Full asymptotic expansion for Pólya structures

Antoine Genitrini¹

¹ Sorbonne Universités, UPMC Univ Paris 06, CNRS, LIP6 UMR 7606, 4 place Jussieu 75005 Paris. Email: Antoine.Genitrini@lip6.fr.

In order to obtain the full asymptotic expansion for Pólya trees, i.e. rooted unlabelled and non-plane trees, Flajolet and Sedgewick observed that their specification could be seen as a slight disturbance of the functional equation satisfied by the Cayley tree function. Such an approach highlights the complicated formal expressions with some combinatorial explanation. They initiated this process in their book but they spared the technical part by only exhibiting the first-order approximation. In this paper we exhibit the university of the method and obtain the full asymptotic expansions for several varieties of trees. We then focus on three different varieties of rooted, unlabelled and non-plane trees, Pólya trees, rooted identity trees and hierarchies, in order to calculate explicitly their full singular expansions and asymptotic expansions.

Keywords: Unlabelled non-plane trees; Full Puiseux expansion; Full asymptotic expansion; Analytic Combinatorics.

1 Introduction

By using either Darboux's method or singularity analysis, we easily get the dominant coefficients of the asymptotic expansions for the number of some specific Pólya structures; a Pólya structure being decomposable by using some Pólya operators like the multiset MSET or the powerset PSET constructions.

For the numbers of hierarchies (a specific class of trees) of size 100 the relative error between the exact number and the first-order approximation is only around 0.01% (note that it is only $10^{-10}\%$ with an 8-order approximation). However for small hierarchies, the first-order approximation is not precise: the relative error for the trees of size 20 is around 0.3% whereas it is only around 0.0004% with the 8-order approximation (cf. Fig. 1).

In a technical report [Fin03c], Finch provided recurrence formulas to compute all the coefficients in the asymptotic expansion for Pólya trees. He developed there the classical Darboux's method to derive the recurrences and computed explicitly the five most important coefficients.

According to Finch's report, Flajolet proposed at that time to study the fundamental equation given by the Weierstrass Preparation Theorem as, somehow, a slight disturbance of

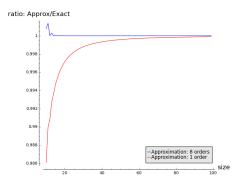


Fig. 1: Ratio between the approximations and the exact numbers of hierarchies

the functional equation satisfied by the Cayley tree function. Using this point of view, the procedure to exhibit the full asymptotic expansion is much more highlighted and the complicated formal expressions can be combinatorially understood. Flajolet and Sedgewick initiated this process in their book [FS09, p. 477] in the context of Pólya trees but they spared the technical part of the proof by only exhibiting the first-order approximation.

In this paper, we explain why such an approach is generic to obtain easily the full asymptotic expansions for several varieties of trees. We focus on varieties that can be seen as a disturbance of the Cayley function in the way that they can be described by their generating function T(z) as:

$$T(z) = \zeta(z) \exp(T(z)),$$

for some constrained function $\zeta(z)$. For such classes of trees, we exhibit the full Puiseux (i.e., singular) expansion of the generating series. We then compute the generic full asymptotic expansion of the number of trees. In Section 3, we then focus on three different varieties of rooted, unlabelled and non-plane trees. The first class of trees is the classical set of Pólya trees that already appears in the papers of Cayley [BLW76], Pólya [Pól37] and Otter [Ott48]. The generating function of Pólya trees is easily described with a functional equation using the multiset construction. By replacing the construction by the powerset operator we get the class of rooted identity trees, the second class we are interested in. Such trees are studied, for example, in the work of Harary *et al.* in [HRS75]. Finally we deal with hierarchies, i.e., rooted unlabelled non-plane trees without nodes of arity 1. This class has been introduced by Cayley too, but it is also directly linked to series-parallel networks in the papers of Riordan and Shannon [RS42] and Moon [Moo87]. In the Section 3.4, we give numerical approximations for the first coefficients of the singular and the asymptotic expansions of each specific variety of trees. We conclude the paper (Section 4) by mentioning several other structures where our generic approach could be applied directly.

