COMBINATORICS AND ASYMPTOTICS ON TREES

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ABSTRACT. The purpose of this article is to present explicit and asymptotic methods to count various kinds of trees. In all cases the use of generating functions is essential. Explicit formulae are derived with help of Lagrange's inversion formula. On the other hand singularity analysis of generating functions leads to asymptotic formulas.

Trees are defined as connected graphs without circles, and their properties are basics of graph theory. For example, a connected graph is a tree if and only if the number of edges equals the number of nodes minus 1. Furthermore, each pair of nodes is connected by a unique path etc.

If we mark a specific node r in a tree T then it is called *rooted tree.* A rooted tree may be easily described in terms of *generations* or *levels.* The root is the 0-th generation. The neighbors of the root constitute the first generation, and in general the nodes of distance k from the root form the k-th generation (or level). If a node of level k has neighbors of level $k+1$ then these neighbors are also called *successors.* Furthermore, if v is a node in a rooted tree T then v may be considered as the root of a subtree T_v of T that consists of all iterated successors of v. This means that rooted trees can be constructed in a recursive way. Due to that property counting problems on rooted trees are usually easier than on unrooted trees.

Rooted trees have also various applications in computer science. They naturally appear as data structures, e.g. the recursive structure of foldes in any computer is just a rooted tree. Furthermore, fundamental algorithms such as Quicksort or the Lempel-Ziv data compression algorithm are closely related to rooted trees, namely to binary and digital search trees which are also used to store (and search for) data. Rooted trees even occur in information theory. For example, prefix free codes on an alphabet of order m are easily encoded as the set of leaves in m-ary trees.

In what follows we will present methods for counting trees that are based on the concept of generating functions. Generatings functions are quite natural in this context since (rooted) trees have a recursive structure which translates to recurrence relations for corresponding counting problems. And generating functions are a proper tool for solving recurrence equations. There are lots of references in the literature concerning tree enumeration with generating functions. We just mention two of them, the book of Harary and Palmer [9] and the article of Vitter and Flajolet [18].

The present article is divided into two main parts. In Section 1 we consider several kinds of trees (binary trees, planted plane trees, simply generated trees, unrooted trees) and show how we can obtain explicit and aymptotic formulas for the numbers of trees of size n. Section 2 is devoted to more involved counting problems, for example one is interested in the number of trees of size n with k leaves etc. Both sections are followed by 2 appendices where some additional material from

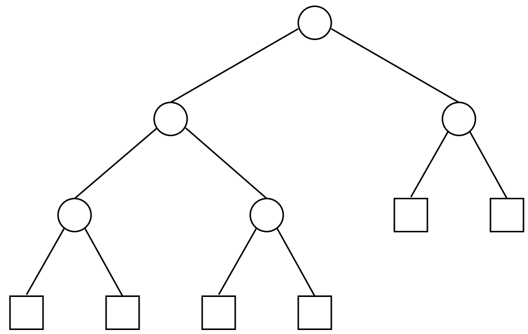

FIGURE 1. Binary tree

combinatorics and asymptotics for generating functions is collected (with proofs) that can be applied to the above mentioned tree enumeration problems on trees.

1. Counting Trees With Generating Functions

1.1. Rooted Trees.

One of the basis objects in the context of trees are *binary trees.* Binary trees are rooted trees, where each node is either a leaf (that is, it has no successor) or it has two successors. Usually these two successors are distinguishable: the left successor and the right successor. The leaves of a binary trees are also called *external* nodes and those nodes with two successors *internal* nodes. It is clear that a binary tree with n internal nodes has $n+1$ external nodes. Thus, the total number of nodes is always odd.

Our first result is an explicit formula for the number of binary trees.

Theorem 1. *The number b_n of binary trees with n internal nodes is given by*

$$b_n = \frac{1}{n+1}\binom{2n}{n}.$$

Proof. Suppose that a binary tree has $n+1$ internal nodes. Then the left and right subtrees are also binary trees (with k resp. $n-k$ internal nodes, where $0 \le k \le n$). Thus, one directly gets the recurrence for the corresponding numbers:

$$b_{n+1} = \sum_{k=0}^{n} b_k b_{n-k}. \tag{1}$$

The inital value is $b_0 = 1$ (where the tree consists just of the root).

This recurrence can easily be solved with help of the generating function

$$B(x) = \sum_{n\ge 0} b_n x^n.$$

By (1) we find the relation

$$B(x) = 1 + xB(x)^2 \tag{2}$$

and consequently an explicit representation of the form

$$B(x) = \frac{1-\sqrt{1-4x}}{2x}. \tag{3}$$

Hence[1]

$$\begin{aligned} b_n &= [x^n]\frac{1-\sqrt{1-4x}}{2x} \\ &= -\frac{1}{2}[x^{n+1}](1-4x)^{\frac{1}{2}} \\ &= -\frac{1}{2}\binom{\frac{1}{2}}{n+1}(-4)^{n+1} \\ &= \frac{1}{n+1}\binom{2n}{n}. \end{aligned}$$

□

Remark . There is also an alternate way of deriving a formula for the coefficients with help of (2). Set $\tilde{B}(x) = B(x) - 1$. Then

$$\tilde{B}(x) = x(1+\tilde{B}(x))^2,$$

and we can use Lagrange's inversion formula (see Theorem 9 of Appendix 1.A) with $\varphi(x) = (1+x)^2$ to obtain (for $n \geq 1$)

$$\begin{aligned} b_n = [x^n]\tilde{B}(x) &= \frac{1}{n}[u^{n-1}](1+u)^{2n} \\ &= \frac{1}{n}\binom{2n}{n-1} = \frac{1}{n+1}\binom{2n}{n}. \end{aligned}$$

By inspecting the proof of Theorem 1 one observes that the recurrence relation (1) – together with its intial condition – is exactly a translation of a recursive description of binary trees:

> A binary trees $\mathcal{B}$ is either just an external node or an internal node (the root) with two subtrees that are again binary trees.

