

Asymptotics of Coefficients of Multivariate Generating Functions

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Preliminaries

Introduction and motivation

- Univariate case

- Multivariate case

Analytic details

- Saddle point approach: geometry

- Computing formulae: Fourier-Laplace integrals

More combinatorial examples

Advanced issues, related and future work

References

- ▶ mvGF site: www.cs.auckland.ac.nz/~mcw/Research/mvGF/ .
- ▶ P. Flajolet and R. Sedgewick, *Analytic Combinatorics*, drafts at algo.inria.fr/flajolet/Publications/ .
- ▶ A. Odlyzko, survey on Asymptotic Enumeration Methods in *Handbook of Combinatorics*, Elsevier 1995, available from www.dtc.umn.edu/~odlyzko/doc/enumeration.html.
- ▶ E. Bender, survey on Asymptotic Enumeration, *SIAM Review* 16:485-515, 1974.

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- ▶ The **generating function** of the sequence is the formal power series $F(\mathbf{z}) = \sum_{\mathbf{r}} a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}}$.
- ▶ If the series converges in a neighbourhood of $\mathbf{0} \in \mathbb{C}^d$, then F defines an analytic function there.

Cauchy integral formula approach

- ▶ Let U be the open disc of convergence, ∂U its boundary, C a circle centred at 0, inside U . Then

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- ▶ Suppose that $\rho < \infty$. Then in the combinatorial case
 - ▶ (Vivanti-Pringsheim) $z = \rho$ is a singularity of F ;
 - ▶ If F is aperiodic, $z = \rho$ is the only singularity on ∂U .

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 - ▶ If ∂U is a natural boundary, use **Darboux' method** or **circle method** or

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- ▶ The integral is $O((1 + \varepsilon)^{-r})$ while the residue equals $-e^{-1}$.
- ▶ Thus $[z^r]F(z) \sim e^{-1}$ as $r \rightarrow \infty$.
- ▶ Since there are no more poles, we can push C to ∞ in this case, so the error in the approximation decays faster than any exponential.

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- ▶ This yields asymptotics for $[z^r]F(z)$ where F looks like $(1-z)^\alpha[-\log(1-z)]^\beta$. “Looks like” means o, O, Θ .
- ▶ Asymptotics for $F(z)$ near $z = 1$ yields asymptotics for $[z^r]F(z)$ automatically. Very useful: singularities in applications are often poles, logarithmic, or square-root.

Darboux' method

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

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

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- ▶ We find that the integral over C_R has most mass near $z = n$, so that

$$\begin{aligned} a_n &= \frac{1}{2\pi n^n} \int_0^{2\pi} \exp(-in\theta) F(ne^{i\theta}) d\theta \\ &\approx \frac{e^n}{2\pi n^n} \int_{-\varepsilon}^{\varepsilon} \exp(-n\theta^2/2 + O(\theta^3)) d\theta. \end{aligned}$$

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- ▶ Now **Laplace's method** gives asymptotics of the integral; leading term is $\sqrt{2\pi/n}$. This gives the first order Stirling formula.

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- ▶ (Flajolet/Sedgewick 200x) “Roughly, we regard here a bivariate GF as a collection of univariate GFs”

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- ▶ Other workers on the project: Yuliy Baryshnikov, Andrew Bressler, Manuel Lladser, Alexander Raichev, Mark Ward.

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- ▶ Analysis: the (Leray) residue formula is much harder to use.

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- ▶ Otherwise: try resolution of singularities or other approach.

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- ▶ We can determine crit and contrib by a combination of algebraic and geometric criteria.
- ▶ For each $\mathbf{z}^* \in \text{contrib}$, there is an asymptotic expansion formula(\mathbf{z}^*) for $a_{\mathbf{r}}$, computable via derivatives of G and H .
- ▶ This yields

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

where $\text{formula}(\mathbf{z}^*)$ is an asymptotic series that depends on the type of geometry of \mathcal{V} near \mathbf{z}^* , and is uniform on compact subsets provided the geometry does not change.

Generic shape of formula(\mathbf{z}^*)

- ▶ (smooth point, or multiple point with $n \leq d$)

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- ▶ (multiple point, $n \geq d$)

$$\mathbf{z}^{*\mathbf{-r}} G(\mathbf{z}^*) P\left(\frac{r_1}{z_1^*}, \dots, \frac{r_d}{z_d^*}\right),$$

P a piecewise polynomial of degree $n - d$.