2 Main results

For each of the varieties under consideration, the fundamental idea consists, from an analytic point of view, at studying its generating function as a disturbance of the classical Cayley tree function (cf. e.g. [FS09, p. 127]). Let C(z) be the Cayley tree function; it satisfies the functional equation

$$C(z) = z \cdot \exp(C(z)). \tag{1}$$

Its dominant singularity is 1/e and C(1/e) = 1. Recall that the Cayley tree function is closely related to the Lambert W function. Many fundamental results about this classical function are given in the paper of Corless *et al.* [CGH⁺96].

In order to obtain generically the full asymptotic expansion of the number of the structures of a variety of trees, let us first compute the full Puiseux expansion (i.e., the full singular expansion) of the Cayley tree function and then study how the disturbance induced by a given variety modifies this behaviour. Let us recall the definition of Bell polynomials, extensively studied in Comtet's book [Com74] and denoted by $B_{n,k}(\cdot)$:

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

The Bell polynomials appear naturally in Faà di Bruno's formula [Com74] that states the value of iterated derivatives of the composition of two functions.

Proposition 1 The full Puiseux expansion of the Cayley tree function is

$$C(z) \underset{z \to 1/e}{=} 1 - \sqrt{2}\sqrt{1 - ez} - \sum_{n \ge 2} \left(\sum_{k=1}^{n-1} (-1)^k B_{n-1,k} \left(\frac{1}{3}, \frac{1}{4}, \dots, \frac{1}{n-k+2} \right) \prod_{i=0}^{k-1} (n+2i) \right) \frac{2^{n/2}}{n!} (1 - ez)^{n/2},$$

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

The calculation of the first terms of the singular expansion gives

$$\begin{split} C(z) &\underset{z \to 1/e}{=} 1 - \sqrt{2}\sqrt{1 - ez} + \frac{2}{3}(1 - ez) - \frac{11}{36}\sqrt{2}(1 - ez)^{3/2} + \frac{43}{135}(1 - ez)^2 - \\ &\frac{769}{4320}\sqrt{2}(1 - ez)^{5/2} + \frac{1768}{8505}(1 - ez)^3 - \frac{680863}{5443200}\sqrt{2}(1 - ez)^{7/2} + \mathcal{O}\left((1 - ez)^4\right). \end{split}$$

Let us recall that the expansion until $\mathcal{O}((1-ez)^{3/2})$ has been derived in [FS09]. We prove the full expansion with their approach but with further precision. Note that, in the formula of Proposition 1, the inner sum of k can be factored in the same way as the classical Ruffini-Horner method for polynomial evaluation. Doing so makes its computations much more efficient.

The second step consists in studying the ordinary generating function $T(z) = \sum_{n\geq 0} T_n z^n$ of the tree variety under consideration as a disturbance of the Cayley tree function. We follow the approach presented in [FS09, p. 477] for Pólya trees. We assume the existence of a function $\zeta(z)$ such that

$$T(z) = \zeta(z) \cdot \exp(T(z)). \tag{2}$$

Theorem 2 Let \mathcal{T} be a variety of trees whose generating function is T(z), and ρ be its dominant singularity. If the generating function T(z) satisfies the Equation (2), if the dominant singularity of $\zeta(z)$ is strictly larger than ρ and if $\zeta^{(1)}(\rho) \neq 0$, then T(z) satisfies the following full Puiseux expansion

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

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

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

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

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

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

Proof key idea: The complete proof follows the strategy of Flajolet and Sedgewick. The main idea is to compose the Puiseux expansion of C(z) at the singularity 1/e and the analytic expansion of $\zeta(z)$ at the dominant singularity of T(z).

In Theorem 2, the assumption $\zeta^{(1)}(\rho) \neq 0$ could be replaced by a weaker assumption that there exists an integer r > 0 such that $\zeta^{(r)}(\rho) \neq 0$. Making this weaker assumption would however make the proof a bit more technical without adding substantial information.

