

Infinity in Combinatorics: Asymptotic Enumeration

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6227020800, 87178291200, 1307674368000

What can we say about these numbers?

They grow very fast.

Aha! The numbers are given by the formula $n!$

How fast do they grow?

We want to compare with some “standard quantities”

Stirling’s formula:

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$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$$

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Stirling: 3598695.61...

30! = 265252859812191058636308480000000

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Definition:

$$a_n \sim b_n$$

as $n \rightarrow \infty$ if

$$\lim_{n \rightarrow \infty} \frac{a_n}{b_n} = 1$$

(asymptotic equivalence)

More precision:

$$a_n = b_n + O(c_n)$$

Meaning:

$$|a_n - b_n| \leq K \cdot c_n$$

This is Bachmann's celebrated big-Oh notation, popularised by Landau.

Why are we interested?

Given

$$S_n = \sum_{k=1}^n \binom{n}{k} \frac{(-1)^{k-1}}{k}.$$

First idea: Simplify!

Indeed

$$S_n = H_n = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} \sim \log n$$

(harmonic number)

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She encounters combinatorial structures, like permutations, compositions, partitions, trees, lattice paths, words, . . .

She wants to know how many objects *of size n* there are. And sometimes, an exact formula does not exist, or, if it exists, it is not conclusive.

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Why would a computer scientist be interested?

Standard answer: It is in Knuth's book, and Knuth is interested . . .

Seriously: Her algorithms depends on an input of size n , and she wants to know the performance. (Sorting, searching, . . .).

Some people: Algorithms performs in $O(n^3)$.

What does that mean? Worst-case behaviour.

Even less precise: "polynomial performance"

People who analyse algorithms:

How does the algorithm perform *on average*, with a precisely defined (probabilistic) input model?

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What shall I do when I encounter an asymptotic problem?

- ▶ Maple knows a little bit: $\text{asympt}(f(n),n)$
- ▶ Concrete Mathematics (Graham/Knuth/Patashnik) has a section on it.
- ▶ Bender wrote a survey in SIAM Review (1974); it is a bit dated.
- ▶ Odlyzko wrote a long chapter in the handbook of combinatorics.
- ▶ The long-awaited book “Analytic Combinatorics” by Flajolet/Sedgewick will answer many questions.
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Use generating functions!

Consider

$$\sum_{n \geq 0} a_n z^n$$

and treat it as a function of a complex variable z .

The shortest path between two truths in the real domain passes through the complex domain.

(Hadamard)

Sometimes it is better to consider

$$\sum_{n \geq 0} a_n \frac{z^n}{n!},$$

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Simple example: Fibonacci numbers.

$$F_n = F_{n-1} + F_{n-2}, F_0 = 0, F_1 = 1.$$

$$F(z) = \sum_{n \geq 0} F_n z^n = \frac{z}{1 - z - z^2}.$$

Partial fraction decomposition:

$$F(z) = \frac{1}{\sqrt{5}} \frac{1}{1 - z\alpha} - \frac{1}{\sqrt{5}} \frac{1}{1 - z\beta},$$

with

$$\alpha = \frac{1 + \sqrt{5}}{2}, \quad \beta = \frac{1 - \sqrt{5}}{2}$$

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$$F_n = [z^n]F(z) = \frac{1}{\sqrt{5}}\alpha^n - \frac{1}{\sqrt{5}}\beta^n.$$

(explicit)

$$F_n \sim \frac{1}{\sqrt{5}}\alpha^n.$$

Why? Since $|\beta| < |\alpha|$, or the pole $1/\alpha$ is closer to the origin than $1/\beta$.

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Rational functions are easy!

For enumerative generating functions, 0 isn't a pole. We can (in principle) perform partial fraction decomposition, and so we only need to know what

$$[z^n] \frac{1}{(1 - z\alpha)^{m+1}}$$

is. A simple shift gives

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$$[z^n] \frac{1}{(1-z)^{m+1}} = \binom{n+m}{m} \sim \frac{n^m}{m!}$$

Even if you cannot locate all poles exactly, you win, if you know that they are far away:

The closer the pole is to the origin, the larger the contribution.

