Asymptotic enumeration in several variables: integration and computation

Mark C. Wilson, UMass Amherst

AMC seminar 2019-10-29

My research profile

- Asymptotics of multivariate generating functions and applications to combinatorial and probabilistic models
- Network science and applications in social science
- Social choice theory, voting and electoral systems
- Relations with computer science: algorithms, data science
- See https://markcwilson.site for more.

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Today's talk

- ✓Asymptotics of multivariate generating functions and applications to combinatorics and probability
- Network science and applications in social science
- Social choice theory, voting and electoral systems
- Relations with computer science: algorithms, data science
- See `http://ACSVproject.org` for more on this project, or talk to me about any project.

Sample applications

- Our machinery has been applied to, among others: quantum walks; queuing systems; RNA secondary structure; sequence alignment; random tilings; special function theory; integrable systems in statistical mechanics.
- Lattice walk models are ubiquitous in combinatorics, owing to nice bijections with many other structures. They also arise in nonparametric statistics, and via random walk models.
- First basic example: estimate a_{rs}, which counts nearest-neighbor walks in $\mathbb{Z}^2$, going from $(0,0)$ to (r,s), with steps in $\{(1,0),(0,1),(1,1)\}$ (Delannoy walks).
- Second basic example: $F = 1/H = \sum_{r,s} a_{rs} x^r y^s$ where

$$H(x,y) = x^2y^2 - 2xy(x+y) + 5\left(x^2+y^2\right) + 14\,xy - 20(x+y) + 19.$$

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Basic steps

1. Compute generating function transform of sequence of interest.
2. Invert transform via Cauchy Integral Formula.
3. Approximate by integral of residue in smaller dimension.
4. Convert to Fourier-Laplace integral by trigonometric substitution.
5. Compute asymptotics of Fourier-Laplace integral.

- Do everything algorithmically and implement in open source software.
- In this talk concentrate on Steps 2–5 and especially 5.

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Basic steps: $d = 1$ example coming up

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Example (Pole: derangements)

- Consider $F(z) = e^{-z}/(1-z)$, the GF for derangements. Integrating over a small circle around $z = 0$ gives by Cauchy's integral theorem

$$a_r = \frac{1}{2\pi i} \int_C z^{-r-1} F(z)\, dz.$$

- Push the circle past the pole $z = 1$. By Cauchy's residue theorem,

$$a_r = \frac{1}{2\pi i} \int_{C_{1+\varepsilon}} z^{-r-1} F(z)\, dz - \operatorname{Res}(z^{-r-1} F(z); z = 1).$$

- The integral is $O((1+\varepsilon)^{-r})$, for any $\varepsilon > 0$, while the residue equals $-e^{-1}$.
- Thus $[z^r]F(z) \sim e^{-1}$ as $r \to \infty$, and error decays superexponentially in r.

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Example (Essential singularity: saddle point method)

- Here $F(z) = \exp(z)$. The Cauchy integral formula on a circle C_R of radius R gives $a_n \leq F(R)/R^n$.
- Consider the "height function" $\log F(R) - n \log R$ and try to minimize over R. In this example, $R = n$ is the minimum.
- The integral over C_n has most mass near $z = n$, so that

$$a_n = \frac{F(n)}{2\pi n^n} \int_0^{2\pi} \exp(-in\theta) \frac{F(ne^{i\theta})}{F(n)} \, d\theta$$

$$\approx \frac{e^n}{2\pi n^n} \int_{-\varepsilon}^{\varepsilon} \exp\left(-in\theta + \log F(ne^{i\theta}) - \log F(n)\right) \, d\theta.$$

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Example (Saddle point example continued)

- The Maclaurin expansion yields

$$-in\theta + \log F(ne^{i\theta}) - \log F(n) = -n\theta^2/2 + O(n\theta^3).$$

- This gives, with $b_n = 2\pi n^n e^{-n} a_n$, Laplace's approximation:

$$b_n \approx \int_{-\varepsilon}^{\varepsilon} \exp(-n\theta^2/2)\, d\theta \approx \int_{-\infty}^{\infty} \exp(-n\theta^2/2)\, d\theta = \sqrt{2\pi/n}.$$