Formally we can write this in the form

$$\mathcal{B} = \Box + \circ \times \mathcal{B} \times \mathcal{B} = \Box + \circ \times \mathcal{B}^2,$$

where we denote an external node by $\Box$ and an internal node by $\circ$. The interesting fact – which is also the key to most of the subsequenct considerations – is that this recursive description directly translates to a corresponding relation (2) for the generating function:

$$B(x) = 1 + xB(x)^2.$$

We will demonstrate this kind of prodecure with *planted plane trees*. Planted plane trees are again rooted trees, where each node has an arbitrary number of successors with a natural left to right order (similarly as above).

Theorem 2. *The number p_n of planted plane trees with $n \geq 1$ nodes is given by*

$$p_n = \frac{1}{n}\binom{2n-2}{n-1}.$$

[1] For a power series $a(x) = \sum_{n\geq 0} a_n x^n$ we will use the notation $[x^n]a(x)$ to denote the coefficient a_n of x^n.

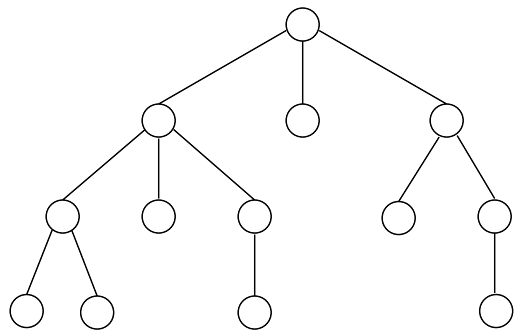

FIGURE 2. Planted plane tree

Proof. We directly proceed in a formal way. Let $\mathcal{P}$ denote the set of planted plane trees. Then from the above description we obtain the recursive relation

$$\mathcal{P} = \circ + \circ \times \mathcal{P} + \circ \times \mathcal{P}^2 + \circ \times \mathcal{P}^3 + \cdots .$$

With

$$P(x) = \sum_{n\ge 1} p_n x^n$$

this translates to

$$P(x) = x + xP(x) + xP(x)^2 + xP(x)^3 = \frac{x}{1-P(x)}.$$

Hence

$$P(x) = \frac{1-\sqrt{1-4x}}{2} = xB(x) \tag{4}$$

and consequently

$$p_n = b_{n-1} = \frac{1}{n}\binom{2n-2}{n-1}.$$

□

Remark 1. As in the case of binary trees we can also use Lagrange's inversion formula (with $\varphi(x) = 1/(1-x)$ to obtain p_n explicitly:

$$p_n = \frac{1}{n}[u^{n-1}](1-u)^{-n} = \frac{1}{n}\binom{-n}{n-1}(-1)^{n-1} = \frac{1}{n}\binom{2n-2}{n-1}.$$

Remark 2. The relation $p_n = b_{n-1}$ has a deeper meaning. There is a *natural bijection* between planted plane trees with n nodes and binary trees with $n-1$ internal nodes: the *rotation correspondance.* Let us start with a planted plane trees with n nodes and apply the following procedure.

1. Delete the root and all edges going to the root.
2. If a node has successors delete all edges to these successors depite one edge to the most left one.
3. Join all theses (previous) successors with a path (by *horizontal edges*).
4. Rotate all these new (horizontal) edges by $\pi/4$ below.
5. The remaining $n-1$ nodes are now considered as internal nodes of a binary tree. Append the (missing) $n+1$ external leaves.

The result is a binary trees with $n-1$ internal nodes. It is easy to verify that this procedure is bijective.

Another kind of rooted trees where we can solve the counting problem directly with help of generating functions are m-ary rooted trees, where $m \ge 2$ is a fixed integer. As in the binary case ($m = 2$) we just take into account the number n of internal nodes. The number of leaves is then given by $(m-1)n+1$ and the total number of leaves by $mn+1$.