Simplest special case in dimension 2

- ▶ Suppose that $F = G/H$ has a simple pole at $P = (z^*, w^*)$ and $F(z, w)$ is otherwise analytic for $|z| \leq |z^*|, |w| \leq |w^*|$. Define

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

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

$$a_{rs} = (z^*)^{-r}(w^*)^{-s} \left[\frac{G(z^*, w^*)}{\sqrt{2\pi}} \sqrt{\frac{-A}{sQ(z^*, w^*)}} + O(s^{-3/2}) \right].$$

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- ▶ This simplest case already covers Pascal, Catalan, Motzkin, Schröder, ... triangles, generalized Dyck paths, ordered forests, sums of IID random variables, Lagrange inversion, ...

Next simplest special case in dimension 2

- ▶ Suppose that $F = G/H$ has a pole at $P = (z^*, w^*)$, which is a double point of \mathcal{V} , $F(z, w)$ is otherwise analytic for $|z| \leq |z^*|, |w| \leq |w^*|$, and $G(P) \neq 0$. Then as $s \rightarrow \infty$ for r/s in a certain cone K ,

$$a_{rs} \sim (z^*)^{-r} (w^*)^{-s} \left[\frac{G(z^*, w^*)}{\sqrt{(z^* w^*)^2 \text{hess}(z^*, w^*)}} + O(e^{-c(r+s)}) \right]$$

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 - ▶ the expansion holds uniformly over compact subcones of K (defined later);
 - ▶ the hypothesis $G(P) \neq 0$ is necessary; when $d > 1$, can have $G(P) = H(P) = 0$ even if G, H are relatively prime.

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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- ▶ Solving, and using the smooth point formula above we obtain (uniformly for $r/s, s/r$ away from 0)

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- ▶ Extracting the diagonal (“central Delannoy numbers”) is now easy:

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

Example: queueing network

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$$F(x, y) = \frac{1}{\left(1 - \frac{2x}{3} - \frac{y}{3}\right)\left(1 - \frac{2y}{3} - \frac{x}{3}\right)}$$

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- ▶ The point $(1, 1)$ is a double point satisfying the above. In the cone $1/2 < r/s < 2$, we have $a_{rs} \sim 3$. Outside, the smooth formula holds.

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- ▶ How does it all work (I want to see the details)?

Book references for this lecture

- ▶ E. Stein, *Harmonic analysis: real-variable methods, orthogonality, and oscillatory integrals*, Princeton, 1993.
- ▶ L. Hörmander, *The analysis of linear partial differential operators. I.*, Springer, 2003.
- ▶ V. Arnol'd, S. Guseĭn-Zade, A. Varchenko, *Singularities of Differentiable Maps*, Birkhäuser 1985, 1988.
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Notation and basic setup

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- ▶ So far we have done this by simple contour changes to use 1-variable residue theorem; convert to Fourier-Laplace integral in remaining $d - 1$ variables; stationary phase/saddle point analysis of these integrals.
- ▶ There may be other ways to compute the residue integral; however they are unlikely to be easy: explicit residue computation for $d > 1$ seems difficult.

Cauchy integral formula

- ▶ We have

$$a_{\mathbf{r}} = (2\pi i)^{-d} \int_T \mathbf{z}^{-\mathbf{r}-1} F(\mathbf{z}) \mathbf{d}\mathbf{z}$$

where $\mathbf{d}\mathbf{z} = dz_1 \wedge \cdots \wedge dz_d$ and T is a small torus around the origin.

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- ▶ The homology of $\mathbb{C}^d \setminus \mathcal{V}$ is the key to decomposing the integral.
- ▶ It is natural to try a saddle point/steepest descent approach.

Stratified Morse theory

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- ▶ Key problem: find the highest critical points with nonzero n_i . These form the set $\text{contrib}(\bar{\mathbf{r}})$. Others give exponentially smaller contributions.

