Full asymptotic expansion for Pólya structures

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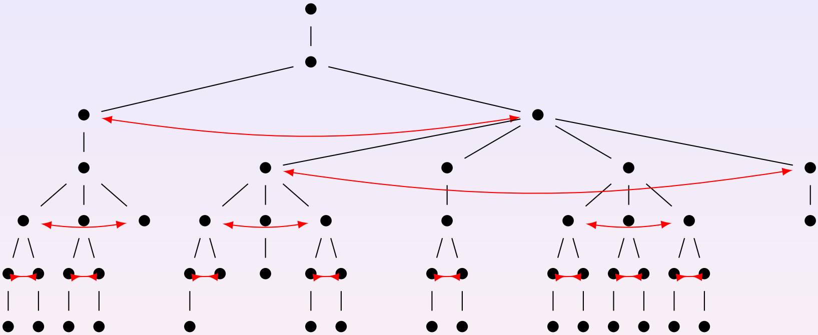
AofA
July 6th, 2016

Pólya trees



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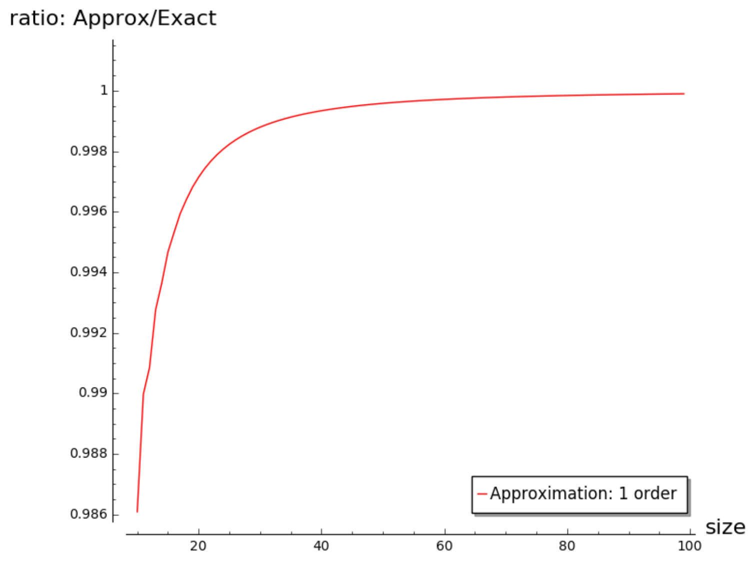
Approximations



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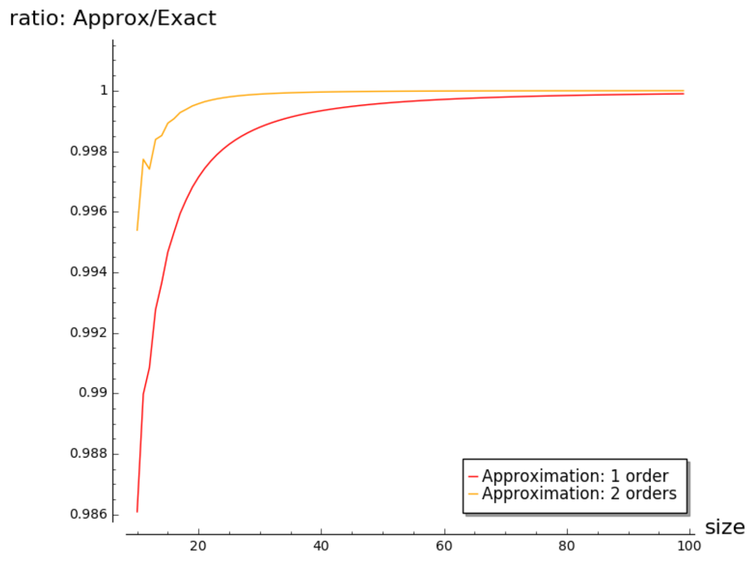

