

# Higher order asymptotics from multivariate generating functions

Mark C. Wilson, University of Auckland  
(joint with Robin Pemantle, Alex Raichev)

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## References

- ▶ Our papers at mvGF site:  
[www.cs.auckland.ac.nz/~mcw/Research/mvGF/](http://www.cs.auckland.ac.nz/~mcw/Research/mvGF/) .
- ▶ P. Flajolet and R. Sedgewick, *Analytic Combinatorics*, Cambridge University Press, 2009.
- ▶ A. Odlyzko, survey on Asymptotic Enumeration Methods in *Handbook of Combinatorics*, Elsevier 1995, available from [www.dtc.umn.edu/~odlyzko/doc/asymptotic.enum.pdf](http://www.dtc.umn.edu/~odlyzko/doc/asymptotic.enum.pdf).
- ▶ E. Bender, survey on Asymptotic Enumeration, *SIAM Review* 16:485-515, 1974.
- ▶ L. Hörmander, *The Analysis of Linear Partial Differential Operators* (Ch 7), Springer, 1983.

## Notation

- ▶ Boldface denotes a multi-index:  $\mathbf{z} = (z_1, \dots, z_d)$ ,  
 $\mathbf{r} = (r_1, \dots, r_d)$ ,  $\mathbf{z}^{\mathbf{r}} = z_1^{r_1} \dots z_d^{r_d}$ ,  $d\mathbf{z} = dz_1 \wedge dz_2 \wedge \dots \wedge dz_d$ .

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- ▶ If the series converges in a neighbourhood of  $\mathbf{0} \in \mathbb{C}^d$ , then  $F$  defines an analytic function there.

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- ▶  $F = G/H$  with  $G, H$  entire functions but  $F$  is not itself entire. Key examples: rational function that is not a polynomial.

## $d = 1$ : analysis is easy

- ▶ Consider the Cauchy integral representation

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

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- ▶ Thus  $a_r = \int_{C'} \omega - \sum_{c \neq 0} \text{Res}(\omega, c)$  and the integral is exponentially smaller than the residues.
- ▶ Note that if  $c \neq 0$ , then  $\text{Res}(\omega, c) = c^{-r} \text{Res}(F, c)$  and so asymptotics are dominated by the pole with smallest modulus. This is positive real (Vivanti-Pringsheim).

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

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- ▶ (Flajolet/Sedgewick 2009) “Roughly, we regard here a bivariate GF as a collection of univariate GFs . . . .”



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- ▶ Other collaborators: Yuliy Baryshnikov, Wil Brady, Andrew Bressler, Timothy DeVries, Manuel Lladser, Alexander Raichev, Mark Ward, . . . .

## Cauchy integral representation

- ▶ Let  $U$  be the open polydisc of convergence,  $\partial U$  its boundary,  $C$  a product of circles centred at  $\mathbf{0}$ , inside  $U$ . Then

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

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- ▶ Good general idea: **saddle point method**: using analyticity, we deform the contour  $C$  to minimize the maximum modulus of the integrand. Usually we minimize only the factor  $|z|^{-|r|}$ .
- ▶ The other main idea is **residue theory**. The **Leray residue formula** and reduces dimension of the integral by 1; we still need to integrate the residue form.

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- ▶ Otherwise: try resolution of singularities or other approach.
- ▶ The analysis depends on the direction  $\bar{r}$  as a parameter. If done right the dependence is as uniform as possible.

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- ▶ Asymptotics in each fixed direction  $\bar{\mathbf{r}}$  are determined by the geometry of the **singular variety**  $\mathcal{V}$  (given by  $H = 0$ ) near a **contributing** point  $\mathbf{z}^*(\bar{\mathbf{r}})$ .

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- ▶ A necessary condition:  $\mathbf{z}^*(\bar{\mathbf{r}}) \in \text{crit}(\bar{\mathbf{r}})$  where the finite subset  $\text{crit}(\bar{\mathbf{r}})$  is geometrically well defined, and algorithmically computable by symbolic algebra.



