singular variety of F.
- $\mathsf{T}(\mathbf{z}), \mathsf{D}(\mathbf{z})$ the torus, polydisc centred at $\mathbf{0}$ and containing $\mathbf{z}$.
- A point of $\mathcal{V}$ is strictly minimal (with respect to the usual partial order on moduli of coordinates) if $\mathcal{V} \cap \mathsf{D}(\mathbf{z}) = \{\mathbf{z}\}$. When $F \geq 0$, such points lie in the positive real orthant.
- A minimal point can be a smooth (manifold), multiple (locally product of n smooth factors H_i) or bad (all other types), depending on local geometry of $\mathcal{V}$.
- For smooth point, dir($\mathbf{z}$) is direction of $(z_1 H_1, \dots, z_d H_d)$ (gradient of H in log-coordinates). Always positive if $\mathbf{z}$ minimal.

Brief outline of methods

- Use Cauchy integral formula in $\mathbb{C}^d$; contour changes (homology/residue theory); convert to Fourier-Laplace integral in remaining d variables; stationary phase analysis of these integrals.
- Must specify a direction $\overline{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$ for asymptotics.
- To each minimal point $\mathbf{z} \in \mathcal{V}$ we associate a cone $\mathsf{K}(\mathbf{z})$ of directions. If $\mathbf{z}$ is smooth, K is a single ray represented by dir($\mathbf{z}$); if $\mathbf{z}$ is multiple, K is nonempty, spanned by K's of smooth factors.
- If $\overline{\mathbf{r}}$ is bounded away from $\mathsf{K}(\mathbf{z})$, then $|\mathbf{z}^{\mathbf{r}} a_{\mathbf{r}}|$ decreases exponentially. We show that if $\overline{\mathbf{r}}$ is in $\mathsf{K}(\mathbf{z})$, then $\mathbf{z}^{-\mathbf{r}}$ is the right asymptotic order, and develop full asymptotic expansions, on a case-by-case basis.

Outline of results

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- For each $\mathbf{z} \in$ contrib, there is an asymptotic expansion formula($\mathbf{z}$) for $a_{\mathbf{r}}$, computable in terms of the derivatives of G and H at $\mathbf{z}$.
- This yields

$$a_{\mathbf{r}} \sim \sum_{\mathbf{z} \in \text{contrib}} \text{formula}(\mathbf{z}) \qquad (1)$$

where formula($\mathbf{z}$) depends on the type of critical point.

Generic shape of leading term of formula(z)

- (smooth/multiple point $n < d$)

$$C(\mathbf{z})G(\mathbf{z})\mathbf{z}^{-\mathbf{r}}|\mathbf{r}|^{-(d-n)/2}$$

where C depends on the derivatives to order 2 of H;

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- (bad point) Not yet done, hence the name.

Specialization to dimension 2 — smooth points

- Suppose that H has a simple pole at $P = (z, w)$ and is otherwise analytic in $\mathrm{D}(z, w)$. Define

  $$Q(z, w) = -A^2 B - AB^2 - A^2 z^2 H_{zz} - B^2 w^2 H_{ww} + ABH_{zw}$$

  where $A = wH_w, B = zH_z$, all computed at P. Then when $r/s = B/A$,

  $$a_{rs} \sim \frac{G(z, w)}{\sqrt{2\pi}} \sqrt{\frac{-A}{sQ(z, w)}}.$$

  The apparent lack of symmetry is illusory, since $A/s = B/r$.

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$$a_{rs} = \left(\frac{G(z, w)}{\sqrt{-z^2 w^2 \det \operatorname{hess}(z, w)}} + O(e^{-c}) \right) \text{ uniformly for } (r, s) \in K$$

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- The uniformity breaks down near the walls of K, but we know the expansion on the boundary.

The combinatorial case

In the combinatorial case ($a_{\mathbf{r}} \geq 0$ for all $\mathbf{r}$), several nice results hold that are not generally true.

- For each $\overline{\mathbf{r}}$ of interest, there is always a unique element $\mathbf{z}(\overline{\mathbf{r}})$ of contrib($\overline{\mathbf{r}}$) lying in the positive orthant $\mathcal{O}^d$. All others lie on the same torus, and generically there are no others.