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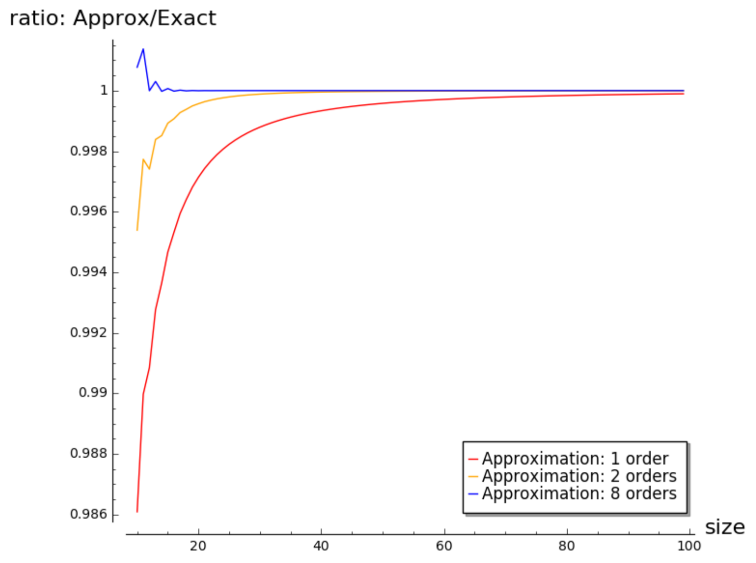

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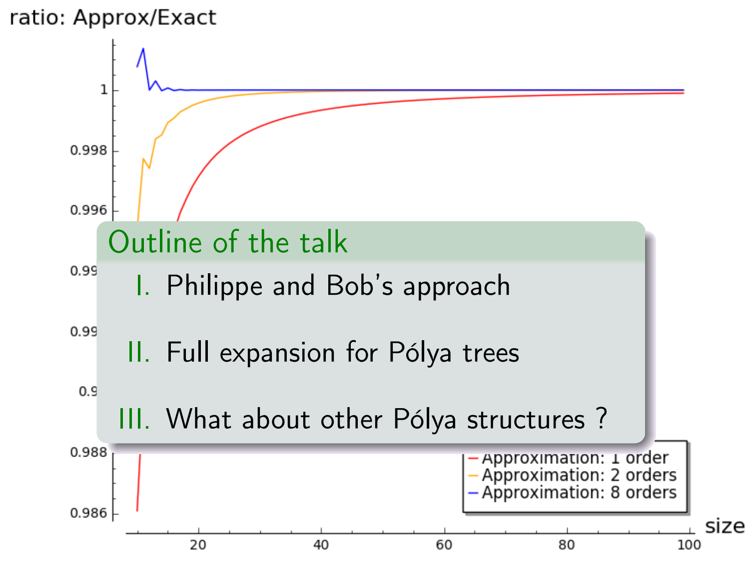

Outline of the talk

I. Philippe and Bob's approach

II. Full expansion for Pólya trees

III. What about other Pólya structures ?

Finch's result [Tech. report 2003]

Two Asymptotic Series

STEVEN FINCH

December 10, 2003

When enumerating trees [1, 2] or prime divisors [3, 4], the leading term of the corresponding asymptotic series is usually sufficient for practical purposes. Greater accuracy is possible by using several more terms, but the coefficients are not as widely known as one might expect. We briefly provide the formulas required to compute the required constants, as well as some theoretical background.

$$T_n \sim r^{-n} n^{-3/2} \left(0.4399240125\ldots + \frac{0.0441699018\ldots}{n} + \frac{0.2216928059\ldots}{n^2} + \frac{0.8676554908\ldots}{n^3} + \cdots \right)$$

Based on Darboux's method, Finch obtains recurrences for the coefficients of the asymptotic expansion of Pólya trees.

Philippe's remark [Finch, Tech. report 2003]

0.3. Addendum I. Philippe Flajolet maintained that the preceding discussion tends to "hide the facts" and provided thoughtful comments. Briefly, the equation $F(x, T(x)) = 0$ can be rearranged as $T(x) = \xi \exp(T(x))$ with

$$\xi(x) = x \exp\left(\sum_{k=2}^{\infty} \frac{T(x^k)}{k}\right).$$

The inverse function of $y \exp(-y)$ is the well-known Cayley tree function τ, an elementary variant of the Lambert W function:

$$\tau(z) = \sum_{n=1}^{\infty} n^{n-1} \frac{z^n}{n!}$$

on the complex plane. In a small disk around the origin, therefore, $T(z) = \tau(\xi(z))$. From here, singularities are easily accessed, making a full asymptotic expansion possible. Writing such conceptual remarks were, in Flajolet's words, an "enjoyable intermezzo" for him despite limited time. These eventually found their way into his treatise [12] with Sedgewick. For completeness, we mention that $C_0 =$ 1.5594900203... for rooted trees (as presented in [12]) and that the corresponding coefficient is 1.1300337163... for binary trees