Theorem 3. *The number $b_n^{(m)}$ of m-ary trees with n internal nodes is given by*

$$b_n^{(m)} = \frac{1}{(m-1)n+1}\binom{mn}{n}.$$

Proof. As in the binary case, m-ary trees $\mathcal{B}_m$ can be formally described by

$$\mathcal{B}_m = \Box + \circ \times \mathcal{B}_m^m.$$

Thus, the generating function

$$B_m(x) = \sum_{n\ge 0} b_n^{(m)} x^n$$

satisfies the relation

$$B_m(x) = 1 + xB_m(x)^m.$$

Setting $\tilde{B}_m(x) = B_m(x) - 1$ we get

$$\tilde{B}_m(x) = x(1+\tilde{B}_m(x))^m$$

and by Lagrange's inversion formula (for $n \ge 1$)

$$\begin{aligned} b_n^{(m)} &= [x^n]\tilde{B}_m(x) = \frac{1}{n}[u^{n-1}](1+u)^{mn} \\ &= \frac{1}{n}\binom{mn}{n-1} = \frac{1}{(m-1)n+1}\binom{mn}{n}. \end{aligned}$$

□

A similar counting procedure applies to labeled (rooted and unrooted) trees, too. The nodes of a *labeled tree* of size n are labeled with the numbers $1, 2, \ldots, n$. An unrooted labeled tree can be also interpreted as a spanning tree on the complete graph C_n with nodes $1, 2, \ldots, n$.

Theorem 4. *The number l_n of rooted labeled trees of size n is given by*

$$l_n = n^{n-1}.$$

Consequently the number of unrooted labeled trees of size n equals n^{n-2}.

Proof. Let $\mathcal{L}$ denote the set of labeled rooted trees. Then $\mathcal{L}$ can be recursively described as a root followed by an unordered k-tuple of labeled rooted trees for some $k \ge 0$. Note that (for example) a pair of labeled trees (of sizes m and n) naturally corresponds to $\binom{m+n}{m}$ pairs which are labeled with the numbers $1, 2, \ldots, m+n$. Thus, it is appropriate to use the exponential generating function

$$L(x) = \sum_{n\ge 0} \frac{l_n}{n!} x^n$$

of l_n, since the above recursive description is then translated to

$$L(x) = x + xL(x) + x\frac{L(x)^2}{2!} + x\frac{L(x)^3}{3!} + \cdots = xe^{L(x)}.$$

With help of Lagrange's inversion formula we thus get

$$\begin{aligned} l_n = n![x^n]L(x) &= \frac{n!}{n}[u^{n-1}]e^{un} \\ &= (n-1)!\frac{n^{n-1}}{(n-1)!} = n^{n-1}. \end{aligned}$$

Note further that the number of unrooted labeled trees of size n equals l_n/n since every node in an unrooted tree can be used as a root (and produces n different rooted trees). □

1.2. **Simply Generated Trees.**

Simply generated trees have been introduced by Meir and Moon [12] and are proper generalizations of several types of rooted trees. Let

$$\varphi(x) = \varphi_0 + \varphi_1 x + \varphi_2 x^2 + \cdots$$

be a power series with non-negative coefficients, in particular we assume that $\varphi_0 > 0$ and $\varphi_j > 0$ for some $j \ge 2$. We then define the weight $\omega(T)$ of a finite rooted tree T by

$$\omega(T) = \prod_{j\ge 0} \varphi_j^{D_j(T)},$$

where $D_j(T)$ denotes the number of nodes in T with j successors. If we set

$$y_n = \sum_{|T|=n} \omega(T)$$

then the generating function

$$y(x) = \sum_{n\ge 1} y_n x^n$$

satisfies the functional equation

$$y(x) = x\varphi(y(x)).$$

In this context y_n denotes a weighted number of trees is size n. For example, if $\varphi_j = 1$ for all $j \ge 0$ (that is, $\varphi(x) = 1/(1-x)$) then all rooted trees have weight $\omega(T) = 1$ and $y_n = p_n$ is the number of planted plane trees. Another example is $\varphi(x) = 1 + x + x^2$ that leads to *Motzkin trees*. Here only rooted trees, where all nodes have less than 3 successors get (a non-zero) weight $\omega(T) = 1$: y_n is the number of Motzkin trees with n nodes.

Binary trees are also covered by this approach. If we set $\varphi(x) = 1 + 2x + x^2 = (1+x)^2$ then nodes with one successor get the weight 2. This takes into account that binary trees (where external nodes are disregarded) have two kinds of nodes with one successor, namely those with a left branch but no right branch and those with a right branch but no left branch. Similarly, m-ary trees are counted with help of $\varphi(x) = (1+x)^m$.

In view of this examples it is convenient to think of simply generated trees $\mathcal{T}$ as a weighted recursive structure of the form

$$\mathcal{T} = \varphi_0 \cdot \circ + \varphi_1 \cdot \circ \times \mathcal{T} + \varphi_2 \cdot \circ \times \mathcal{T}^2 + \cdots .$$

If all φ_j are (non-negative) integers then the *weighted* number y_n is actually a number of certain rooted trees of size n.

Interestingly there is an intimate relation to Galton-Watson branching processes. Let ξ be a non-negative integer valued random variable. The Galton-Watson branching process $(Z_k)_{k\geq 0}$ is then given by $Z_0 = 1$, and for $k \geq 1$ by

$$Z_k = \sum_{j=1}^{Z_{k-1}} \xi_j^{(k)},$$

where the $(\xi_j^{(k)})_{k,j}$ are iid random variables distributed as ξ.