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- ▶ When  $\mathbf{z}^*(\bar{\mathbf{r}})$  is a smooth point (simple pole) of  $\mathcal{V}$ ,

$$a_{\mathbf{r}} \sim \mathbf{z}^*(\bar{\mathbf{r}})^{-\mathbf{r}} \sum_{q \geq 0} b_q(\mathbf{z}^*) |\mathbf{r}|^{-(d-1)/2-q}$$

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- ▶ Leading term can be expressed in terms of outward normal to, and Gaussian curvature of,  $\mathcal{V}$  in appropriate coordinates.

$d = 2$ , smooth point, explicit leading term

- ▶ 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

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

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

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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, transfer matrix method, ....

## Example: Delannoy numbers

- ▶ Consider walks in  $\mathbb{Z}^2$  from  $(0,0)$ , steps in  $(1,0), (0,1), (1,1)$ . Here  $F(z, w) = (1 - z - w - zw)^{-1}$ .

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- ▶ Note  $\mathcal{V}$  is globally smooth and crit turns out to be given by  $1 - z - w - zw = 0, z(1 + w)s = w(1 + z)r$ . There is a unique solution for each  $r, s$ .

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

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

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

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

## Extensions, jargon, applications

Check out the following in the references — no time here!

- ▶ higher order poles (“multiple points”, e.g. queueing networks);
- ▶ other nonsmooth points (“cone points”, e.g. tilings);
- ▶ non-generic directions (“Airy phenomena”, e.g. maps);
- ▶ periodicity (“torality”, e.g. quantum random walks);
- ▶ (Gaussian) limit laws follow directly from the analysis;

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- ▶ Higher order terms are useful for many reasons (e.g. better approximations for smaller indices, cancellation of lower terms).
- ▶ There are many “formulae” in the literature for asymptotic expansions, but higher order terms are universally acknowledged to be hard to compute.



## Explicit integral: Delannoy numbers

- ▶ The integral of the residue turns out to be

$$\int_{-\varepsilon}^{\varepsilon} \exp \left[ ir\theta - s \log \left( \frac{1 + z^* e^{i\theta}}{1 + z^*} \frac{1 - z^*}{1 - z^* e^{i\theta}} \right) \right] \frac{1}{1 - z^* e^{i\theta}} d\theta.$$

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

## Fourier-Laplace integrals

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  - ▶ typically  $\det g''(\mathbf{0}) \neq 0$  and there are no other **stationary points** of the phase on  $D.$
- ▶ Difficulties in analysis: interplay between exponential and oscillatory decay, nonsmooth boundary of simplex.

## Low-dimensional examples of F-L integrals

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- ▶ Multiple point with  $n = 2, d = 1$  gives an 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.

## Asymptotics from F-L integrals

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- ▶ If  $u(\mathbf{0}) \neq 0$  then the leading term is given by  $b_0 = u(\mathbf{0})$ . This is fine, but how to compute the higher order terms?

## Explicit series: Hörmander's formula

We want the coefficients  $b_q$  from above. Define

$$L_q(u, g) := \sum_{l=0}^{2q} \frac{\mathcal{H}^{q+l}(\underline{u}g^l)(\mathbf{0})}{(-1)^q 2^{q+l} l! (q+l)!},$$

$$\underline{g}(\theta) = g(\theta) - \frac{1}{2} \theta g''(\mathbf{0}) \theta^T$$

$$\mathcal{H} = - \sum_{a,b} (g''(\mathbf{0})^{-1})_{a,b} \partial_a \partial_b.$$

Then  $b_q = L_q(u, g)$ .