Philippe and Bob's approach [FS09, pp. 475...]

the main diagonal. The series $S = \frac{z}{2}(1 + D)$ enumerates Schröder's generalized parenthesis systems (Chapter I, p. 69): $S := z + S^2/(1 - S)$, and the asymptotic formula

$$Y_{2n-1} = S_n = \frac{1}{2} D_{n-1} \sim \frac{1}{4\sqrt{\pi n^3}} \left(3 - 2\sqrt{2}\right)^{-n+1/2}$$

follows straightforwardly. ◁

VII. 5. Unlabelled non-plane trees and Pólya operators

Essentially all the results obtained earlier for simple varieties of trees can be extended to the case of non-plane unlabelled trees. *Pólya operators* are central, and their treatment is typical of the asymptotic theory of unlabelled objects obeying symmetries (i.e., involving the unlabelled MSET, PSET, CYC constructions), as we have seen repeatedly in this book.

Binary and general trees. We start the discussion by considering the enumeration of two classes of non-plane trees following Pólya [488, 491] and Otter [466], whose articles are important historic sources for the asymptotic theory of non-plane tree enumeration—a brief account also appears in [319]. (These authors used the more traditional method of Darboux instead of singularity analysis, but this distinction is immaterial here, as calculations develop under completely parallel lines under both theories.) The two classes under consideration are those of general and binary non-plane unlabelled trees. In both cases, there is a fairly direct reduction to the enumeration of Cayley trees and of binary trees, which renders explicit several steps of the calculation. The trick is, as usual, to treat values of $f(z^2)$, $f(z^3)$, ..., arising from Pólya operators, as "known" analytic quantities.

Proposition VII.5 (Special unlabelled non-plane trees). *Consider the two classes of* unlabelled non-plane trees

$$\mathcal{H} = \mathcal{Z} \times \text{MSET}(\mathcal{H}), \quad \mathcal{W} = \mathcal{Z} \times \text{MSET}_{\{0,2\}}(\mathcal{W}),$$

respectively, of the general and binary type. Then, with constants γ_H, A_H and γ_W, A_W given by Notes VII.21 and VII.22, one has

$$(49) \qquad H_n \sim \frac{\gamma_H}{2\sqrt{\pi n^3}} A_H^n, \qquad W_{2n-1} \sim \frac{\gamma_W}{2\sqrt{\pi n^3}} A_W^n.$$

Proof. (*i*) *General case*. The OGF of non-plane unlabelled trees is the analytic solution to the functional equation

$$(50) \qquad H(z) = z \exp\left(\frac{H(z)}{1} + \frac{H(z^2)}{2} + \cdots\right).$$

Let T be the solution to

$$(51) \qquad T(z) = z e^{T(z)},$$

that is to say, the Cayley function. The function $H(z)$ has a radius of convergence ρ strictly less than 1 as its coefficients dominate those of $T(z)$, the radius of convergence of the latter being exactly $e^{-1} \doteq 0.367$. The radius ρ cannot be 0 since the number of trees is bounded from above by the number of plane trees whose OGF has radius 1/4. Thus, one has $1/4 \le \rho \le e^{-1}$.

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Rewriting the defining equation of $H(z)$ as

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we observe that $\zeta = \zeta(z)$ is analytic for $|z| < \rho^{1/2}$; that is, ζ is analytic in a disc that properly contains the disc of convergence of $H(z)$. We may thus rewrite $H(z)$ as

$$H(z) = T(\zeta(z)).$$

Since $\zeta(z)$ is analytic at $z = \rho$, a singular expansion of $H(z)$ near $z = \rho$ results from composing the singular expansion of T at e^{-1} with the analytic expansion of ζ at ρ. In this way, we get:

$$(52) \qquad H(z) = 1 - \gamma\left(1 - \frac{z}{\rho}\right)^{1/2} + O\left(\left(1 - \frac{z}{\rho}\right)\right), \qquad \gamma = \sqrt{2e\rho\zeta'(\rho)}.$$

Thus,

$$[z^n]H(z) \sim \frac{\gamma}{2\sqrt{\pi n^3}}\rho^{-n}.$$

(*ii*) *Binary case*. Consider the functional equation

$$(53) \qquad f(z) = z + \frac{1}{2}f(z)^2 + \frac{1}{2}f(z^2).$$

This enumerates non-plane binary trees with size defined as the number of external nodes, so that $W(z) = \frac{1}{z}f(z^2)$. Thus, it suffices to analyse $[z^n]f(z)$, which dispenses us from dealing with periodicity phenomena arising from the parity of n.