It is clear that Galton-Watson branching processes can be represented by ordered (finite or infinite) rooted trees T such that the sequence Z_k is just the number of nodes at level k and $\sum_{k\geq 0} Z_k$ (which is called the *total progeny*) is the number of nodes $|T|$ of T. We will denote by $\nu(T)$ the probability that a specific tree T occurs. The generating function $y(x) = \sum_{n\geq 1} y_n x^n$ of the numbers

$$y_n = \mathbf{Pr}[|T| = n] = \sum_{|T|=n} \nu(T)$$

satisfies the functional equation

$$y(x) = x\varphi(y(x)),$$

where $\varphi(t) = \mathbf{E}\, t^{\xi} = \sum \varphi_j t^j$ with $\varphi_j = \mathbf{Pr}[\xi = j]$. Note that

$$\nu(T) = \prod_{j\geq 0} \varphi_j^{D_j(T)} = \omega(T).$$

The *weight* of T is now the *probability* of T.

By Lagrange's inversion formula we get for all simply generated trees (and for all Galton-Watson branching processes)

$$y_n = \frac{1}{n}[u^{n-1}]\varphi(u)^n. \tag{5}$$

But there are only few cases where we can use this formula to obain *nice* explicit expressions for y_n. Nevertheless there is a quite general asymptotic result which relies on the fact that (under certain conditions) the generating function $y(x)$ has a finite radius r of convergence and that $y(x)$ has a singularity of square root type at $x_0 = r$, that is, $y(x)$ has a represenation of the form

$$y(x) = g(x) - h(x)\sqrt{1 - \frac{x}{x_0}} = c_0 + c_1\sqrt{x - x_0} + c_2(x - x_0) + \mathcal{O}\left(|x - x_0|^{3/2}\right),$$

where $g(x)$ and $h(x)$ are analytic at x_0. For binary and planted plane trees this has been made explicit, see (3) and (4). Of course, such representations can be used to derive asymototic expansions for the coefficients y_n (for details see the proof of Theorem 10 in the Appendix 1.B). It should be further mentioned that formula (5) can be also used to derive asymptotics for y_n via a saddle point method applied to the integral $\int (\varphi(u)/u)^n \, du$, where the contour of integration is the circle $|u| = \tau$ (compare also with Theorem 17). Of course, one gets the same result. But the method presented in Theorem 10 is much more general. It works for *general* functional equations of the form $y = F(x,y)$ and not only for equations of the form $y = x\varphi(y)$.

Theorem 5. *Let R denote the radius of convergence of $\varphi(t)$ and suppose that there exists τ with $0 < \tau < R$ that satisfies $\tau\varphi'(\tau) = \varphi(\tau)$. Set $d = \gcd\{j > 0 : \varphi_j > 0\}$. Then*

$$y_n = d\sqrt{\frac{\varphi(\tau)}{2\pi\varphi''(\tau)}}\frac{\varphi'(\tau)^n}{n^{3/2}}\left(1 + \mathcal{O}\left(n^{-1}\right)\right) \qquad (n \equiv 1 \bmod d) \tag{6}$$

and $y_n = 0$ if $n \not\equiv 1 \bmod d$.

Proof. We apply Theorem 10 for $F(x,y) = x\varphi(y)$ and assume first for simplicity that $d = 1$. Then all assumptions are satisfied. In particular we have $x_0 = 1/\varphi'(\tau)$ and $y_0 = \tau$.

If $d > 1$ then it is easy to see that $y_n = 0$ if $n \not\equiv 1 \bmod d$. Consequently we have $y(x) = \tilde{y}(x^d)/x^{d-1}$ and (of course) $\varphi(x) = \tilde{\varphi}(x^d)$ for analytic functions $\tilde{y}(x)$ and $\tilde{\varphi}(x)$. They satisfy $\tilde{y}(x) = x\tilde{\varphi}(\tilde{y}(x))$ and the corresponding gdc $\tilde{d} = 1$. Thus, Theorem 10 can be directly applied to this equation and we obtain (6) in general. □

Note that for m-ary trees and for planted plane trees this asymptotic formula also follows from the explicit formulae for $b_n^{(m)}$ and p_n via Stirling's formula.

1.3. Unrooted Trees.

Let $\tilde{\mathcal{T}}$ denote the set of unlabeled unrooted trees and $\mathcal{T}$ the set of unlabeled rooted trees. The corresponding cardinalities of these trees (of size n) are denoted by $\tilde{t}_n$ and t_n, and the generating functions by

$$\tilde{t}(x) = \sum_{n\ge 1}\tilde{t}_n x^n \quad \text{and} \quad t(x) = \sum_{n\ge 1} t_n x^n.$$

The structure of these trees is much more difficult than that of rooted trees, where the successors have a left to right order. It turns out that one has to apply Pólya's theory of counting and an amazing observation (8) by Otter [15].