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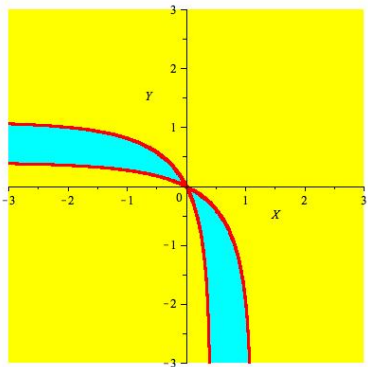
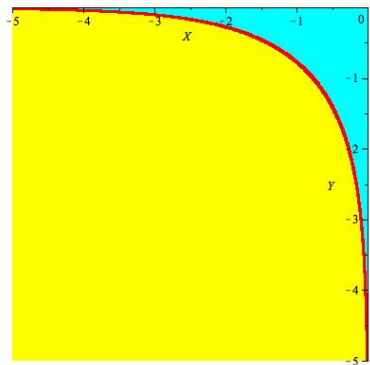
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- ▶ The cone spanned by normals to supporting hyperplanes at $\mathbf{x}^* \in \partial \log U$ we denote by $K(\mathbf{z}^*)$. If \mathbf{z}^* is smooth, this is a single ray determined by $\text{dir}(\mathbf{z}^*)$, the image of \mathbf{z}^* under the **logarithmic Gauss map**.

Picture of $\log U$ for Delannoy and queueing examples



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- ▶ Note: for general F , there may not be any minimal points in contrib.

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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 $\text{formula}(\mathbf{z}^*)$ to compute asymptotics in direction $\bar{\mathbf{r}}$. Provided the geometry does not change, the above expansion is uniform (over compact subsets) in $\bar{\mathbf{r}}$.

Sample reduction to iterated integral in simple case

Suppose (WLOG) $(1, 1)$ 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.

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

To proceed we need a formula for the residue sum.

Dealing with the residues

- ▶ In smooth case, use local parametrization $wv(z) = 1$. Then $R(z; s; \varepsilon) = v(z)^s \operatorname{Res}(F/w)|_{w=1/v(z)} := v(z)^s \psi(z)$. So above has the form

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- ▶ In the multiple case there are $n + 1$ poles $1/v_0(z), \dots, 1/v_n(z)$ in the ε -annulus and we use the following nice lemma: Let $h : \mathbb{C} \rightarrow \mathbb{C}$ and let μ be the normalized volume measure on the unit simplex \mathcal{S}_n . Then

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

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$$i \left(\frac{r(z^*)^2 + 2sz^* - r}{(z^*)^2 - 1} \right) \theta + \frac{sz^*(1 + (z^*)^2)}{(1 - (z^*)^2)^2} \theta^2 + \dots$$

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- ▶ Thus $f(0) = 0$, and $f'(0) = 0$ because (z^*, w^*) is a critical point for direction $\overline{(r, s)}$.

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

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- ▶ 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.

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 - ▶ (change of variables/contour moving) ensure that phase has nice form allowing explicit computation of integral.
 - ▶ Integration by parts.
- ▶ The **stationary phase approximation** for the leading term, given a quadratically nondegenerate stationary point in the interior of $D \subseteq \mathbb{R}^m$ is

$$\psi(\mathbf{0}) \left(\frac{2\pi}{\lambda} \right)^{m/2} (\det f''(\mathbf{0}))^{-1/2}.$$

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- ▶ Many of our applications to generating function asymptotics do not fit into this framework. In some cases, we need to extend what is known.

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- ▶ For multiple points with $n < d$ we have a higher-dimensional stationary phase set (more difficult).

References for this lecture

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 - ▶ compute its minimal polynomial using the **multiplication matrix** approach.

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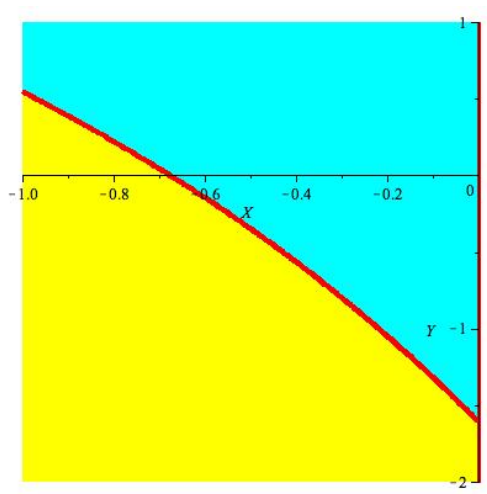
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- ▶ Note that

$$F(x, y) = \frac{\phi(x)}{1 - yv(x)}.$$

Above analysis extends to GFs of this form (**Riordan arrays**).

