Analytic Combinatorics (in Several Variables)

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Please note!

- This is a general overview of a big area, so necessarily omits most details and citations.
- Also, I work on several other research topics, mostly centered around collective decision-making:
  - social choice, voting, resource allocation (relevant to AI and ML)
  - network science, diffusion of beliefs, preferences, etc
  - scientometrics, improving science
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What is Analytic Combinatorics?

- It presumably means the use of mathematical analysis to study problems in combinatorics.
- Analysis has many branches: real, complex, functional, differential equations, measure theory, ... There are many possible ways to apply it to combinatorics!
- The most common usage of the term refers to the application of complex analysis to combinatorial enumeration (counting, discrete probability).

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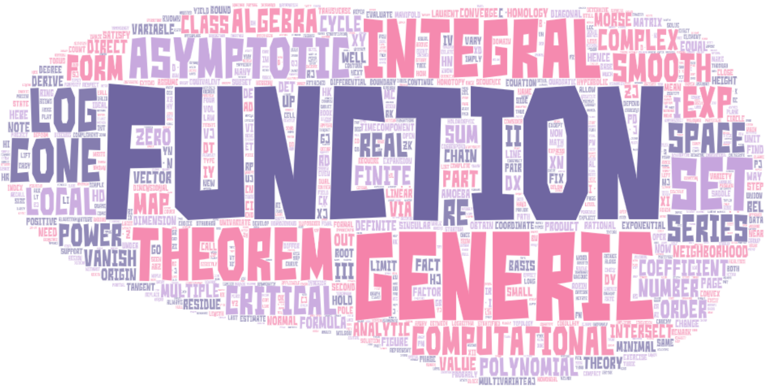
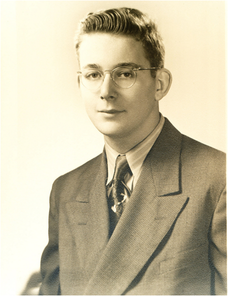
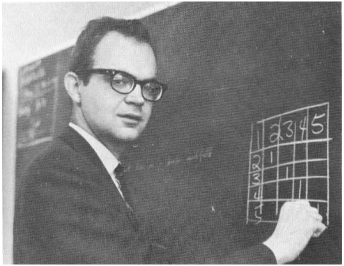
Word cloud from our book



Karp vs Knuth?





- Very roughly, there have been two schools of algorithms researchers.
- One (related to Complexity Theory) cares about P vs NP and big-O (or looser) approximation.
- The other (Analysis of Algorithms — AofA) cares about constant factors and improving polynomial-time algorithms. Big names: Knuth, Sedgewick, Flajolet.

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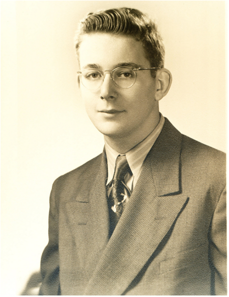

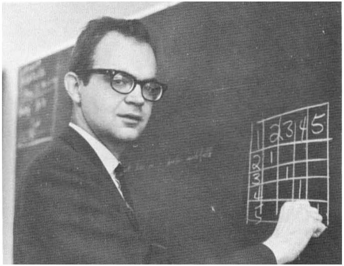

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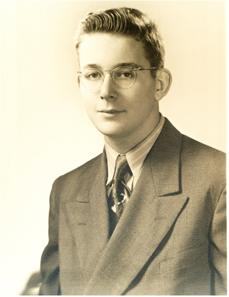 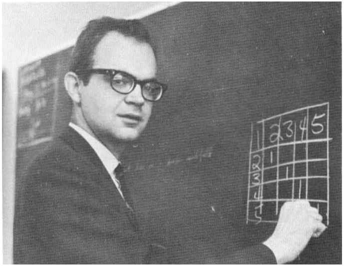

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AofA and analytic combinatorics

- Basic principle of AofA: detailed probabilistic analysis of large combinatorial structures gives insight into performance of algorithms.
- Basic mathematical question: Given a sequence (a_n) of relevance, derive a tight asymptotic approximation for a_n.
- That is, find a simply understood sequence (b_n) with $\lim_{n\to\infty} a_n/b_n = 1$. Goes beyond big-O and even big-Theta.
- Analytic combinatorics developed for AofA also helps to devise random generation algorithms and test random number generators.
- Analytic combinatorics has many applications to information theory, statistical physics, probability and stochastic processes, bioinformatics . . . .