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- All steps but the last are straightforward polynomial algebra for rational F; the last is harder but usually doable.
- We can now use formula($\mathbf{z}$) to compute asymptotics in direction $\overline{\mathbf{r}}$. Provided the geometry does not change, the above expansion is locally uniform in $\overline{\mathbf{r}}$.

Concrete example: Delannoy numbers

- Consider walks in $\mathbb{Z}^2$ from $(0, 0)$, steps in $(1, 0), (0, 1), (1, 1)$. Here $F(x, y) = (1 - x - y - xy)^{-1}$.

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- Using these relations we obtain x, y in terms of r, s, then use smooth formula to give

$$a_{rs} \sim \left[\frac{\Delta - s}{r}\right]^{-r} \left[\frac{\Delta - r}{s}\right]^{-s} \sqrt{\frac{rs}{2\pi\Delta(r+s-\Delta)^2}}.$$

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  where $\Delta = \sqrt{r^2+s^2}$.
- Extracting the diagonal ("central Delannoy numbers") is now easy:

$$a_{rr} \sim (3+2\sqrt{2})^r \frac{1}{4\sqrt{2}(3-2\sqrt{2})} r^{-1/2}.$$

Riordan arrays

- A Riordan array is a triangular array a_{nk} with GF of the form

$$F(x, y) = \sum_{n,k} a_{nk} x^n y^k = \frac{\phi(x)}{1 - yv(x)},$$

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- Closely linked with Lagrange inversion: $v(x) = xA(v(x))$ for some unique A. Lots of interesting identities.
- Examples: number triangles (Pascal, Catalan, Motzkin, Schröder, . . .); various 2-D lattice walks, generalized Dyck paths; ordered forests; many sequence enumeration problems; sums of IID random variables; Lagrange inversion; kernel method.

Basic theorem on Riordan array asymptotics

Let (v, ϕ) determine a Riordan array. Generically (v has radius of convergence $R > 0$, $v \geq 0$, v not periodic, ϕ has radius of convergence at least R), we have

$$a_{rs} \sim v(y)^r y^{-s} r^{-1/2} \sum_{k=0}^{\infty} b_k(s/r) r^{-k} \tag{2}$$

where y is the unique positive real solution to $\mu(v; y) = s/r$.

- Here $b_0 = \frac{\phi(y)}{\sqrt{2\pi\sigma^2(v;y)}} \neq 0$.
- The asymptotic approximation is uniform for s/r in a compact subset of (A, B), where A is the order of v at 0 and B its order at infinity. We suspect it is usually uniform even on $[A, B)$.

Multiple point example — Cayley graph diameters

- (J. Siran et al. 2004) Fix t disjoint pairs from $[n] := \{1, \ldots, n\}$. Now choose $S \subseteq n$, $|S| = k$, uniformly at random. What is prob(no pair belongs to S)?

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- Relevant GF turns out to be

$$\begin{aligned} F(x,y,z) &= \sum a(n,k,t) x^n y^k z^t \\ &= \left(1 - z(1 - x^2 y^2)\right)^{-1} (1 - x(1+y))^{-1}. \end{aligned}$$

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$$= \left(1 - z(1 - x^2 y^2)\right)^{-1} \left(1 - x(1 + y)\right)^{-1}.$$

- Here $a(n, k, t)$ can be negative for large t, so we are not in the combinatorial case. But crit has two elements, both multiple points with $n = 2, d = 3$. One point can be eliminated from contrib since it leads to negative asymptotics for a positive sequence. Answer is asymptotic to

$$C \binom{n}{k}^{-1} x^{-k} y^{-n} z^{-t} n^{-1/2}$$

where x, y, z are quadratic over $\mathbb{Z}[r, s]$.

Fourier-Laplace integrals

We are quickly led via $\mathbf{z} = e^{i\boldsymbol{\theta}}$ to large-λ analysis of integrals of the form

$$I(\lambda) = \int_D e^{-\lambda f(\mathbf{x})} \psi(\mathbf{x})\, dV(\mathbf{x})$$

where:

- $f(0) = 0$, $f'(0) = 0$ iff $\overline{\mathbf{r}} \in \mathsf{K}(\mathbf{z})$.
- $\operatorname{Re} f \geq 0$; the phase f is analytic, the amplitude $\psi \in C^\infty$.
- D is an $(n + d)$-dimensional product of real tori, intervals and simplices; dV the volume element.