- This recaptures Stirling's approximation, since $n! = 1/a_n$:

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Multivariate asymptotics — some quotations

- (Bender 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."
- (Odlyzko 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."
- (Flajolet/Sedgewick 2009) "Roughly, we regard here a bivariate GF as a collection of univariate GFs ...."
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Standing assumptions

- We use boldface to denote a multi-index: $\mathbf{z} = (z_1, \dots, z_d)$, $\mathbf{r} = (r_1, \dots, r_d)$. Similarly $\mathbf{z}^{\mathbf{r}} = z_1^{r_1} \dots z_d^{r_d}$.
- A (multivariate) sequence is a function $a : \mathbb{N}^d \to \mathbb{C}$ for some fixed d. Usually write $a_{\mathbf{r}}$ instead of $a(\mathbf{r})$.
- The generating function (GF) is the formal power series

$$F(\mathbf{z}) = \sum_{\mathbf{r} \in \mathbb{N}^d} a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}}.$$

- Assume $F(\mathbf{z}) = G(\mathbf{z})/H(\mathbf{z})$ where G, H are polynomials. The singular variety $\mathcal{V} := \{\mathbf{z} : H(\mathbf{z}) = 0\}$ consists of poles.
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Outline of ACSV project results (steps 3–5)

- Given a direction $\bar{\mathbf{r}}$, to compute asymptotics of $a_{\mathbf{r}}$ in that direction we first restrict to a variety $\mathrm{crit}(\bar{\mathbf{r}})$ of critical points.
- A subset $\mathrm{contrib}(\bar{\mathbf{r}}) \subseteq \mathrm{crit}(\bar{\mathbf{r}})$ contributes to asymptotics.
- For $\mathbf{p} \in \mathrm{contrib}(\bar{\mathbf{r}})$, there is a full asymptotic series $\mathcal{A}(\mathbf{p})$ depending on the type of singularity at $\mathbf{p}$. Each term is computable from finitely many derivatives of G and H at $\mathbf{p}$.
- This yields an asymptotic expansion

$$a_{\mathbf{r}} \sim \sum_{\mathbf{p} \in \mathrm{contrib}(\bar{\mathbf{r}})} \mathbf{p}^{-\mathbf{r}} \mathcal{A}(\mathbf{p})$$

  that is uniform on compact subsets of directions, provided the geometry at $\mathbf{p}$ does not change.

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Simplest geometries: generic shape of $\mathcal{A}(\mathbf{p})$

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

$$\sum a_k |\mathbf{r}|^{-(d-n)/2-k}$$

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

$$a_0 = G(\mathbf{p})C(\mathbf{p})$$

where C depends on the derivatives to order 2 of H;
- (multiple point, $n = d$)

$$a_0 = G(\mathbf{p})(\det J(\mathbf{p}))^{-1}$$

where J is the Jacobian matrix $(\partial H_i / \partial z_j)$, other a_k are zero;
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$$G(\mathbf{p})P\left(\frac{r_1}{p_1}, \dots, \frac{r_d}{p_d}\right),$$

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

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$$a_0 = G(\mathbf{p})C(\mathbf{p})$$

  where C depends on the derivatives to order 2 of H;
- (multiple point, $n = d$)

$$a_0 = G(\mathbf{p})(\det J(\mathbf{p}))^{-1}$$

  where J is the Jacobian matrix $(\partial H_i / \partial z_j)$, other a_k are zero;
- (multiple point, $n \geq d$)