Theorem 6. *The generating functions $t(x)$ and $\tilde{t}(x)$ satisfy the functional equations*

$$t(x) = x\exp\left(t(x) + \frac{1}{2}t(x^2) + \frac{1}{3}t(x^3) + \cdots\right) \tag{7}$$

and

$$\tilde{t}(x) = \sum_{n\ge 1}\tilde{t}_n x^n = t(x) - \frac{1}{2}t(x)^2 + \frac{1}{2}t(x^2). \tag{8}$$

They have a common radius of convergence $\rho \approx 0.338219$ which is given by $t(\rho) = 1$, that is, $t(x)$ is convergent at $x = \rho$. Furthermore, they have a local expansion of the form

$$t(x) = 1 - b(\rho - x)^{1/2} + c(\rho - x) + d(\rho - x)^{3/2} + \mathcal{O}\left((\rho - x)^2\right) \tag{9}$$

and

$$\tilde{t}(x) = \frac{1 + t(\rho^2)}{2} + \frac{b^2 - \rho t'(\rho^2)}{2}(\rho - x) + bc(\rho - x)^{3/2} + \mathcal{O}\left((\rho - x)^2\right), \tag{10}$$

where $b \approx 2.6811266$ and $c = b^2/3 \approx 2.3961466$, and $x = \rho$ is the only singularity on the circe of convergence $|x| = \rho$. Finally, t_n and $\tilde{t}_n$ are asymptotically given by

$$t_n = \frac{b\sqrt{\rho}}{2\sqrt{\pi}} n^{-3/2} \rho^{-n} \left(1 + \mathcal{O}\left(n^{-1}\right)\right) \tag{11}$$

and

$$\tilde{t}_n = \frac{b^3 \rho^{3/2}}{4\sqrt{\pi}} n^{-5/2} \rho^{-n} \left(1 + \mathcal{O}\left(n^{-1}\right)\right). \tag{12}$$

Remark . In 1937 Pólya [16] already discussed the generating function $t(x)$ and showed that the radius of convergence ρ satisfies $0 < \rho < 1$ and that $x = \rho$ is the only singularity on the circle of convergence $|x| = \rho$. Later Otter [15] showed that $t(\rho) = 1$ and used the representation (9) to deduce the asymptotics for t_n. He also calculated $\rho \approx 0.338219$ and $b \approx 2.6811266$. However, his main contribution was to show (8). Consequently he derived (10) and (12).

Proof. We first show (7). As in the previous cases we can think of rooted trees in a recursive way, that is, $\mathcal{T}$ is a root followed by a *set of rooted trees*. However, these rooted subtrees are not ordered from left to right and there are no labels. In other words a subtree structure and all its permutations just count once. On the level of generating functions this can be managed with help Pólya's theory of counting. Let $Z(S_k; x_1, x_2, \ldots, x_k)$ denote the cycle index of the symmetric group S_k then we get

$$t(x) = x \sum_{k \ge 0} Z(S_k; t(x), t(x^2), \ldots, t(x^k)).$$

Since

$$\sum_{k \ge 0} Z(S_k; x_1, x_2, \ldots, x_k) = \exp\left(x_1 + \frac{1}{2}x_2 + \frac{1}{3}x_3 + \cdots\right)$$

we also obtain (7).

The radius of convergence ρ of $t(x)$ surely satisfies $\frac{1}{4} \le \rho \le 1$. (This follows from $t_n \le p_n$ and $t_n \to \infty$.) Next we show that $t(\rho)$ is finite (although $x = \rho$ is a singularity of $t(x)$) and that $\rho < 1$. From (7) it follows that $\log(t(x)/x) \ge t(x)$ for $0 < x < \rho$. Hence,

$$\frac{t(x)/x}{\log(t(x)/x)} \le \frac{1}{x}$$

and consequently $t(\rho)$ has to be finite. If $\rho = 1$ then $t(\rho^k) = t(\rho)$ for all $k \ge 1$ and it would follow that

$$\lim_{x \to \rho-} e^{t(x) + \frac{1}{2}t(x^2) + \frac{1}{3}t(x^3) + \cdots} = \infty$$

which is impossible. Thus, $\rho < 1$ and consequently the functions $t(x^2), t(x^3), \ldots$ are regular at $x = \rho$. Moreover, they are analytic for $|x| \le \rho + \varepsilon$ (for some sufficiently small $\varepsilon > 0$) and are also bounded by $|t(x^k)| \le C|x^k|$ in this range. Hence, $t(x)$ may be considered as the solution of the functional equation $y = F(x, y)$, where

$$F(x, y) = x \exp\left(y + \frac{1}{2}t(x^2) + \frac{1}{3}t(x^3) + \cdots\right).$$

This function satisfies the assumptions of Theorem 10. In particular, the singularity $x = \rho$ and $\eta = t(\rho)$ satisfy the system of equations

$$\eta = \rho \exp\left(\eta + \frac{1}{2}t(\rho^2) + \frac{1}{3}t(\rho^3) + \cdots\right),$$
$$1 = \rho \exp\left(\eta + \frac{1}{2}t(\rho^2) + \frac{1}{3}t(\rho^3) + \cdots\right)$$

that directly gives $\eta = t(\rho) = 1$. Now, by using the expansion (9) and (7) we also get $c = b^2/3$ by comparing coefficients. So get obtain (10) and (11). Note also that Theorem 10 implies that $x = \rho$ is the only singularity on the circle of convergence of $t(x)$.

Next, observe that (9) and (8) imply (10) and (with help of the transfer lemma (Lemma 1) (12). Therefore it remains to prove (8).