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Classic AofA problems

- $a_n =$ expected running time of your particular flavor of quicksort on randomly shuffled input: internal path length of binary search tree;
- $a_n =$ expected number of occurrences of a given pattern (substring, regular expression) in a large random text, or waiting time until first occurrence;
- $a_n =$ expected number of entries in an open addressing hash table before first collision occurs: random mappings, balls in bins;
- $a_n =$ expected height of a binary search tree grown by random insertions.

Precise answers to these are known, and the variance and entire limiting distributions are known in most cases.

The foundational method of analytic combinatorics

1. Given a sequence (a_n) of interest, express it recursively somehow.
2. Express a_n as the Maclaurin coefficient of an analytic function, the generating function.
3. Using the form of this function, derive information about a_n.

This procedure goes back at least to de Moivre (1730) in the study of discrete probability. Step 2 is the discrete analog of the Laplace transform and Step 3 to inverting it — typical techniques in solving differential equations.

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Example (Fibonacci)

- Consider the Fibonacci numbers defined by the recurrence relation

$$a_n = \begin{cases} a_{n-1} + a_{n-2} & n \geq 2 \\ n & n \in \{0, 1\}. \end{cases}$$

- The generating function $F(x) = \sum_{n\geq 0} a_n x^n$ is easily seen to satisfy the linear equation $(1 - x - x^2)F(x) = x$ and hence is a rational function.
- Partial fraction decomposition yields $\frac{x}{1-x-x^2} = \frac{1}{\sqrt{5}}\left(\frac{1}{1-\theta x} - \frac{1}{1+\theta^{-1}x}\right)$ where $\theta = \frac{1+\sqrt{5}}{2} \approx 1.618$ is the reciprocal of the positive root of the denominator.
- Thus by geometric series expansion

$$a_n = \frac{1}{\sqrt{5}}\left(\theta^n - (-\theta)^{-n}\right) \sim \frac{1}{\sqrt{5}}\theta^n.$$

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The key principles of coefficient extraction

- The location of dominant points of the singular variety $\mathcal{V}$ of the GF determines the exponential growth rate of coefficients;
- The type of singularity determines subexponential factors.

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Example (Finding GF the modern way)

- A binary tree is either a single external node or an internal node connected to a pair of binary trees. Let $\mathcal{T}$ be the class of binary trees:

$$\mathcal{T} = \{ext\} \cup \{int\} \times \mathcal{T} \times \mathcal{T}.$$

- In terms of a formal grammar

$$< tree >=< ext > | < int >< tree >< tree > .$$

- Give $< ext >$ weight a and $< int >$ weight b to obtain the GF enumerating binary trees by total weight:

$$T(z) = z^a + z^b T(z)^2.$$

- Special cases: $a = 0, b = 1$ counts trees by internal nodes; $a = 1, b = 0$ by external nodes; $a = b = 1$ by total nodes.
- Every unambiguous context-free language leads to an algebraic equation for the GF in a similar way.

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Alternative method of deriving asymptotics from GF

- A more general method uses Cauchy's Integral Formula

$$a_n = \frac{1}{2\pi i} \int_{\mathcal{C}} F(z) z^{-n} \frac{dz}{z}$$

for some small circle $\mathcal{C}_\varepsilon$ of radius ε enclosing the origin.