Difficulties in analysis: interplay between exponential and oscillatory decay, nonsmooth boundary of simplex.

Low-dimensional examples of F-L integrals

- Typical smooth point example looks like

$$\int_{-1}^{1} e^{-\lambda(1+i)x^2}\, dx.$$

  Isolated nondegenerate critical point, exponential decay

- Simplest double point example looks roughly like

$$\int_{-1}^{1}\int_{0}^{1} e^{-\lambda(x^2+2ixy)}\, dy\, dx.$$

  Note Re $f = 0$ on $x = 0$ so rely on oscillation for smallness.

- Multiple point with $n = 2, d = 1$ gives integral like

$$\int_{-1}^{1}\int_{0}^{1}\int_{-x}^{x} e^{-\lambda(z^2+2izy)}\, dy\, dx\, dz.$$

Simplex corners now intrude, continuum of critical points.

Sample reduction to F-L in simple case

Suppose $(1, 1)$ is a smooth or multiple strictly minimal point. Here C_a is the circle of radius a centred at 0, $R(z; s; \varepsilon)$ = residue sum in annulus, N a nbhd of 1.

$$\begin{aligned} a_{rs} &= (2\pi i)^{-2} \int_{C_1} z^{-r-1} \int_{C_{1-\varepsilon}} w^{-s-1} F(z, w) \, dw \, dz \\ &= (2\pi i)^{-2} \int_N z^{-r-1} \left[\int_{C_{1+\varepsilon}} w^{-s-1} F(z, w) - 2\pi i R(z; s; \varepsilon) \right] dz \\ &\cong -(2\pi i)^{-1} \int_N z^{-r-1} R(z; s; \varepsilon) \, dz \\ &= (2\pi)^{-1} \int_N \exp(-ir\theta + \log(-R(z; s; \varepsilon)) \, d\theta. \end{aligned}$$

To proceed we need a formula for the residue sum.

Dealing with the residues

- In smooth case $R(z;\varepsilon) = v(z)^s \operatorname{Res}(F/w)_{|w=1/v(z)} := v(z)^s \phi(z)$. So above has the form

$$(2\pi)^{-1} \int_N \exp(-s(ir\theta/s - \log v(z) - \log(-\phi(z))\, d\theta.$$

- In multiple case there are $n+1$ poles in the ε-annulus and we use the following nice lemma:
  Let $h : \mathbb{C} \to \mathbb{C}$ and let μ be the normalized volume measure on $\mathcal{S}_n$. Then

$$\sum_{j=0}^{n} \frac{h(v_j)}{\prod_{r \neq j}(v_j - v_r)} = \int_{\mathcal{S}_n} h^{(n)}(\boldsymbol{\alpha v})\, d\mu(\boldsymbol{\alpha}).$$

Comparing approaches for small singularities

- (GF-sequence methods) Treat $F(z_1, \ldots, z_d)$ as a sequence of $d-1$ dimensional GFs, use probability limit theorems. Pro: can use 1-D methods. Con: complete expansions hard to get, only works well for smooth singularities (below).
- (diagonal method) For each rational slope p/q, consider singularities of $f(t) := F(z^q, t/z^p)$. Pro: gives complete GF for each diagonal using 1-D methods. Con: only works in dimension 2; complexity of computation depends on slope; only rational slopes, so uniform asymptotics impossible.
- (genuinely multivariate methods) Try to use Cauchy residue approach, then convert to Fourier-Laplace integrals. Pro: uniform asymptotics, complete expansions, general approach. Con: geometry of singular set is hard.

Open problems

- Complete analysis of F-L integrals in general case (large stationary phase set).
- How to find and classify minimal singularities algorithmically? Note: a minimal point is a Pareto optimum of the functions $|z_1|, \dots, |z_{d+1}|$.
- Computer algebra of multivariate asymptotic expansions.
- Patching together asymptotics at cone boundaries; uniformity, phase transitions.
- Compute expansions controlled by bad points.