The the first terms of the singular expansion of T(z) are given by

$$\begin{split} T(z) &\underset{z \to \rho}{=} 1 - \sqrt{2e\rho\zeta^{(1)}(\rho)} \sqrt{1 - \frac{z}{\rho}} + \frac{2e\rho\zeta^{(1)}(\rho)}{3} \left(1 - \frac{z}{\rho}\right) - \left(\frac{11\sqrt{2}(e\rho\zeta^{(1)}(\rho))^{3/2}}{36} - \frac{\sqrt{2e}\rho^{3/2}\zeta^{(2)}(\rho)}{4\sqrt{\zeta^{(1)}(\rho)}}\right) \left(1 - \frac{z}{\rho}\right)^{3/2} \\ &+ \left(\frac{43(e\rho\zeta^{(1)}(\rho))^2}{135} - \frac{e(\rho\zeta^{(2)}(\rho))^2}{3}\right) \left(1 - \frac{z}{\rho}\right)^2 - \left(\frac{769\sqrt{2}(e\rho\zeta^{(1)}(\rho))^{5/2}}{4320} - \frac{11\sqrt{2}\rho^{5/2}(e\zeta^{(1)}(\rho))^{3/2}\zeta^{(2)}(\rho)}{48\zeta^{(1)}(\rho)} - \frac{\sqrt{2}\rho^{5/2}\sqrt{e\zeta^{(1)}(\rho)}}{96} \left(\frac{3(\zeta^{(2)}(\rho))^2}{(\zeta^{(1)}(\rho))^2} - \frac{8\zeta^{(3)}(\rho)}{\zeta^{(1)}(\rho)}\right)\right) \left(1 - \frac{z}{\rho}\right)^{5/2} + \mathcal{O}\left(\left(1 - \frac{z}{\rho}\right)^3\right). \end{split}$$

We are now ready to compute the full asymptotic expansion for the class \mathcal{T} .

Theorem 3 Let \mathcal{T} be a variety of trees whose generating function is T(z), and ρ be its dominant singularity. If the generating function T(z) satisfies the Equation (2), if the dominant singularity of $\zeta(z)$ is strictly larger than ρ and if $\zeta^{(1)}(\rho) \neq 0$, then asymptotically when n tends to infinity,

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

where

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

with the sequence (t_i) defined in Theorem 2, $R_0 = 1$ and

$$R_{\ell} = \sum_{\substack{r=1 \\ r \equiv \ell \bmod 2}}^{\ell} \sum_{\substack{k_1, \dots, k_r \ge 1 \\ k_j \in \frac{\ell+r}{2}}} \prod_{i=1}^{r} \frac{(2^{-2k_i} - 1) \sum_{s=0}^{2k_i} \frac{1}{s+1} \sum_{j=0}^{s} (-1)^j {s \choose j} j^{2k_i}}{(\ell - 2k_1 - \dots - 2k_{i-1} + i - 1)k_i} \quad \text{for all } \ell > 0.$$

In particular, the first few terms in the asymptotic expansion of T_n are given by

$$T_{n} = \int_{n \to \infty}^{n} \frac{\rho^{-n}}{\sqrt{\pi n^{3}}} \left(-\frac{t_{1}}{2} - \frac{3(t_{1} - 4t_{3})}{16n} - \frac{5(5t_{1} - 72t_{3} + 96t_{5})}{256n^{2}} - \frac{105(t_{1} - 44t_{3} + 160t_{5} - 128t_{7})}{2048n^{3}} - \frac{21(79t_{1} - 10800t_{3} + 81600t_{5} - 161280t_{7} + 92160t_{9})}{65536n^{4}} + \mathcal{O}\left(\frac{1}{n^{5}}\right) \right),$$

where the t_i 's are given in the Theorem 2.

3 Different varieties of rooted unlabelled and non-plane trees

In the following three sections, we will show how both Theorems 2 and 3 directly apply to three families of trees, namely the Pólya trees, the rooted identity trees and the hierarchies. In each of these sections, we will use the same notations \mathcal{T} , T(z) and $\zeta(z)$ to refer to the family of considered trees.

For each of the three examples, we proceed in two steps. First we focus on efficient recurrences in order to compute the first numbers of the sequence $(T_n)_{n\in\mathbb{N}}$ that encodes for each positive integer n the number of trees of size n. Second, by using the numerical procedure given in [FS09, p. 477], we compute an approximation of the dominant singularity of T(z).