The OGF $f(z)$ has a radius of convergence ρ that is at least $1/4$ (since there are fewer non-plane trees than plane ones). It is also at most $1/2$, which is seen from a comparison of f with the solution to the equation $g = z + \frac{1}{2}g^2$. We may then proceed as before: treat the term $\frac{1}{2}f(z^2)$ as a function analytic in $|z| < \rho^{1/2}$, as though it were known, then solve. To this effect, set

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$$f(z) = 1 - \sqrt{1 - 2\zeta(z)}.$$

The singularity ρ is the smallest positive solution of $\zeta(\rho) = 1/2$. The singular expansion of f is obtained by combining the analytic expansion of ζ at ρ with $\sqrt{1-2\zeta}$. The usual square-root singularity results:

$$f(z) \sim 1 - \gamma\sqrt{1 - z/\rho}, \qquad \gamma := \sqrt{2\rho\zeta'(\rho)}.$$

This induces the $\rho^{-n}n^{-3/2}$ form for the coefficients $[z^n]f(z) \equiv [z^{2n-1}]W(z)$. ■

The argument used in the proof of the proposition may seem partly non-constructive. However, numerically, the values of ρ and γ can be determined to great accuracy. See the notes below as well as Finch's section on "Otter's tree enumeration constants" [211, Sec. 5.6].

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6. A singular expansion of $T(z)$ at ρ is obtained by composing the singular expansion of $C(z)$ at e^{-1} with the analytic expansion of $\zeta(z)$ at ρ.

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Lemma: Full Puiseux expansion of the Cayley tree function

$$C(z) \underset{z\to 1/e}{=} 1 - \sqrt{2}\sqrt{1-ez}$$

$$- \sum_{n\geq 2} \left(\sum_{k=1}^{n-1} (-1)^k B_{n-1,k} \left(\frac{1}{3}, \frac{1}{4}, \dots, \frac{1}{n-k+2} \right) \prod_{i=0}^{k-1} (n+2i) \right) \frac{2^{n/2}}{n!} (1-ez)^{n/2},$$

where the functions $B_{n,k}(\cdot)$ are the Bell polynomials.

Key ideas:

The Cayley tree function satisfies: $C(z) = z\exp(C(z))$.

Reverse the singular expansion of $C(z)\exp(-C(z))$.

- Lagrange inversion formula
- Faà di Bruno's formula

$$B_{n,k}(x_1,\dots,x_{n-k+1}) = \sum_{\substack{c_1,\dots,c_{n-k+1}\geq 0 \\ \sum_i c_i = k \\ \sum_i ic_i = n}} \frac{n!}{c_1!\cdots c_{n-k+1}!} \left(\frac{x_1}{1!}\right)^{c_1} \cdots \left(\frac{x_{n-k+1}}{(n-k+1)!}\right)^{c_{n-k+1}}$$

Pólya trees: key ideas of the proof

$$T(z) = z \exp\left(\frac{T(z)}{1} + \frac{T(z^2)}{2} + \frac{T(z^3)}{3} + \dots\right) = \zeta(z) \exp(T(z)),$$

with $\zeta(z) = z \exp\left(\frac{T(z^2)}{2} + \frac{T(z^3)}{3} + \dots\right)$.

Let ρ be the dominant singularity of $T(z)$.

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The dominant singularity of $\zeta(z)$ is strictly larger than ρ. Thus

$$\zeta(z) \underset{z\to\rho}{=} \frac{1}{e} + \sum_{i\geq 1} \frac{(-\rho)^i\ \zeta^{(i)}(\rho)}{i!} \left(1 - \frac{z}{\rho}\right)^i,$$

with $\zeta^{(i)}(\cdot)$ the i-th differentiate of ζ.