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$$1 + 2 + 2$$

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From a composition of $n = c_1 + \cdots + c_k$ we can create 2 compositions of $n + 1$:

$$c_1 + \cdots + (c_k + 1)$$

and

$$c_1 + \cdots + c_k + 1.$$

Hence, since for $n = 1$, there is 1 composition, the answer is 2^{n-1} .
This was too easy, no asymptotics needed.

Carlitz Compositions:

Additional restriction: Always $c_i \neq c_{i+1}$. Now it is not so easy to find the generating function $f(z)$. Trick: Use $K(z, u)$, where the coefficient of $z^n u^k$ is the number of Carlitz compositions of n with last summand k . One derives:

$$K(z, u) = \frac{uz}{1 - uz} + \frac{uz}{1 - uz} K(z, 1) - K(z, zu).$$

This functional equation can be solved by iteration; specialising $u = 1$ eventually leads to

$$f(z) = K(z, 1) = \left(1 + \sum_{j \geq 1} \frac{(-z)^j}{1 - z^j} \right)^{-1}$$

This is not a rational function, but “almost”

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$$K(z, u) = \frac{uz}{1 - uz} + \frac{uz}{1 - uz} K(z, 1) - K(z, zu).$$

This functional equation can be solved by iteration; specialising $u = 1$ eventually leads to

$$f(z) = K(z, 1) = \left(1 + \sum_{j \geq 1} \frac{(-z)^j}{1 - z^j} \right)^{-1}$$

This is not a rational function, but “almost”

There is a dominant pole ρ : The smallest positive root of the equation

$$\sum_{j \geq 1} \frac{\rho^j}{1 + \rho^j} = 1.$$

This can be computed numerically. Consequently

$$[z^n]f(z) \sim C \cdot \beta^n,$$

with 0.45636 , $\beta = 1.75024$. (Unrestricted case: 2)

Derangements:

D_n is the number of fix-point free permutations.

In elementary courses, one derives by inclusion-exclusion:

$$D_n = n! \left(\frac{1}{0!} - \frac{1}{1!} + \frac{1}{2!} - \dots + \frac{(-1)^n}{n!} \right).$$

One notices the truncated series for $1/e$, and thus $D_n/n! \sim \frac{1}{e}$.

More elegantly, one uses (exponential) generating functions:

Permutations are a collection of cycles, and from basic principles of exponential generating functions:

$$\exp \left(\log \frac{1}{1-z} \right) = \frac{1}{1-z}.$$

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But: We can handle restrictions: Forbidding fixpoints, means:

$$f(z) := \exp\left(\log \frac{1}{1-z} - z\right) = \frac{e^{-z}}{1-z}.$$

Again: This is not a rational function, but almost: There is a dominant pole at 1.

$$f(z) \sim \frac{e^{-1}}{1-z},$$

and

$$[z^n]f(z) \sim [z^n] \frac{e^{-1}}{1-z} = e^{-1}.$$

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Binary trees.

Recursion definition: A root and a left resp. right subtree.

Consequently

$$B(z) = 1 + zB^2(z)$$

(this is almost a context-free grammar).

Solving

$$B(z) = \frac{1 - \sqrt{1 - 4z}}{2z}.$$

This is not rational, but has a square-root singularity at $z = \frac{1}{4}$.

Local expansion: (Puiseux)

$$B(z) \sim 2 - 2\sqrt{1 - 4z}.$$

Coefficients:

$$[z^n]\sqrt{1 - z} \sim \frac{n^{-3/2}}{\Gamma(-\frac{1}{2})}.$$

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More generally:

$$[z^n](1-z)^{-\alpha} \sim \frac{n^{\alpha-1}}{\Gamma(\alpha)}.$$

For us (binary trees)

$$\sim \frac{1}{\sqrt{\pi n^{3/2}}} 4^n$$

(Also from the explicit formula $\frac{1}{n+1} \binom{2n}{n}$).

Local expansions can be *translated* into asymptotic expansions of the coefficients. (Under mild technical conditions.)

SINGULARITY ANALYSIS OF GENERATING FUNCTIONS.

(Flajolet and Odlyzko)

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SINGULARITY ANALYSIS OF GENERATING FUNCTIONS.