Finally, at the end of the section, we exhibit two Tables 1 and 2 to compare the numerical approximations (according to each class of trees) of the coefficients given in the Theorems 2 and 3. We also exhibit the typical gain in the relative error obtained by using a more precise asymptotic approximation.

3.1 Pólya trees

A Pólya tree is a rooted unlabelled and non-plane tree. Let us denote by \mathcal{T} the set of Pólya trees. It satisfies the following unambiguous specification :

$$\mathcal{T} = \mathcal{Z} \times MSET \mathcal{T}$$
,

because a Pólya tree is by definition a root, specified by \mathcal{Z} (of size 1), followed by a multiset of Pólya trees (we refer the reader to [FS09] for more details). By the *symbolic method* (cf. [FS09]), we get

$$T(z) = z \exp\left(\sum_{i>0} \frac{T(z^i)}{i}\right),\tag{3}$$

with T(z) being the ordinary generating function enumerating \mathcal{T} . The latter formula already appears in Pólya's paper [Pól37] and has been sketched by Cayley ([BLW76, p. 67]) as an introduction to the counting theory for unlabelled objects. This method takes into account symmetries of the objects and thus quantifies isomorphisms. We have a classical alternative definition: cf. e.g. [FS09, p. 71].

$$T(z) = z \cdot \prod_{n > 0} \frac{1}{(1 - z^n)^{T_n}},\tag{4}$$

with T_n the number of trees of size n in \mathcal{T} . Some combinatorial arguments, given in [FS09, p. 27–30], prove that both definitions are equivalent. From the latter Equation (4), we deduce a recurrence for the sequence $(T_n)_{n\in\mathbb{N}}$ for Pólya trees.

Fact 4 The sequence $(T_n)_{n\in\mathbb{N}}$ enumerating Pólya trees satisfies

$$T_{n} = \begin{cases} n & \text{if } n \in \{0, 1\} \\ \frac{1}{n-1} \sum_{i=1}^{n-1} iT_{i} \left(\sum_{m=1}^{\lfloor \frac{n-1}{i} \rfloor} T_{n-mi} \right) & \text{if } n > 1. \end{cases}$$

This result is given as an exercise by Knuth [Knu97, p. 395]. Furthermore, Otter [Ott48] proved a very similar recurrence for unrooted trees. The first values of the sequence, given in OEIS⁽ⁱ⁾ sequence A000081, are

$$0, 1, 1, 2, 4, 9, 20, 48, 115, 286, 719, 1842, 4766, 12486, 32973, 87811, \dots$$

The number of Pólya trees from each size from 1 to n can be computed in $\mathcal{O}(n^2)$ arithmetic operations (by using memoization).

Proof of Fact 4: Several authors, in particular, Flajolet and Sedgwick obtained such a recurrence by using the logarithmic derivative of T(z): for all n > 1

$$z\frac{T'(z)}{T(z)} = 1 + \sum_{n>0} T_n \frac{nz^n}{1 - z^n}.$$

We rewrite this equation as

$$zT'(z) = \left(1 + \sum_{n > 0} nT_n \frac{z^n}{1 - z^n}\right) T(z).$$

Extracting the n-th coefficient of the generating functions gives:

$$nT_n = T_n + \sum_{i=1}^{n-1} \left([z^i] \sum_{m>0} mT_m \frac{z^m}{1-z^m} \right) T_{n-i}.$$

Since $[z^k](1-z^m)^{-1}$ equals 1 if m divides k and 0 otherwise, we get

$$(n-1)T_n = \sum_{i=1}^{n-1} \left(\sum_{m|i} mT_m\right) T_{n-i}.$$

The notation m|i corresponds to the condition that the integer m divides the integer i. The stated formula is obtained by interchanging the two sums.