We consider three sets of trees, the set $\mathcal{T}$ of rooted trees, the set $\tilde{\mathcal{T}}$ of unrooted trees and the set $\mathcal{T}^{(p)}$ of (unordered) pairs $\{T_1, T_2\}$ of rooted trees of $\mathcal{T}$ with $T_1 \neq T_2$. (It will be convenient to consider the pair $\{T_1, T_2\}$ as a tree that is *rooted* by an additional edge joining the roots of T_1 and T_2.) Let $t_n^{(p)}$ denote the number of pairs of that kind with a total number of n nodes, and let $t^{(p)}(x)$ denote the generating function of $t_n^{(p)}$. Then by Pólya's theory we have (see [9])

$$t^{(p)}(x) = \frac{1}{2}t(x)^2 - \frac{1}{2}t(x^2). \tag{13}$$

We will now show that there is a bijection between $\mathcal{T}$ and $\tilde{\mathcal{T}} \cup \mathcal{T}^{(p)}$.[2] In view of (13) such a bijection implies (8).

Recall that an arbitrary (finite) tree has either a *cental node* or a *central edge*. The central edge $e = (v, w)$ is called *symmetry* line if the two subtrees rooted at the endpoints v and w are equal.

We first partition the set $\mathcal{T}$ into 6 subsets:

1. Let $\mathcal{T}_1$ denote those rooted trees that are rooted at the central node.
2. Let $\mathcal{T}_2$ denote those rooted trees that have a central node that is different from the root.
3. Let $\mathcal{T}_3$ denote those rooted trees that have a central edge which is not a symmetry line and where one of the two endpoints of the central edge is the root.
4. Let $\mathcal{T}_4$ denote those rooted trees that have a central edge which is not a symmetry line and where the root is not one of the two endpoints of the central edge.
5. Let $\mathcal{T}_5$ denote those rooted trees that have a central edge which is a symmetry line and where one of the two endpoints is the root.
6. Let $\mathcal{T}_6$ denote those rooted trees that have a central edge which is a symmetry line and where the root is not one of the two endpoints of the central edge.

In a similar way we partition the unrooted trees $\tilde{\mathcal{T}}$:

1. Let $\tilde{\mathcal{T}}_1$ denote those unrooted trees that have a central node.
2. Let $\tilde{\mathcal{T}}_2$ denote those unrooted trees that have a central edge, that is not a symmetry line.
3. Let $\tilde{\mathcal{T}}_3$ denote those unrooted trees that have a symmetry line as a central edge.

[2]This bijection was pointed out to me by Bernhard Gittenberger.

Finally we partition $\mathcal{T}^{(p)}$, that we consider as trees *rooted* at an edge.

1. Let $\mathcal{T}_1^{(p)}$ be the set of pairs $\{T_1, T_2\}$ with $T_1 \neq T_2$ with the propery that if we join the roots of T_1 and T_2 by an edge then the resulting tree has a central node.
2. Let $\mathcal{T}_2^{(p)}$ be the set of pairs $\{T_1, T_2\}$ with $T_1 \neq T_2$, such that the tree that results from T_1 and T_2 by joining the roots by an edge has a central edge that is not a symmetry line and that is different from the edge joining T_1 and T_2.
3. Let $\mathcal{T}_3^{(p)}$ be the set of pairs $\{T_1, T_2\}$ with $T_1 \neq T_2$, such that the tree that results from T_1 and T_2 by joining the roots by an edge has a central edge that is not a symmetry line and that is different from the the edge joining T_1 and T_2.
4. Let $\mathcal{T}_4^{(p)}$ be the set of pairs $\{T_1, T_2\}$ with $T_1 \neq T_2$, such that the tree that results from T_1 and T_2 by joining the roots by an edge has symmetry line as a central edge that is different from the the edge joining T_1 and T_2.

Now there is a natural bijection between $\mathcal{T}_1$ and $\tilde{\mathcal{T}}_1$. We only have to take the central node as the root.

Next, there is a bijection betwenn $\mathcal{T}_2$ and $\mathcal{T}_1^{(p)}$. We identify the first edge from the path connecting the root and the central node with the edge joining T_1 and T_2.

Next, there is a trivial bijection between sets $\tilde{\mathcal{T}}_2$ and $\mathcal{T}_2^{(p)}$. Furthermore, by marking one of the two endpoints of the central edge in the trees of $\tilde{\mathcal{T}}_2$ we obtain $\mathcal{T}_3$. Of course, this can be *rewritten* as a bijection between $\mathcal{T}_3$ and $\tilde{\mathcal{T}}_2 \cup \mathcal{T}_2^{(p)}$.

Next, there is a bijection betwenn $\mathcal{T}_4$ and $\mathcal{T}_3^{(p)}$. We identify the first edge from the path connecting the root and the central edge with the edge joining T_1 and T_2. Similarly there is a bijection between $\mathcal{T}_6$ and $\mathcal{T}_4^{(p)}$.

Finally, there is a natural bijection between $\mathcal{T}_5$ and $\tilde{\mathcal{T}}_3$. □

In a similar (but easier) way one can also treat planar trees $\tilde{\mathcal{P}}$. We already discussed planted plane trees $\mathcal{P}$ and their generating function $p(x)$ which satisfies $p(x) = x/(1-p(x))$. If $\tilde{p}(x)$ denotes the generating function of the numbers $\tilde{p}_n$ of planar (unrooted) trees of size n then the following relations hold.