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with $\zeta^{(i)}(\cdot)$ the i-th differentiate of ζ.
By composition of both expansions of $C(z)$ and $\zeta(z)$

$$C(\zeta(z)) \underset{z\to\rho}{=} 1 - \sum_{n\geq 1} \frac{B(n)}{n!} (2e\rho\zeta^{(1)}(\rho))^{n/2} \left(1 - \frac{z}{\rho}\right)^{n/2} \left(1 + \sum_{i\geq 1} \frac{(-\rho)^i\ \zeta^{(i+1)}(\rho)}{(i+1)!\ \zeta^{(1)}(\rho)} \left(1 - \frac{z}{\rho}\right)^i\right)^{n/2}.$$

Theorem: Puiseux expansion for Pólya trees $T(z) = \zeta(z)\exp(T(z))$

$$T(z) \underset{z\to\rho}{=} 1 + \sum_{n\geq 1} t_n \left(1 - \frac{z}{\rho}\right)^{n/2},$$

with $t_1 = -\sqrt{2e\rho\zeta^{(1)}(\rho)}$; and, for all $n > 1$

$$t_n = -\frac{B(n)}{n!}\left(2e\rho\zeta^{(1)}(\rho)\right)^{n/2} - \sum_{\substack{\ell=1 \\ n\equiv \ell \bmod 2}}^{n-1} (-1)^{(n-\ell)/2}\rho^{n/2}\cdot\frac{B(\ell)}{\ell!}\left(2e\zeta^{(1)}(\rho)\right)^{\ell/2}$$

$$\cdot \sum_{r=1}^{\frac{n-\ell}{2}} \binom{\ell/2}{r}\frac{1}{(\zeta^{(1)}(\rho))^r} \sum_{\substack{i_1,\dots,i_r\geq 1 \\ \sum_j i_j = \frac{n-\ell}{2}}} \frac{\zeta^{(i_1+1)}(\rho)}{(i_1+1)!}\cdots\frac{\zeta^{(i_r+1)}(\rho)}{(i_r+1)!},$$

where $\zeta^{(i)}(z)$ stands for the ith derivative of $\zeta(z)$, $B(1)=1$, and for all $\ell > 1$,

$$B(\ell) = \sum_{k=1}^{\ell-1}(-1)^k B_{\ell-1,k}\left(\frac{1}{3},\frac{1}{4},\dots,\frac{1}{\ell-k+2}\right)\prod_{i=0}^{k-1}(\ell+2i).$$

Theorem: Asymptotic expansion for Pólya trees

$$T_n \underset{n\to\infty}{\sim} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \sum_{\ell\geq 0} \frac{1}{n^\ell} \cdot \left(\sum_{r=1}^{\ell+1} Q_r R_{\ell+1-r} \right),$$

where

$$Q_r = \sum_{j=0}^{r-1} (-1)^{j+1} t_{2j+1} \sum_{\substack{\ell_0,\ldots,\ell_j \geq 1 \\ \sum_i \ell_i = r}} \prod_{i=0}^{j} \left(i + \frac{1}{2} \right)^{\ell_j} \qquad \text{for all } r > 0;$$

$R_0 = 1$ and for all $\ell > 0$

$$R_\ell = \sum_{\substack{r=1 \\ r \equiv \ell \bmod 2}}^{\ell} \sum_{\substack{k_1,\ldots,k_r \geq 1 \\ \sum_j k_j = \frac{\ell+r}{2}}} \prod_{i=1}^{r} \frac{(2^{-2k_i}-1)\sum_{s=0}^{2k_i} \frac{1}{s+1} \sum_{j=0}^{s} (-1)^j \binom{s}{j} j^{2k_i}}{(\ell - 2k_1 - \cdots - 2k_{i-1} + i - 1) k_i}.$$

Approximation of the asymptotic expansion for Pólya trees

$$\rho \approx 0.3383218568992076951961126257170170531837746075329 7\ldots$$

$$T_n \underset{n\to\infty}{=} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \left(0.7797450101873204419\ldots + \frac{0.0782891126106109613 3\ldots}{n} + \frac{0.3929402676631860168\ldots}{n^2} + \frac{1.5378793159788380 92\ldots}{n^3} + \frac{8.2008440904355961 94\ldots}{n^4} + O\left(\frac{1}{n^5}\right)\right).$$

And other Pólya structures ?