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So one needs a catalogue of known expansions:

$$\frac{1}{(1-z)^\alpha} \log^\beta \frac{1}{1-z}$$

and perhaps other ones.

Another occurrence of a square-root singularity: the tree function.

Implicitly defined: $y = ze^y$.

$$y(z) = \sum_{n \geq 1} a_n \frac{z^n}{n!}$$

Where is a singularity?

Where the implicit function theorem ceases to apply!

Differentiate w.r.t y :

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$$y = ze^y$$

$$1 = ze^y$$

Consequently $y = \tau = 1$, and $z = \rho = \frac{1}{e}$. The singularity is at $z = 1/e$, and there is a local expansion

$$y(z) \sim 1 - \sqrt{2}\sqrt{1 - ez}$$

It is a fact that the precise knowledge of the behaviour of an analytic function in the vicinity of its singular points is a source of arithmetic properties. (Erich Hecke)

Basic principle:

- ▶ location and type of singular points
- ▶ local expansion
- ▶ translate (“Transfer theorems”)

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Longest runs in binary words.

We are interested in binary words (letters a, b), such that no run of k consecutive a 's can be found.

$$a^{<k} = \varepsilon + a + a^2 + \cdots + a^{k-1}$$

Decomposition:

$$L = a^{<k} (ba^{<k})^*$$

Translate into generating functions:

$$f(z) = \frac{1 - z^k}{1 - z} \frac{1}{1 - z \frac{1 - z^k}{1 - z}} = \frac{1 - z^k}{1 - 2z + z^{k+1}}$$

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This is a rational function, but where are the poles?

Equation:

$$z = \frac{1}{2}(1 + z^{k+1})$$

“bootstrapping”:

$$\rho_k \sim \frac{1}{2}$$

Now plug in $\rho_k = \frac{1}{2} + \varepsilon_k$

$$\frac{1}{2} + \varepsilon_k \sim \frac{1}{2}\left(1 + \frac{1}{2^{k+1}}\right) \quad \text{or} \quad \varepsilon_k \sim \frac{1}{2^{k+2}}$$

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One can show that the other poles are “far away” (Rouché’s theorem!)

$$\frac{1 - z^k}{1 - 2z + z^{k+1}} \sim \frac{\text{constant}}{1 - z/\rho_k}$$

The coefficient of z^n :

$$\sim \text{constant} \rho_k^{-n}$$

Probabilities: divide by 2^n

$$\sim \text{constant} (2\rho_k)^{-n} \sim \text{constant} \left(1 + \frac{1}{2^{k+1}}\right)^{-n} \sim \text{constant} \exp\left(-\frac{n}{2^{k+1}}\right)$$

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If one works out the details, in order to compute the average of the longest run of a 's:

$$E_n \sim \sum_{k \geq 1} \left(1 - e^{-n/2^k}\right).$$

The asymptotics of this is harder than what we have seen so far!

Something similar is of relevance in von Neumann's addition scheme.

Two binary numbers x and y of length n are added as follows: $s = s_n \dots s_0$, where $s_i = x_i + y_i \bmod 2$. The carries will be collected into a separate string (number) c . The process is repeated by adding s and c . It stops when no more carries are there.

The number of iterations is the parameter of interest. If one adds x and y bitwise, it is the longest sequence of 1's, which has a 2 at the right end.

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The height of planar trees.

The average (planar trees with $n + 1$ nodes):

$$E_n = (n + 1) \sum_{k \geq 1} d(k) \frac{\binom{2n}{n+1-k} - 2\binom{2n}{n-k} + \binom{2n}{n-1-k}}{\binom{2n}{n}}$$

$d(k)$ is the number of (positive) divisors of k .

Approximation:

$$E_n \sim \sum_{k \geq 1} d(k) \left(-2 + 4 \frac{k^2}{n} \right) e^{-k^2/n}$$

The technique for this and the average length of the longest run of ones is the Mellin transform!

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Ramanujan's Q -function.

$$Q(n) = 1 + \frac{n-1}{n} + \frac{(n-1)(n-2)}{n^2} + \dots$$

$$Q(n) \sim ?$$

Not so easy. It is also related to a famous open question by Ramanujan (that I solved together with some coauthors). The function appears in many contexts, e.g., in the birthday paradox.