By using Flajolet and Sedgewick's numerical procedure (cf. [FS09, p. 477]) with n=200 terms, we get the following 50-digits approximation of ρ :

$$\rho \approx 0.33832185689920769519611262571701705318377460753297\dots$$

We are now interested in the full Puiseux expansion of the generating function of Pólya trees. In view of Equations (2) and (3), we define have

$$T(z) = \zeta(z) \cdot \exp(T(z)), \quad \text{where } \zeta(z) = z \cdot \exp\left(\sum_{n \ge 2} \frac{T(z^n)}{n}\right).$$
 (5)

Fact 5 The function $\zeta(z)$ defined for Pólya trees satisfies the assumptions of the Theorems 2 and 3.

⁽i) OEIS: On-line Encyclopedia of Integer Sequences

This fact has already been proved by Cayley as mentioned in [BLW76, p. 67]. We recall here the arguments given in [FS09, p. 477].

Proof: The definition of $\zeta(z)$ given in Equation (??) implies that its dominant singularity is $\sqrt{\rho}$, (with the constant ρ being the dominant singularity of T(z)). Since 1/e is the dominant singularity of the Cayley tree function C(z) and $[z^n]T(z)>[z^n]C(z)$ (by using Equation (3)) for n sufficiently large, we get $\rho \leq 1/e$. Thus $\sqrt{\rho} > \rho$ and we finally infer that the function $\zeta(z)$ is analytic beyond the disc of convergence of T(z). Finally we easily get $\zeta'(\rho)>0$.

Theorem 2 and the above approximation for ρ give the first coefficients for the Puiseux expansion of Pólya trees presented in the Table 1. The computations of the numbers t_i 's have been done with an approximation of the function $\zeta(z)$, computed with the truncation of the series T(z) after the 100-th first coefficients. Experimentally, it seems that the accuracy is actually much larger than the 20 digits given in Table 1.

Finally the previous approximations and the result of Theorem 3 give

$$T_n = \int_{n \to \infty}^{\rho - n} \left(0.7797450101873204419 \dots + \frac{0.07828911261061096133 \dots}{n} + \frac{0.3929402676631860168 \dots}{n^2} + \frac{1.537879315978838092 \dots}{n^3} + \frac{8.200844090435596194 \dots}{n^4} + \mathcal{O}\left(\frac{1}{n^5}\right) \right).$$
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Note that, from here, it is then easy to get back the first evaluations exhibited by Finch [Fin03c].

3.2 Rooted identity trees

A rooted identity tree is a rooted unlabelled (non-plane) tree for which the only automorphism preserving the root node is the identity. Harary $et\ al.$ studied this class of trees in [HRS75]. In his book [Fin03a], Finch also mentions this class. Intuitively, whereas a Pólya tree can be seen as a root followed by a multiset of Pólya trees, a rooted identity tree can be seen as a root followed by a set of rooted identity trees (i.e., no repetition is allowed). Let us denote by $\mathcal T$ the set of rooted identity trees. It satisfies the following unambiguous specification

$$\mathcal{T} = \mathcal{Z} \times PSET \mathcal{T}.$$

The symbolic method gives the functional equation

$$T(z) = z \exp\left(\sum_{i>0} (-1)^{i-1} \frac{T(z^i)}{i}\right).$$

An equivalent formula for the function T(z) is

$$T(z) = z \cdot \prod_{n>0} (1+z^n)^{T_n}.$$

In order to obtain an efficient recurrence relation satisfied by the numbers of rooted identity tree, we use the same strategy as above (for Pólya trees), and thus obtain:

Proposition 6 The sequence $(T_n)_{n\in\mathbb{N}}$ enumerating rooted identity trees satisfies

$$T_n = \begin{cases} n & \text{if } n \in \{0, 1\} \\ \frac{1}{n-1} \sum_{i=1}^{n-1} iT_i \left(\sum_{m=1}^{\lfloor \frac{n-1}{i} \rfloor} (-1)^{m+1} T_{n-mi} \right) & \text{if } n > 1. \end{cases}$$

The first values of the sequence, see in OEIS A004111, are

$$0, 1, 1, 1, 2, 3, 6, 12, 25, 52, 113, 247, 548, 1226, 2770, 6299, \dots$$

The number of rooted identity trees from each size from 1 to n can be computed in $\mathcal{O}(n^2)$ arithmetic operations. Once we are able to compute efficiently the first numbers T_n we can estimate the dominant singularity of T(z) to be approximately

$$\rho \approx 0.39721309688424004148565407022739873422987370995276\dots$$

Obviously this dominant singularity is larger than the one for Pólya trees because there are less rooted identity trees than Pólya trees.