Theorem 7. *The generating functions $\tilde{p}(x)$ is given by*

$$\tilde{p}(x) = x \sum_{k\geq 0} Z(C_k; p(x), p(x^2), \dots, p(x^k)) - \frac{1}{2}p(x)^2 + \frac{1}{2}p(x^2), \tag{14}$$

where $Z(C_k; x_1, x_2, \dots, x_k) = \frac{1}{k}\sum_{d|k}\varphi(d)x_d^{k/d}$ denotes the cycle index of the cyclic group C_k of k elements. The numbers $\tilde{p}_n$ of planar (unrooted) trees of size n are asymptotically given by

$$\tilde{p}_n = \frac{1}{8\sqrt{\pi}} 4^n n^{-5/2} \left(1 + \mathcal{O}\left(n^{-1}\right)\right). \tag{15}$$

Proof. First of all, the generating function $r(x)$ of rooted planar trees is given by

$$r(x) = x \sum_{k\geq 0} Z(C_k; p(x), p(x^2), \dots, p(x^k)).$$

This is due to the fact that the subtrees of the root in planted plane trees have a left-to-right order but rotations around the root are not allowed. Second, as in the proof of Theorem 6 one has

$$\tilde{p}(x) = r(x) - \frac{1}{2}p(x)^2 + \frac{1}{2}p(x^2).$$

Consequently $\tilde{p}(x)$ has a local expansion of the form

$$\tilde{p}(x) = \frac{1}{6}(1-4x)^{3/2} + \cdots$$

which gives (15) with help of the transfer lemma (Lemma 1). □

1.4. **Other Types of Trees.**

We just want to mention that there are several other types of trees, for expample *recursice trees, binary search trees, digital search trees, tries, quad-trees* etc. that will not be discussed in this paper. Nevertheless, in all these cases the concept of generating functions can be used to rephrase the counting problem into this more analytic language (for details see Flajolet et al. [7] and Sedgewick and Flajolet [17]).

Appendix 1.A: Lagrange Inversion Formula.

Let $a(x) = \sum_{n\ge 0} a_n x^n$ be a power series with $a_0 = 0$ and $a_1 \ne 0$. The Lagrange inversion formula provides an expicit representation of the coefficients of inverse power series $a^{[-1]}(x)$ which is defined by $a(a^{[-1]}(x)) = a^{[-1]}(a(x)) = x$.

Theorem 8. *Let $a(x) = \sum_{n\ge 0} a_n x^n$ be a formal power series with $a_0 = 0$ and $a_1 \ne 0$. Let $b(x) = a^{[-1]}(x)$ be the inverse power series and $g(x)$ an arbitrary power series. Then the n-th coefficient of $g(b(x))$ is given by*

$$[x^n]g(b(x)) = \frac{1}{n}[u^{n-1}]g'(u)\left(\frac{u}{a(u)}\right)^n \qquad (n \ge 1).$$

In tree enumeration problems the following variant is more appropriate. Note that Theorems 8 and 9 are equivalent. If $a(x) = x/\phi(x)$ then $a^{[-1]}(x) = y(x)$, where $y(x)$ satisfies the equation $y(x) = x\phi(y(x))$.

Theorem 9. *Let $\phi(x)$ be a power series with $\phi(0) \ne 0$ and $y(x)$ the (unique) power series solution of the equation*

$$y(x) = x\phi(y(x)).$$

Then $y(x)$ is invertible and the n-th coefficient of $g(y(x))$ (where $g(x)$ is an arbitrary power series) is given by

$$[x^n]g(y(x)) = \frac{1}{n}[u^{n-1}]g'(u)\phi(u)^n \qquad (n \ge 1).$$

Proof. Since Theorems 8 and 9 are equivalent we only have to prove Theorems 8. We also present an analytic proof for complex coefficients. Of course, the resulting analytic identities are formal ones, too.

We start with Cauchy's formula and use the substitution $u = b(x)$. Note that if γ is a contour with winding number 1 around the origin the $\gamma' = b(\gamma)$ has the same property:

$$
\begin{aligned}
[x^n]g(b(x)) &= \frac{1}{2\pi i}\int_\gamma \frac{g(b(x))}{x^{n+1}}\,dx \\
&= \frac{1}{2\pi i}\int_{\gamma'} g(u)\frac{a'(u)}{a(u)^{n+1}}\,du.
\end{aligned}
$$

Since

$$\left(g(u)\frac{1}{a(u)^n}\right)' = g'(u)\frac{1}{a(u)^n} - n\,g(u)\frac{a'(u)}{a(u)^{n+1}}$$

it follows that

$$\int_{\gamma'} g(u)\frac{a'(u)}{a(u)^{n+1}}\,du = \frac{1}{n}\int_{\gamma'} g'(u)\frac{1}{a(u)^n}\,du$$

and consequently

$$
\begin{aligned}
[x^n]g(b(x)) &= \frac{1}{n}\int_{\gamma'} g'(u)\frac{u^n}{a(u)^n}\,\frac{du}{u^n} \\
&= \frac{1}{n}[u^{n-1}]g'(u)\left(\frac{u}{a(u)}\right)^n.
\end{aligned}
$$

□

Appendix 1.B: Functional Equations.

Let $y(x)$ be a power series that is the solution of a funtional equation of the form $y = F(x,y)$, where F is function with certain properties. In this section we show how we can obtain asymptotic expansions for the coefficients of $y(x)$. One major *ingredience* of the proof of Theorem 10 is the *transfer lemma* of Flajolet and Odlyzko [8].