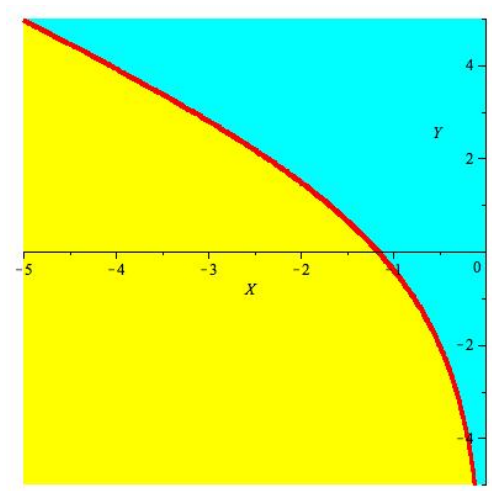
Maximum number of distinct subsequences: $\log U$ 

Polyominoes

- ▶ The GF for horizontally convex polyominoes ($k =$ rows, $n =$ squares) is

$$F(x, y) = \sum_{n,k} a_{nk} x^n y^k = \frac{xy(1-x)^3}{(1-x)^4 - xy(1-x-x^2+x^3+x^2y)}.$$

- ▶ Generically, $\text{crit}(\bar{\mathbf{r}})$ has 4 points. For each direction with $n/k \geq 1$, there is a contributing point in \mathcal{O}^2 .
- ▶ There are no more (can check that the others are on the wrong torus).

Polyominoes: $\log U$ 

Multiple point example — Cayley graph diameters I

- ▶ Fix t disjoint pairs from $[n] := \{1, \dots, n\}$. Let $a(n, k, t)$ be the number of subsets of $[n]$ of size k that do not contain any of the t pairs.

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- ▶ 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 $n = 2, d = 3$.

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- ▶ More detailed analysis using (parameter-varying) F-L integrals gives results in the sublinear case too.

Alignments example

- ▶ A (d, r_1, \dots, r_d) -alignment is a d -row binary matrix with j th row sum r_j and no zero columns.
- ▶ The generating function for the number of (d, \cdot) -alignments is

$$F(\mathbf{z}) = \sum a(r_1, \dots, r_d) \mathbf{z}^{\mathbf{r}} = \frac{1}{2 - \prod_{i=1}^d (1 + z_i)}.$$

- ▶ \mathcal{V} is globally smooth, and we are in the aperiodic combinatorial case. For each $\bar{\mathbf{r}}$, $\text{contrib}(\bar{\mathbf{r}})$ consists of a single element $\mathbf{z}^*(\bar{\mathbf{r}}) \in \mathcal{O}^d$.
- ▶ For the diagonal direction we have $\mathbf{z}^*(\bar{\mathbf{1}}) = (2^{1/d} - 1)\mathbf{1}$, so the number of “square” alignments satisfies

$$a(n, n, \dots, n) \sim (2^{1/d} - 1)^{-dn} \frac{1}{(2^{1/d} - 1) 2^{(d^2-1)/2d} \sqrt{d} (\pi n)^{d-1}}$$

- ▶ Confirms result of [GHOW1990], with less work, and extends to generalized alignments.

Comparing approaches for small singularities

- ▶ (GF-sequence methods) Treat $F(z_1, \dots, z_d)$ 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).

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- ▶ (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.

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- ▶ CLT holds only in the smooth case where the Hessian is nondegenerate.
- ▶ Our work also yields a CLT when it applies, but doesn't improve over previous work (nor is it worse). We cover many more general situations too.

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- ▶ Patch together asymptotics at cone boundaries; uniformity, phase transitions.
- ▶ Describe quantities in our formulae geometrically (e.g. using Gauss map).

Work in progress

- ▶ (Pemantle, Bressler) Applications to quantum random walks. Here crit is sometimes an entire torus. Treated by a variant of above analysis.
- ▶ (Raichev, Wilson) Extending theory to algebraic functions. Currently using reduction of Safonov, which increases dimension by 1, and necessitates higher-order asymptotics.
- ▶ (Raichev, Wilson) Explicit higher-order asymptotics for F-L integrals. Applications to algebraic functions and higher moments.
- ▶ (Pemantle, Baryshnikov) Derivation of asymptotic formulae controlled by certain bad points (quadratic cones).
- ▶ (Lladser, Wilson) Uniform asymptotics near the coordinate planes.