To describe
$$T(z)$$
 like in Equation (2), we get $\zeta(z) = z \cdot \exp\left(\sum_{n \geq 2} (-1)^{n-1} \frac{T(z^n)}{n}\right)$.

Proposition 7 The function $\zeta(z)$ defined in the context of rooted identity trees satisfies the assumptions of the Theorems 2 and 3.

The approximations of the first coefficients of the Puiseux expansion for rooted identity trees are given in the Table 1. The second Table 2 gives the approximations of the asymptotic expansion of T_n :

$$T_n \underset{n \to \infty}{=} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \left(0.6425790797442694714 \dots - \frac{0.1851197977766337056 \dots}{n} - \frac{0.4272427290060978745 \dots}{n^2} - \frac{2.255455568987212079 \dots}{n^3} - \frac{16.60970953335647846 \dots}{n^4} + \mathcal{O}\left(\frac{1}{n^5}\right) \right).$$

It seems that these numbers do not appear elsewhere in the literature.

3.3 Hierarchies

A hierarchy is a rooted unlabelled and non-plane tree with no node of arity 1. The size notion for hierarchies is the number of leaves. This class already appears in the work of Cayley (cf. [BLW76, p. 43]. Using the notations from [FS09, p. 72] for hierarchies, we have both following specification and functional equation for its generating function

$$\mathcal{T} = \mathcal{Z} + \mathsf{MSET}_{\geq 2} \mathcal{T}, \qquad T(z) = rac{1}{2} \left(z - 1 + \exp\left(\sum_{i > 0} rac{T(z^i)}{i}
ight)
ight).$$

Again, we obtain a recurrence formula that computes the numbers T_n .

Proposition 8 The sequence $(T_n)_{n\in\mathbb{N}}$ enumerating hierarchies satisfies

$$T_{n} = \begin{cases} n & \text{if } n \in \{0, 1\} \\ \frac{1}{n} \sum_{\substack{m \mid n \\ m \neq n}} mT_{m} + \frac{2}{n} \left(\sum_{i=1}^{n-1} iT_{i} \sum_{m=1}^{\lfloor \frac{n-1}{i} \rfloor} T_{n-mi} - \frac{1}{2} \delta_{\{n-mi=1\}} \right) & \text{if } n > 1, \end{cases}$$

with the notation $\delta_{\{n-mi=1\}}$ evaluates to 1 if n-mi=1 and to 0 otherwise.

The first values of the sequence, see in OEIS A000669, are given by

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0, 1, 1, 2, 5, 12, 33, 90, 261, 766, 2312, 7068, 21965, 68954, 218751, 699534, \dots
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They are stored (there the sequence is shifted by 1). We note that in this context, we cannot easily simplify the recurrence in order to avoid a sum over the divisors of n (for T_n). However here, the sum is not inside another one, thus the complexity (in the number of arithmetic operations) to compute T_n is quadratic. We estimate the dominant singularity of T(z) to be approximately

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\rho \approx 0.28083266698420035539318755911632333333736599643391\dots
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In order to fall under the framework described by Equation (2), we need to consider the generating function $\tilde{T}(z) = T(z) - \frac{1}{2}(1-z)$. The two generating functions T(z) and $\tilde{T}(z)$ have the same dominant singularity. Thus we get

$$\tilde{T}(z) = \zeta(z) \cdot \exp(\tilde{T}(z)),$$

with

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

Proposition 9 The function $\zeta(z)$ defined in the class of objects associated to $\tilde{T}(z)$ satisfies the assumptions of the Theorems 2 and 3.

It remains to slightly modify the 2 first coefficients in the singular expansion of $\tilde{T}(z)$ to obtain the singular expansion of T(z) and fill both Tables 1. and 2. In particular we get

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

It seems that these numbers do not appear elsewhere in the literature.