$$G(\mathbf{p})P\left(\frac{r_1}{p_1}, \ldots, \frac{r_d}{p_d}\right),$$

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

Simplest geometries: generic shape of $\mathcal{A}(\mathbf{p})$

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

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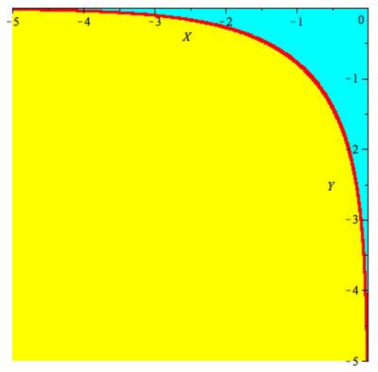
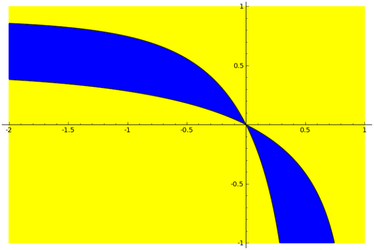
$d = 2$ examples: geometry





Sample problem solutions

1. Estimate a_{rs}, which counts nearest-neighbor walks in $\mathbb{Z}^2$, going from $(0,0)$ to (r,s), with steps in $\{(1,0),(0,1),(1,1)\}$ (Delannoy walks).
   - Uniformly for $r/s, s/r$ away from 0

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

   where $\Delta = \sqrt{r^2+s^2}$.

2. $F = 1/H = \sum_{r,s} a_{rs} x^r y^s$ where

$$H(x,y) = x^2y^2 - 2xy(x+y) + 5\left(x^2+y^2\right) + 14\,xy - 20(x+y) + 19.$$

   - When $1/2 < r/s < 2$, in fact $a_{rs} \sim 1/6$ with exponentially small error.

Basic steps: $d = 2$ example coming up

1. Compute generating function transform of sequence of interest.
2. Invert transform via Cauchy Integral Formula.
3. Approximate by integral of residue in smaller dimension.
4. Convert to Fourier-Laplace integral by trigonometric substitution.
5. Compute asymptotics of F-L integral.

Step 3(a): localization

- Suppose that (z_*, w_*) is a smooth strictly minimal pole with nonzero coordinates, and let $\rho = |z_*|, \sigma = |w_*|$. Let C_a denote the circle of radius a centred at 0.
- By Cauchy, for small $\delta > 0$,

$$a_{rs} = (2\pi i)^{-2} \int_{C_\rho} z^{-r} \int_{C_{\sigma-\delta}} w^{-s} F(z, w) \, \frac{dw}{w} \, \frac{dz}{z}.$$

- The inner integral is small away from z_*, so that for some small neighbourhood N of z_* in C_ρ,

$$a_{rs} \approx I := (2\pi i)^{-2} \int_{N} z^{-r} \int_{C_{\sigma-\delta}} w^{-s} F(z, w) \, \frac{dw}{w} \, \frac{dz}{z}.$$

- Note that this is because of strict minimality: off N, the function $F(z, \cdot)$ has radius of convergence greater than σ, and compactness allows us to do everything uniformly.

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Step 3(b): residue

- By smoothness, there is a local parametrization $w = g(z) := 1/v(z)$ near z_*.
- If δ is small enough, the function $w \mapsto F(z, w)/w$ has a unique pole in the annulus $\sigma - \delta \le |w| \le \sigma + \delta$. Let $\Psi(z)$ be the residue there.
- By Cauchy,

$$I = I' + (2\pi i)^{-1} v(z)^s \Psi(z),$$

where

$$I' := (2\pi i)^{-2} \int_N z^{-r} \int_{C_{\sigma+\delta}} w^{-s} F(z, w) \, \frac{dw}{w} \, \frac{dz}{z}.$$

- Clearly $|z_*^r I'| \to 0$, and hence

$$a_{rs} \approx (2\pi i)^{-1} \int_N z^{-r} v(z)^s \Psi(z) \, dz.$$

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Step 4: Fourier-Laplace integral

- We make the substitution

$$f(\theta) = -\log \frac{v(z_* e^{i\theta})}{v(z_*)} + i\frac{r\theta}{s}$$
$$A(\theta) = \Psi(z_* \exp(i\theta)).$$

- This yields

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Order of vanishing of f

- Let $\alpha := r/s$, so that

$$f'(0) = -i\left(\frac{z_* v'(z_*)}{v(z_*)} - \alpha\right).$$

If $zv'(z_*)/v(z_*) \neq \alpha$, our "reduction" is of no use, owing to oscillation.