It can be attacked by the Laplace method for integrals, or otherwise.

$$Q(n) \sim \sqrt{\frac{\pi n}{2}}$$

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In discrete mathematics, we deal more with sums than with integrals.

However, Cauchy's integral formula extracts coefficients from power series:

$$[z^n]f(z) = \frac{1}{2\pi i} \int_C f(z) \frac{dz}{z^{n+1}}.$$

A carefully crafted path of integration (going through saddle-points via steepest descents) can be used to estimate the integral.

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Mellin analysis

$$E_n \sim \sum_{k \geq 1} d(k) \left(-2 + 4 \frac{k^2}{n} \right) e^{-k^2/n}$$

$$E_n \sim \sum_{k \geq 1} \left(1 - e^{-n/2^k} \right).$$

Another one:

$$E_n \sim \sum_{k \geq 1} v_2(k) \left(-2 + 4 \frac{k^2}{n} \right) e^{-k^2/n}$$

where $v_2(k)$ is the number of trailing zeroes of k when written in binary. Equivalently, the highest j such that 2^j divides k . The last expression occurs in the analysis of the *register function*. This is the minimal number of extra registers (optimal strategy) to evaluate a given binary (expression) tree. This was invented by Ershov, but appeared earlier in the natural sciences (Horton, Strahler).

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Shape:

$$F(x) = \sum_{k \geq 1} a_k f(b_k x)$$

(“harmonic sum”)

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$$f^*(s) = \int_0^{\infty} f(x)x^{s-1}dx$$

Inversion formula

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} f^*(s)x^{-s}ds,$$

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A simple change of variable:

$$f(ax) \longrightarrow a^{-s} f^*(s)$$

and therefore

$$F(x) = \sum_{k \geq 1} a_k f(b_k x) \longrightarrow \sum_{k \geq 1} a_k b_k^{-s} \cdot f^*(s).$$

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is a (generalised) *Dirichlet* series and often admits a nice form in terms of classical functions.

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Example:

$$\sum_{k \geq 1} d(k) \left(-2 + 4k^2 x^2 \right) e^{-k^2 x^2} \longrightarrow$$
$$\sum_{k \geq 1} d(k) k^{-s} \left(\left(-2 + 4x^2 \right) e^{-x^2} \right)^* (s)$$

Both parts are readily computed:

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So

$$\begin{aligned} & \sum_{k \geq 1} d(k) \left(-2 + 4k^2 x^2 \right) e^{-k^2 x^2} \\ &= \frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \zeta^2(s) (s-1) \Gamma\left(\frac{s}{2}\right) x^{-s} ds \end{aligned}$$

The integral is computed (with an error) by *residues*.

(Technical remark. The line of integration is either shifted to the left or right, depending on $x \rightarrow 0$ or $x \rightarrow \infty$.)

The average height of a random planar tree with n nodes is
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If one does the same for the register instance, one gets

$$\begin{aligned} & \sum_{k \geq 1} v_2(k) \left(-2 + 4k^2 x^2 \right) e^{-k^2 x^2} \\ &= \frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \frac{\zeta(s)}{2^s - 1} (s-1) \Gamma\left(\frac{s}{2}\right) x^{-s} ds \end{aligned}$$

And now, there are poles at $\frac{2\pi ik}{\log 2}$ (solutions of $2^s = 1$).
The corresponding residues altogether can be collected into a periodic function.

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Final answer: The average number of registers is asymptotic to

$$\log_4 n + \delta(\log_4 n),$$

with $\delta(x)$ a 1-periodic function.

Such a periodic term appears also in the average of the maximal runs.

One of my favourites (and of M Archibald, the next speaker):
Rice's method:

$$\sum_{k=1}^n \binom{n}{k} (-1)^k f(k) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{n!(-1)^n}{z(z-1)\dots(z-n)} f(z) dz$$

" n -th difference of the sequence $f(n)$ "

Looks like a curiosity, but appears surprisingly often.

Example: study of tries and patricia tries, $f(k) = \frac{k-1}{2^{k-1}-1}$, etc.

Integral is again evaluated by changing the contour and evaluating residues.

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Thank you!