Let us conclude this section on hierarchies by mentioning the OEIS sequence A000084, that is directly related. It counts the number of series-parallel networks with n unlabelled edges; both generating functions are essentially the same (up to a simple factor). We thus get the Puiseux expansions and the asymptotic expansion for these objects as a by-product.

3.4 Approximations

In order to obtain the following approximations for the coefficients in the Puiseux expansions or for the asymptotic expansions of the numbers of trees, we have used the open-source mathematics software Sage [Dev15] and the Python library MPmath [J⁺14] for some specific high precision calculations.

The first table synthesises the first elements of the sequences $(t_n)_{n\in\mathbb{N}}$ satisfying the Puiseux expansions for the previous Pólya structures:

$$T(z) = \sum_{n \ge 0} t_n \left(1 - \frac{z}{\rho} \right)^{n/2}.$$

Coeff.	Pólya trees	Rooted identity trees	Hierarchies
t_0	1.0000000000000000000	1.0000000000000000000	0.6404163334921001777
t_1	-1.559490020374640884	-1.285158159488538943	-0.7316031724762238750
t_2	0.8106697078826992796	0.5505438316333229659	0.03799806716699161541
t_3	-0.2854870216128456058	-0.5681159369076463432	0.1384103018915147449
t_4	0.1653723657120838943	0.4261261857916583247	-0.07387395031732463851
t_5	-0.3424599704021542007	-0.1312888430707878210	-0.05428300802019698042
t_6	0.3174072259465285628	0.1224152517144394163	0.03800381072191918081
t_7	-0.1077788002916310083	-0.3225499663026797778	0.03109684705422999274
t_8	0.06138495705583510410	0.2539454170234272677	-0.02381831461193008886
t_9	-0.1952123835975564636	0.04875363678533678081	-0.02078556533052714092
t_{10}	0.2059848312779074186	-0.00002800001023286558041	0.01666265537126027377
t_{11}	-0.05272470849819056138	-0.3631594631270670335	0.01611178365047090583
t_{12}	0.01702656875495366861	0.2637344037695510765	-0.01295368177079785790
t_{13}	-0.1523706243663253961	0.2617035123807709629	-0.01338408339711046374
t_{14}	0.1737028832998504627	-0.1368754575043169801	0.01075691931570711729
t_{15}	-0.01447370373952704466	-0.5927534134371262366	0.01183388780152404393
t_{16}	-0.02189951761121556237	0.3911340105112945142	-0.009441457380326882677
t_{17}	-0.1445471935709097045	0.6832510269350502136	-0.01084956346194149131
t ₁₈	0.1760771088850177779	-0.3902593892984113718	0.008607637481105329431

Tab. 1: Approximation of the Puiseux expansions for Pólya trees, rooted identity trees and hierarchies

The following Table 2 contains the first numbers $(\tau_n)_{n\in\mathbb{N}}$ satisfying the asymptotic expansions for the previous Pólya structures:

$$T_n \underset{n \to \infty}{\sim} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \sum_{i \ge 0} \frac{\tau_i}{n^i}.$$

Coeff.	Pólya trees	Rooted identity trees	Hierarchies
τ_0	0.7797450101873204419	0.6425790797442694714	0.3658015862381119375
τ_1	0.07828911261061096133	-0.1851197977766337056	0.2409833212579280352
τ_2	0.3929402676631860168	-0.4272427290060978745	0.3678657493849431861
τ_3	1.537879315978838092	-2.255455568987212079	0.9991064877914853523
τ_4	8.200844090435596194	-16.60970953335647846	4.137777553476907813
τ_5	57.29291473494343825	-157.9003693373302727	23.43410248921570084
τ_6	503.0445050262735854	-1840.110517359351172	170.1188811511555370
τ_7	5359.600933884326064	-25387.34869954017854	1514.745295656330186
τ_8	67342.06920114653067	-404610.0663959841556	16007.82637588106931
τ_9	975425.4970695924728	-7.313377058487246593e6	195812.3506172274875
τ_{10}	1.599693249293173348e7	-1.477949138517813328e8	2.719234685827618831e6
τ_{11}	2.928225313353392698e8	-3.301794456762036735e9	4.222444465223140109e7
τ_{12}	5.914523441293936053e9	-8.080229604228356791e10	7.243861962702191648 <i>e</i> 8
τ_{13}	1.305991927898973201e11	-2.149826267241085239e12	1.359774926415692519e10
τ_{14}	3.128498399789526502e12	-6.179075814699061934e13	2.770908644498957323e11
τ_{15}	8.078305401468914384e13	-1.908151484770832703e15	6.089496262810801422e12
τ_{16}	2.236301680891647428e15	-6.301063280436556255e16	1.435269254893331074e14
$ au_{17}$	6.605960869699262787e16	-2.215767775919040241e18	3.610881990157578400e15
τ_{18}	2.073828085209932615e18	-8.267080545525264413e19	9.656755540184967275e16