- We can expand it just beyond $z = \theta^{-1}$, picking up a residue:

$$a_n = \frac{1}{2\pi i} \int_{\mathcal{C}_{\theta^{-1}+\varepsilon}} F(z) z^{-n} \frac{dz}{z} - \operatorname{Res}(F(z) z^{-n-1}; \theta^{-1}).$$

- The residue at the simple pole is easily calculated as

$$(\theta^{-1})^{-n} \operatorname{Res}(zF(z); \theta^{-1}) = \theta^n \lim_{z \to \theta^{-1}} (z - \theta^{-1}) zF(z) = -\theta^n \frac{1}{\theta + \theta^{-1}}$$

and the integral is exponentially smaller because it is bounded by $K(\theta^{-1} + \varepsilon)^{-n}$. Thus we eventually get the same asymptotic result.

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Generic case: asymptotics from univariate GFs

- Rational GF: $a_n \sim \alpha \rho^n$ where $1/\rho$ is the smallest modulus root of the denominator.
- Catalan numbers have an algebraic irrational GF, the asymptotics look like $4^n/\sqrt{\pi n^3}$, which is typical.
- Periodicity can be handled easily, as can exponentially smaller correction terms.
- Everything is effectively computable for rational and algebraic GFs.

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Sample of interesting multivariate problems

- Enumerating lattice paths restricted to the positive quadrant (generalized gambler's ruin problems).
- Quantum random walk in d dimensions: determine the feasible region.
- Tiling models from statistical physics: determine the frozen region.
- Partition functions in queueing networks: numerical approximation for large parameter values.
- Probability limit laws (e.g. limiting distribution of the number k of occurrences of a fixed substring in a random string of length n).

Example (Delannoy walks)

- We count walks on the lattice $\mathbb{Z}^2$ starting at $(0,0)$ and ending at (r,s), with each step chosen from $\{\uparrow, \rightarrow, \nearrow\}$.
- The recurrence is

$$a_{rs} = \begin{cases} a_{r-1,s-1} + a_{r-1,s} + a_{r,s-1} & \text{if } r > 1, s > 1 \\ 1 & (r,s) = (0,0) \\ 0 & \text{otherwise.} \end{cases}$$

  and GF is $(1 - x - y - xy)^{-1}$.
- How to compute asymptotics for $a_{r,s}$ for large $r + s$?

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Technical difficulties in the multivariate case

- Deriving multivariate GFs is often not much harder than in the univariate case.
- However analysing them is much harder, even for rational functions:
  - Model: how should we go to infinity, to take asymptotics?
  - Algebra: partial fraction decomposition does not apply in general.
  - Geometry: the singular variety $\mathcal{V}$ is more complicated.
    - it does not consist of isolated points, and may self-intersect;
    - Topology of $\mathbb{C}^d \setminus \mathcal{V}$ is much more complicated.
  - Analysis: the (Leray) residue formula is much harder to use.
  - Computation: harder owing to the curse of dimensionality.

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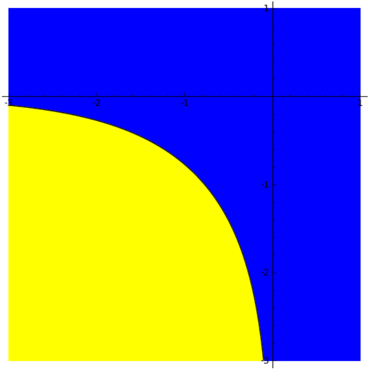
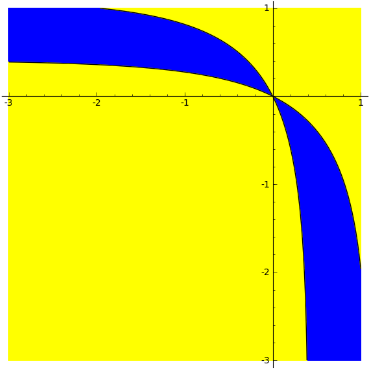
Singular varieties (log coordinates)





The ACSV project

- Robin Pemantle (UPenn) and I began a systematic analysis of multivariate rational GFs — see `https://acsvproject.org`.
- Currently producing – with Steve Melczer (Waterloo) – the 2nd edition of our monograph with Cambridge University Press.
- Methods and results have been used in coding/information theory, number theory, string theory, statistical physics, quantum gravity, mathematical biology, chemistry, ...
- Formulae require substantial computer algebra computation, unlike the univariate case. We have Sage code implementing many of the calculations.