- If $zv'(z_*)/v(z_*) = \alpha$ (critical point equation), we definitely get a result of order $|z_*|^{-r}|w_*|^{-s}$ as $r \to \infty$ with $r/s = \alpha$.
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$$f''(0) = \frac{z_*^2 v''(z_*)}{v(z_*)} + \frac{z_* v'(z_*)}{v(z_*)} - \left(\frac{z_* v'(z_*)}{v(z_*)}\right)^2$$

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- Similar to above example, but get a sum of residues in the inner integral.
- The residues are not individually integrable so we need to keep the sum.
- The sum can be rewritten as an integral over a simplex.
- So we still get an integral of the same general form in the end, with a trickier domain.
- Other local geometries still lead via different routes to similar integrals.

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Fourier-Laplace integrals

- We have reduced to asymptotic ($\lambda >> 0$) analysis of Fourier-Laplace integrals of the form

$$I(\lambda) = \int_D e^{-\lambda f(\mathbf{t})} A(\mathbf{t})\, d\mathbf{t}$$

  where:
  - $\mathbf{0} \in D \subset \mathbb{R}^d$, $f(\mathbf{0}) = f'(\mathbf{0}) = 0$.
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Low-dimensional examples of Fourier-Laplace 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 $f = 1$ on $x = 0$; tricky interplay of decay and oscillation.

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Simplex corners now intrude, continuum of critical points.

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Higher order terms

- These are necessary when any of the following occur:
  - leading term cancels in deriving other formulae;
  - leading term is zero because of numerator;
  - we want accurate numerical approximations in the non-asymptotic regime.
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Hörmander's explicit formula

The asymptotic contribution of an isolated nondegenerate stationary point is

$$\left(\det\left(\frac{\lambda f''(\mathbf{0})}{2\pi}\right)\right)^{-1/2} \sum_{k\geq 0} \lambda^{-k} L_k(A, f)$$

where L_k is a differential operator of order $2k$ evaluated at $\mathbf{0}$. Specifically,

$$\begin{aligned} \underline{f}(t) &= f(t) - (1/2) t f''(0) t^T \\ \mathcal{D} &= \sum_{a,b} (f''(\mathbf{0})^{-1})_{a,b} (-\mathrm{i}\partial_a)(-\mathrm{i}\partial_b) \\ L_k(A, f) &= \sum_{l\leq 2k} \frac{\mathcal{D}^{l+k}(A\underline{f}^l)(0)}{(-1)^k 2^{l+k} l!(l+k)!}. \end{aligned}$$

Example (Binomial coefficients)

The binomial coefficient $\binom{r+s}{s}$ has generating function $(1-x-y)^{-1}$, so the diagonal coefficients yield $\binom{2r}{r}$.

The relative error in our approximation is:

n	1st	2nd	3rd	4th
1	-0.128	0.013	0.004	-0.002
2	-0.063	0.003	0.0006	-8×10^{-5}
4	-0.032	0.0005	7×10^{-5}	-4×10^{-6}
8	-0.016	0.0001	9×10^{-6}	-2×10^{-7}
16	-0.008	3×10^{-5}	1.2×10^{-6}	-1.1×10^{-8}
32	-0.004	8×10^{-6}	1.5×10^{-7}	-6.6×10^{-10}

There is plenty to be done

- Asymptotics for Fourier-Laplace integrals with degenerate singularities.
- Phase transitions as the direction varies.
- Probabilistic limit laws: beyond generic Gaussian case.
- Making everything algorithmic, implementation in Sage.
- Second edition of monograph with Pemantle scheduled for 2021.