Tab. 2: Asymptotic expansion of the number of Pólya trees, rooted identity trees and hierarchies

It is interesting to note that, in Table 2, for n sufficiently large and due to the sign of the values of the

 (τ_i) , all truncations after the nth term in the full expansions (for $n=1\dots 17$) correspond to lower bounds for the case of Pólya trees and hierarchies and all of them are upper bounds for rooted identity trees.

Size	10	20	50	100	200	500
Order-1 approximation	$1.391 \cdot 10^{-2}$	$2.859 \cdot 10^{-3}$	$4.204 \cdot 10^{-4}$	$1.027 \cdot 10^{-4}$	$2.540 \cdot 10^{-5}$	$4.039 \cdot 10^{-6}$
Order-4 approximation	$1.039 \cdot 10^{-3}$	$3.448 \cdot 10^{-5}$	$2.383 \cdot 10^{-7}$	$6.872 \cdot 10^{-9}$	$2.071 \cdot 10^{-10}$	$2.078 \cdot 10^{-12}$
Order-8 approximation	$7.722 \cdot 10^{-4}$	$3.369 \cdot 10^{-6}$	$3.822 \cdot 10^{-10}$	$6.195 \cdot 10^{-13}$	$1.123 \cdot 10^{-15}$	$2.611 \cdot 10^{-18}$

Tab. 3: Relative error induced by approximations for hierarchies

Finally, by using only 20 digits of precision in our approximations of the values $\zeta^{(r)}(\rho)$'s we cannot hope to obtain a better approximation than the one of order 8 (Table 3) for the number of large trees (i.e. with size larger than 500).

4 Conclusion

The strength of the approach presented here is its universality. We have shown, in full detail, how it applies to Pólya trees, rooted identity trees and hierarchies but many other examples fill in our framework.

- 1. Rooted oriented trees and series-reduced planted trees. The OEIS sequences A000151 and A001678 can be directly studied.
- 2. Series-parallel networks. In the context of [RS42], [Moo87] and [Fin03b] we get back several generating functions (listed in OEIS A058385, A058386 and A058387) that can be studied in the same vein as hierarchies. Let us recall that many links between trees and series-parallel graphs have already been exhibited, thus the fact that the behaviours of their generating series are analogous is not a surprise.
- 3. Phylogenetic trees and also total partitions. The OEIS sequence A000311, counting phylogenetic trees and also total partitions that are labelled objects, can also be analysed with our technique. Note here that the function $\zeta(z)$ does not explicitly depend on T(z) and thus every derivative is explicit. Just put a factor n! in front of T_n to obtain its full asymptotic expansion. We thus exhibit the polynomials whose existence has been stated in [Com74, p. 224].
- 4. The unrooted versions of the previous rooted trees. With some further work, we are able to exhibit the full asymptotic expansion of the unrooted versions of the previous rooted trees we were interested in. In fact their generating functions P(z) satisfy some equation of the form

$$P(z) = T(z) - \frac{1}{2}T^{2}(z) + \frac{1}{2}T(z^{2}).$$

Since we have the full Puiseux expansion of the series T(z), we can compute the one of the series P(z). Some examples of such series correspond to the following sequences A000055, A000238, A000014.... An open question would be to be able to write a functional equation for P(z) as a disturbance of the Cayley tree function, and then to use directly an analogous approach as the one studied in Section 2. There, we would get $\zeta^{(1)}=0$ since we know that these trees are unrooted.

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