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General procedure for coefficient asymptotics

1. Express $a_{\mathbf{r}}$ using the Cauchy Integral Formula.
2. Choose direction of asymptotics.
3. Use residue theory to express $a_{\mathbf{r}}$ in terms of integrals over small cycles around contributing points.
4. Asymptotically approximate by the dominant integrals.
5. Evaluate the dominant integrals somehow!

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Outline of (generic) results achieved so far in ACSV project

- Asymptotics in direction $\overline{\mathbf{r}}$ are determined by the geometry of $\mathcal{V}$ near a (finite) set, $\mathrm{crit}(\overline{\mathbf{r}})$, of critical points which is computable via polynomial algebra.
- To compute asymptotics in direction $\overline{\mathbf{r}}$, we may restrict to a single contributing point $\mathbf{z}_*(\overline{\mathbf{r}})$ lying in the positive orthant.
- There is an asymptotic series $\mathcal{A}(\mathbf{z}_*)$ for $a_\mathbf{r}$, depending on the local geometry of $\mathcal{V}$ near $\mathbf{z}_*$; each term is computable from finitely many derivatives of G and H at $\mathbf{z}_*$.
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Asymptotic formula in simplest case

Theorem (Smooth point formula in dimension 2)

Suppose that $F = G/H$ has a strictly minimal simple pole at $\mathbf{p} = (z^*, w^*)$.
Then when $r, s \to \infty$ on the ray $(rwH_w - szH_z)_{|\mathbf{p}} = 0$,

$$a_{rs} = (z^*)^{-r}(w^*)^{-s} C s^{-1/2} \left(1 + O(s^{-1})\right)$$

and if the Hessian Q of $H \circ \exp$ is nonzero then

$$C = \left[\frac{G(\mathbf{p})}{\sqrt{2\pi}} \sqrt{\frac{-wH_w(\mathbf{p})}{sQ(\mathbf{p})}} \right].$$

- The lack of symmetry is illusory, since $wH_w/s = zH_z/r$ at $\mathbf{p}$.
- Here $\mathbf{p}$ is given, but we can vary $\mathbf{p}$ and obtain asymptotics that are uniform in the direction.
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Delannoy walk asymptotics

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

- Vastly many problems involving walks, sequences, sums of IID random variables are of similar difficulty level.

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Delannoy continued — numerical precision

$$F_{4n,3n} = 432^n \left(a_1 n^{-1/2} + a_2 n^{-3/2} + O(n^{-5/2}) \right) \qquad \text{as } n \to \infty$$

where

$$a_1 = \frac{\sqrt{2}\sqrt{3}\sqrt{5}}{10\sqrt{\pi}} \approx 0.3090193616$$

$$a_2 = -\frac{\sqrt{2}\sqrt{3}\sqrt{5}}{288\sqrt{\pi}} \approx -0.01072983895$$

Compare with actual values:

n	1	2	4	8	16
$F_{n\alpha} c^{n\alpha}$	0.299	0.215	0.153	0.109	0.077
$a_1 n^{-1/2}$	0.309	0.219	0.155	0.109	0.077
$a_1 n^{-1/2} + a_2 n^{-3/2}$	0.299	0.215	0.153	0.109	0.077
1-term rel. % error	3	1.7	0.87	0.43	0.22
2-term rel. % error	0.1	0.025	0.006	0.0014	0.00035

Next simplest case - double point

Theorem (Transverse double point formula in dimension 2)

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 there is a nonempty cone $\mathrm{K}(\mathbf{p})$ of directions such that as $r, s \to \infty$ with (r, s) in $\mathrm{K}(\mathbf{p})$,

$$a_{rs} \sim (z_*)^{-r} (w_*)^{-s} \left[C + O(e^{-c(r+s)}) \right]$$

where $C = \frac{G(\mathbf{p})}{\sqrt{(z_* w_*)^2 \, \mathrm{Q}(\mathbf{p})}}$ and Q is the Hessian of H.