Almost 100 examples

Theorem: Puiseux expansion for ~~Pólya trees~~ $T(z) = \zeta(z)\exp(T(z))$

$$T(z) \underset{z\to\rho}{=} 1 + \sum_{n\geq 1} t_n \left(1 - \frac{z}{\rho}\right)^{n/2},$$

with $t_1 = -\sqrt{2e\rho\zeta^{(1)}(\rho)}$; and, for all $n > 1$

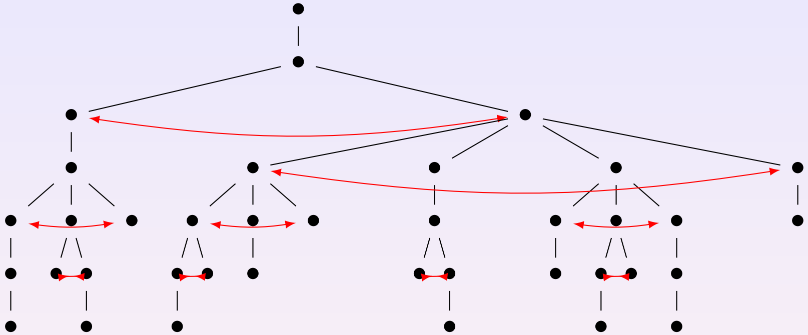
$$t_n = -\frac{B(n)}{n!}\left(2e\rho\zeta^{(1)}(\rho)\right)^{n/2} - \sum_{\substack{\ell = 1 \\ n \equiv \ell \bmod 2}}^{n-1} (-1)^{(n-\ell)/2}\rho^{n/2} \cdot \frac{B(\ell)}{\ell!}\left(2e\zeta^{(1)}(\rho)\right)^{\ell/2}$$

$$\cdot \sum_{r=1}^{\frac{n-\ell}{2}} \binom{\ell/2}{r} \frac{1}{(\zeta^{(1)}(\rho))^r} \sum_{\substack{i_1,\dots,i_r \geq 1 \\ \sum_j i_j = \frac{n-\ell}{2}}} \frac{\zeta^{(i_1+1)}(\rho)}{(i_1+1)!} \cdots \frac{\zeta^{(i_r+1)}(\rho)}{(i_r+1)!},$$

where $\zeta^{(i)}(z)$ stands for the ith derivative of $\zeta(z)$, $B(1) = 1$, and for all $\ell > 1$,

$$B(\ell) = \sum_{k=1}^{\ell-1} (-1)^k B_{\ell-1,k}\left(\frac{1}{3}, \frac{1}{4}, \dots, \frac{1}{\ell-k+2}\right) \prod_{i=0}^{k-1} (\ell + 2i).$$

Rooted identity trees



$\mathcal{T} = \mathcal{Z} \times \mathrm{PSet}\,\mathcal{T}.$

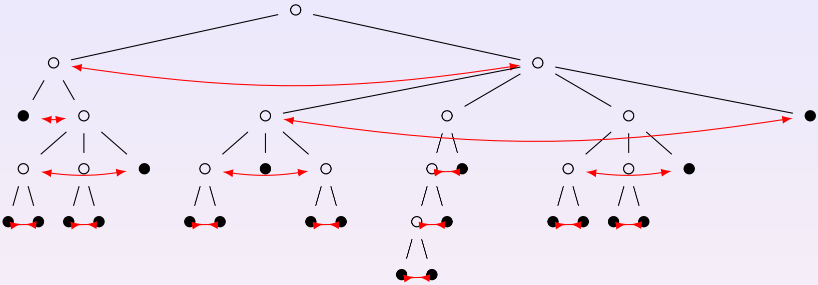
$$T(z) = z \exp\left(\sum_{i>0} (-1)^{i-1} \frac{T(z^i)}{i}\right) \qquad \zeta(z) = z \cdot \exp\left(\sum_{i\geq 2} (-1)^{i-1} \frac{T(z^i)}{i}\right)$$

Approximation of the asymptotic expansion for rooted identity trees

$$\rho \approx 0.3972130968842400414856540702273987342298737099527 6\dots$$

$$T_n \underset{n\to\infty}{=} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \Bigg(0.642579079744269471 4\dots - \frac{0.1851197977663370 56\dots}{n} - \frac{0.4272427290060978745\dots}{n^2} - \frac{2.2554556898721207 9\dots}{n^3} - \frac{16.6097095333564784 6\dots}{n^4} + \left(\frac{1}{n^5}\right)\Bigg).$$