## Consequence of Hörmander for our mvGF application



$$a_{\mathbf{r}} \sim \mathbf{z}^{*\mathbf{-r}} \left[ (2\pi)^{(n-d)/2} (\det M(\mathbf{z}^*))^{-1/2} \sum_{0 \leq q} c_q r_d^{(n-d)/2-q} \right],$$

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as  $n \rightarrow \infty$ , where

$$c_1^{-3}c_2^{-2} \approx 71.16220050$$

$$b_0 = \frac{13^{3/4}\sqrt{3}}{156\sqrt{\pi}}(5 + \sqrt{13}) \approx 0.36906$$

$$b_1 = -(5/1898208)13^{3/4}\sqrt{3}(79\sqrt{13} + 767)/\sqrt{\pi} \approx -0.018536$$

## Delannoy example: improved numerics

Here  $E_1, E_2$  denote the relative error when using the 1- and 2-term approximations  $A_1, A_2$ .

$n$	1	2	4	8	16
$a_{2n,3n}$	25	1289	$4.673 \cdot 10^6$	$8.528 \cdot 10^{13}$	$3.978 \cdot 10^{28}$
$A_1$	26.263	1321.542	$4.732 \cdot 10^6$	$8.581 \cdot 10^{13}$	$3.990 \cdot 10^{28}$
$A_2$	24.944	1288.355	$4.673 \cdot 10^6$	$8.527 \cdot 10^{13}$	$3.978 \cdot 10^{28}$
$E_1$	-5%	-2.5%	-1.3%	-0.6%	-0.3%
$E_2$	0.2%	0.05%	0.01%	0.003%	0.0007%

## Example: cancellation in variance computation

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- ▶  $W$  counts words over a  $d$ -ary alphabet  $X$ , where  $x_j$  marks occurrences of letter  $j$  of  $X$  and  $y$  marks snaps (occurrences of nonoverlapping pairs of duplicate letters).

## Example: variance computation II

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- ▶ However the first order terms cancel out in the computation of the variance. So we require at least a 2-term expansion for the mean and second moment.
- ▶ The answer is (for  $d = 3$ ):

$$E[\psi_n] = \frac{3}{4}n - \frac{15}{32} + O\left(\frac{1}{n}\right)$$

$$E[\psi_n^2] = \frac{9}{16}n^2 - \frac{27}{64}n + O(1)$$

$$V[\psi_n] = \frac{9}{32}n + O(1)$$

## Application: algebraic functions

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- ▶ The construction is algorithmic but quite involved and uses a sequence of **blowups** to resolve singularities.

## Example: Narayana numbers

- ▶ The GF for the Narayana numbers (enumerating Dyck paths by length and number of peaks) is

$$F(z, w) = \frac{1}{2} \left( 1 + z(w - 1) - \sqrt{1 - 2z(w + 1) + z^2(w - 1)^2} \right).$$



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- ▶ Interestingly the whole process commutes with the specialization  $w = 1$ , which gives an analogous result for the (shifted) Catalan numbers  $C_n$ , agreeing with what is known from other methods:

$$C_n = 4^n \left[ \frac{1}{4\sqrt{\pi}} n^{-3/2} + \frac{3}{32\sqrt{\pi}} n^{-5/2} + O(n^{-7/2}) \right].$$

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- ▶ Contributing points can lie at infinity (more topology!)
- ▶ Plenty of stimulus for further research, even if Safonov proves to be less effective than other approaches (such as directly resolving the Cauchy integral).

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- ▶ The number of (partial) derivatives needed to evaluate the  $n$ th term is likely superpolynomial in the number of terms. Using Hörmander we need to go to order  $2n$  (or  $6n - 6$  if completely naive), and the partials are indexed by partitions.

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- ▶ There are many “formulae” for higher order terms in the literature but Hörmander’s is the only useful one we have found.
- ▶ Of course we do not require a formula, only an algorithm. The coefficients are given implicitly by the Morse lemma’s change of variables and can be found by solving a triangular system of equations.
- ▶ The number of (partial) derivatives needed to evaluate the  $n$ th term is likely superpolynomial in the number of terms. Using Hörmander we need to go to order  $2n$  (or  $6n - 6$  if completely naive), and the partials are indexed by partitions.
- ▶ However the error reduces quickly with the number of terms, so not many terms are needed in practice it seems.

## Open problems

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- ▶ Patch together asymptotics in different regimes: uniformity, phase transitions.