- Note that
  - the expansion holds uniformly away from the boundary of $\mathrm{K}(\mathbf{p})$;
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Example (Number of successes in a coin-flipping game)

- Consider repeatedly flipping a biased coin where heads and tails are swapped partway through. In other words the coin will be biased so that $p = 2/3$ for the first n flips, and $p = 1/3$ thereafter.
- A player desires to get r heads and s tails and is allowed to choose n. On average, how many choices of $n \le r + s$ will be winning choices?
- The GF is readily computed to be

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

- By Theorem 2 the answer is asymptotically 3 up to exponentially small error, whenever $r/(r + s)$ stays in any compact subinterval of $(1/3, 2/3)$.

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Example (diameters of random Cayley graphs)

- From the set $[n] := \{1, ..., n\}$, a collection of t disjoint pairs is named. Then a k element subset, $S \subseteq [n]$ is chosen. Let $a(n, k, t)$ be the number of such S that fail to contain as a subset any of the t pairs.
- The GF turns out to be

$$\frac{1}{(1 - x(1+y))\,(1 - zx^2(1+2y))}.$$

- From a general result similar to the last two, we obtain

$$a(n, k, t) \sim C\left(\frac{k}{n}, \frac{t}{n}\right) n^{-1/2} x_*^{-n} y_*^{-k} z_*^{-t}$$

where x_*, y_*, z_* each satisfy an explicitly given quadratic in n, k and C is explicitly given.

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- Noncombinatorial problems (finding dominant points is harder; need Morse theory, probably)
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Example (Stationary distribution in an edge-flipping model on graphs)

- Choose an edge uniformly at random and with probability p (resp. $1-p$) turn both its endpoints blue (resp. red).
- The stationary distribution of this Markov chain (due to Diaconis) is (up to a simple transformation) encoded for complete graphs by

$$f(x,y) = \frac{1 - x(1+y)}{\sqrt{1 - 2x(1+y) - x^2(1-y)^2}}.$$

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Work in progress on algebraic GFs

- Conjecturally (Christol 1990), every "not obviously ruled out" GF arises as a diagonal of a rational function.
- Every algebraic d-variate GF arises as the diagonal of a rational function in $2d$ variables, and if we relax the definition of diagonal we can replace this by $d + 1$ (Safonov, 2000).
- The main problem is that the rational GF may not preserve nice properties of the original:
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Example (Binary trees)

- Binary trees are counted by $f(x) = \sum_n a_n x^n = (1 - \sqrt{1-4x})/2$ with minimal polynomial $P(x,y) = y^2 - y + x$.
- By standard methods (Furstenberg 1967) $a_n = b_{nn}$ where b is the coefficient sequence of $F(x,y) = y(1-2y)/(1-x-y)$.
- This falls under our results above, EXCEPT the relevant dominant point is $(1/2, 1/2)$ and the numerator vanishes there.
- We needed to derive explicit formulae for higher order terms.
- This turns out to be doable, and we obtain the correct answer

$$a_n \sim 4^{n-1}/\sqrt{\pi n^3}.$$

Example (Binary trees)

- Binary trees are counted by $f(x) = \sum_n a_n x^n = (1 - \sqrt{1-4x})/2$ with minimal polynomial $P(x, y) = y^2 - y + x$.
- By standard methods (Furstenberg 1967) $a_n = b_{nn}$ where b is the coefficient sequence of $F(x, y) = y(1 - 2y)/(1 - x - y)$.
- This falls under our results above, EXCEPT the relevant dominant point is $(1/2, 1/2)$ and the numerator vanishes there.
- We needed to derive explicit formulae for higher order terms.
- This turns out to be doable, and we obtain the correct answer

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References

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- Contact me if you are interested in learning more!