Hierarchies



$$\mathcal{T} = \mathcal{Z} + \text{MSet}_{\geq 2}\mathcal{T}.$$

$$T(z) = \frac{1}{2}\left(z - 1 + \exp\left(\sum_{i>0}\frac{T(z^i)}{i}\right)\right) \qquad \zeta(z) = \frac{1}{2}\exp\left(\frac{1}{2}(1-z) + \sum_{n\geq 2}\frac{T(z^i)}{i}\right).$$

Approximation of the asymptotic expansion for hierarchies

$$\rho \approx 0.28083266698420035539318755911632333337365996433 91\dots$$

$$T_n \underset{n\to\infty}{=} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \left(0.3658015862381119375\dots - \frac{0.2409833212579280352\dots}{n} - \frac{0.3678657493849431861\dots}{n^2} - \frac{0.9991064877914853523\dots}{n^3} - \frac{4.137777553476907813\dots}{n^4} + O\left(\frac{1}{n^5}\right)\right).$$

OEIS sequence A000084

- Series-parallel networks with unlabelled edges (multiple edges allowed)
- Unlabeled cographs
- Non-equivalent And/Or Boolean functions

For $n > 1$,

$$T_n = \frac{1}{2} \#\text{Hierarchies}(n).$$

OEIS sequence A000151

- Oriented rooted trees
- Rooted trees whose non-root nodes are 2-colored

$$T(z) = z \exp\left(\frac{2T(z)}{1} + \frac{2T(z^2)}{2} + \frac{2T(z^3)}{3} + \dots\right).$$

OEIS sequence A001678

Series-reduced planted trees

$$T(z) = \frac{z^2}{1+z} \exp\left(\frac{T(z)}{z} + \frac{T(z^2)}{2z^2} + \frac{T(z^3)}{3z^3} + \dots\right).$$

OEIS sequences

- A058385: Essentially parallel series-parallel networks with unlabeled edges (multiple edges not allowed)
- A058386: Essentially series series-parallel networks with unlabeled edges (multiple edges not allowed)
- A058387: Series-parallel networks with unlabeled edges (multiple edges not allowed)

OEIS sequences

- A058385: Essentially parallel series-parallel networks with unlabeled edges (multiple edges not allowed)
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- A058387: Series-parallel networks with unlabeled edges (multiple edges not allowed)

- A000311: Phylogenetic tree; also Total partitions

$$T(z) = \frac{z-1}{2} + \frac{1}{2}\exp(T(z)) \qquad T(z) - \frac{z-1}{2} =: U(z) = \frac{1}{2}\exp\left(U(z) + \frac{z-1}{2}\right).$$

The functions $\zeta(z)$ does not explicitly depend on $U(z)$ and thus every derivative is explicit.

And a second story ...

(*ii*) *Binary case*. Consider the functional equation

$$f(z) = z + \frac{1}{2} f(z)^2 + \frac{1}{2} f(z^2). \tag{53}$$

This enumerates non-plane binary trees with size defined as the number of external nodes, so that $W(z) = \frac{1}{z} f(z^2)$. Thus, it suffices to analyse $[z^n]f(z)$, which dispenses us from dealing with periodicity phenomena arising from the parity of n.

The OGF $f(z)$ has a radius of convergence ρ that is at least $1/4$ (since there are fewer non-plane trees than plane ones). It is also at most $1/2$, which is seen from a comparison of f with the solution to the equation $g = z + \frac{1}{2} g^2$. We may then proceed as before: treat the term $\frac{1}{2} f(z^2)$ as a function analytic in $|z| < \rho^{1/2}$, as though it were known, then solve. To this effect, set

$$\zeta(z) := z + \frac{1}{2} f(z^2),$$

which exists in $|z| < \rho^{1/2}$. Then, the equation (53) becomes a plain quadratic equation, $f = \zeta + \frac{1}{2} f^2$, with solution

$$f(z) = 1 - \sqrt{1 - 2\zeta(z)}.$$

The singularity ρ is the smallest positive solution of $\zeta(\rho) = 1/2$. The singular expansion of f is obtained by combining the analytic expansion of ζ at ρ with $\sqrt{1 - 2\zeta}$. The usual square-root singularity results:

$$f(z) \sim 1 - \gamma \sqrt{1 - z/\rho}, \qquad \gamma := \sqrt{2\rho\zeta'(\rho)}.$$

This induces the $\rho^{-n} n^{-3/2}$ form for the coefficients $[z^n]f(z) \equiv [z^{2n-1}]W(z)$. ∎