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Example (Gessel walks)

- Walks with steps in $\{E, NE, W, SW\}$ restricted to lie in the positive quadrant.
- A notoriously tough class to enumerate, done via huge amounts of computer algebra.
- We can express the number of such walks as the diagonal coefficients of a rational function in 2 variables.
- Geometry of the singular variety is more complicated, leading to more complicated geometry of phase.
- Phase looks locally like $u^3 + v^3 + uv^2 + u^2v$ instead of $u^2 + v^2$.

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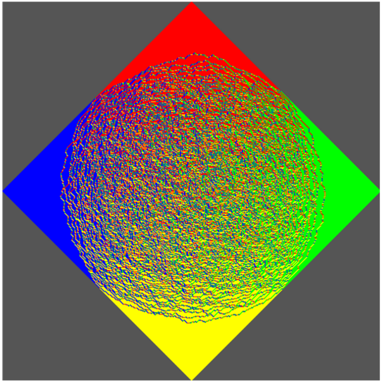
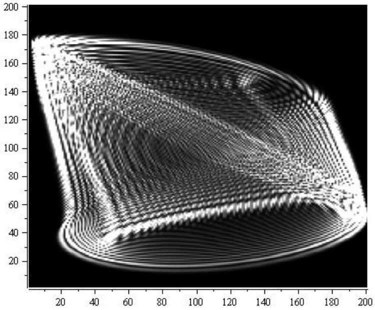
Phase transitions and limit laws





Algorithmic implementation

- The expansions based on Hörmander's results are now included in the core implementation of Sage.
- The current implementation is quite slow, with obvious algorithmic inefficiencies.
- Higher order asymptotics are important but we only have an algorithm for the nondegenerate case.
- Interesting issue: we need to factor in the local analytic ring but we can only factor algorithmically in the algebraic local ring (?).

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Example (local factorization of lemniscate)

- Given $F = 1/H$ where
  $H(x, y) = 19 - 20x - 20y + 5x^2 + 14xy + 5y^2 - 2x^2y - 2xy^2 + x^2y^2$.
- Here $\mathcal{V}$ is smooth at every point except $(1, 1)$, which we see by solving the system $\{H = 0, \nabla H = 0\}$.
- At $(1, 1)$, changing variables to $h(u, v) := H(1 + u, 1 + v)$, we see that $h(u, v) = 4u^2 + 10uv + 4v^2 + C(u, v)$ where C has no terms of degree less than 3.
- The quadratic part factors into distinct factors, showing that $(1, 1)$ is a transverse multiple point.
- Note that our double point formula does not require details of the individual factors. However this is not the case for general multiple points.

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Generic smooth point asymptotics in dimension 2

Theorem

Suppose that $F = G/H$ has a strictly minimal simple pole at $\mathbf{p} = (z^*, w^*)$. If $Q(\mathbf{p}) \neq 0$, then when $s \to \infty$ with $(rwH_w - szH_z)_{|\mathbf{p}} = 0$,

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

The apparent lack of symmetry is illusory, since $wH_w/s = zH_z/r$ at $\mathbf{p}$.

- This, the simplest multivariate case, already covers hugely many applications.
- Here $\mathbf{p}$ is given, which specifies the only direction in which we can say anything useful. But we can vary $\mathbf{p}$ and obtain asymptotics that are uniform in the direction.

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Generic double point in dimension 2

Theorem

Suppose that $F = G/H$ has a strictly minimal pole at $\mathbf{p} = (z_*, w_*)$, which is a double point of $\mathcal{V}$ such that $G(\mathbf{p}) \neq 0$. Then as $s \to \infty$ for r/s in $\mathrm{K}(\mathbf{p})$,

$$a_{rs} \sim (z_*)^{-r}(w_*)^{-s}\left[\frac{G(\mathbf{p})}{\sqrt{(z_* w_*)^2\,\mathrm{Q}(\mathbf{p})}} + O(e^{-c(r+s)})\right]$$

where Q is the Hessian of H.

- Note that
  - the expansion holds uniformly over compact subcones of K;
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