Lemma 1. *Let*

$$A(x) = \sum_{n\ge 0} a_n x^n$$

be analytic in a region

$$\Delta = \{x : |x| < x_0 + \eta,\ |\arg(x - x_0)| > \delta\},$$

in which x_0 and η are positive real numbers and $0 < \delta < \pi/2$. Furthermore suppose that there exists a real number α such that

$$A(x) = \mathcal{O}\left((1 - x/x_0)^{-\alpha}\right) \qquad (x \in \Delta).$$

Then

$$a_n = \mathcal{O}\left(x_0^{-n} n^{\alpha-1}\right).$$

Proof. One uses Cauchy's formula

$$a_n = \frac{1}{2\pi i}\int_\gamma \frac{A(z)}{z^{n+1}}\,dz,$$

where γ is a suitable chosen path of integration around the origin. In particular one can use $\gamma = \gamma_1 \cup \gamma_2 \cup \gamma_3 \cup \gamma_4$, where

$$\begin{aligned}
\gamma_1 &= \left\{ x = x_0 + \frac{z}{n} : |z| = 1,\ \delta \le |\arg(z)| \le \pi \right\}, \\
\gamma_2 &= \left\{ x = x_0 + te^{i\delta} : \frac{1}{n} \le t \le \eta \right\}, \\
\gamma_3 &= \left\{ x = x_0 + te^{-i\delta} : \frac{1}{n} \le t \le \eta \right\}, \\
\gamma_4 &= \left\{ x : |x| = \left| x_0 + e^{i\delta}\eta \right|,\ \arg\left(x_0 + e^{i\delta}\eta\right) \le |\arg x| \le \pi \right\}.
\end{aligned}$$

It is easy to show that the bound $|A(z)| \le C|1 - z/x_0|^{-\alpha}$ directly proves that

$$\left| \int_{\gamma_1 \cup \gamma_2 \cup \gamma_3} \frac{A(z)}{z^{n+1}}\, dz \right| = \mathcal{O}\left(x_0^{-n} n^{\alpha-1} \right),$$

whereas the integal over γ_4 is exponentially smaller: $\mathcal{O}\left((x_0+\eta)^{-n}\right)$. □

Remark . Suppose that a function is analytic in a region of the form Δ and that it has an expansion of the form

$$a(x) = C\left(1 - \frac{x}{x_0}\right)^{-\alpha} + \mathcal{O}\left(\left(1 - \frac{x}{x_0}\right)^{-\beta}\right) \qquad (x \in \Delta),$$

where $\beta < \alpha$. Then we have

$$a_n = [x^n]a(x) = C\frac{n^{\alpha-1}}{\Gamma(\alpha)} x_0^{-n} + \mathcal{O}\left(x_0^{-n} n^{\max\{\alpha-2,\beta-1\}} \right). \tag{16}$$

This is due to the fact that

$$(-1)^n \binom{-\alpha}{n} = \frac{n^{\alpha-1}}{\Gamma(\alpha)} + \mathcal{O}\left(n^{\alpha-2}\right).$$

Theorem 10. *Suppose that $F(x,y)$ is an analytic function in x,y around $x = y = 0$ such that $F(0,y) = 0$ and that all Taylor coefficients of F around 0 are real and non-negative. Then there exists a unique analytic solution $y = y(x)$ of the functional equation*

$$y = F(x,y) \tag{17}$$

with $y(0) = 0$ that has non-negative Taylor coefficients around 0.

If the region of convergence of $F(x,y)$ is large enough such that there exist positive solutions $x = x_0$ and $y = y_0$ of the system of equations

$$\begin{aligned}
y &= F(x,y), \\
1 &= F_y(x,y).
\end{aligned}$$

with $F_x(x_0,y_0) \ne 0$ and $F_{yy}(x_0,y_0) \ne 0$ then $y(x)$ is analytic for $|x| < x_0$ and there exist functions $g(x)$, $h(x)$ that are analytic around $x = x_0$ such that $y(x)$ has a representation of the form

$$y(x) = g(x) - h(x)\sqrt{1 - \frac{x}{x_0}} \tag{18}$$

locally around $x = x_0$. We have $g(x_0) = y(x_0)$, and

$$h(x_0) = \sqrt{\frac{2x_0 F_x(x_0, y_0)}{F_{yy}(x_0, y_0)}}.$$

Moreover, (18) provides a local analytic continuation of $y(x)$ (for $\arg(x - x_0) \neq 0$).

If we further assume that $[x^n]y(x) > 0$ for $n \geq n_0$ then $x = x_0$ is the only singularity of $y(x)$ on the circle $|x| = x_0$ and we obtain an asymptotic expansion for $[x^n]y(x)$ of the form

$$[x^n]y(x) = \sqrt{\frac{x_0 F_x(x_0, y_0)}{2\pi F_{yy}(x_0, y_0)}} x_0^{-n} n^{-3/2} \left(1 + \mathcal{O}\left(n^{-1}\right)\right). \tag{19}$$

Remark 3. Note that the assumptions $F_x(x_0, y_0) \neq 0$ and $F_{yy}(x_0, y_0) \neq 0$ are really necessary to obtain a representation of the form (18). If $F_x(x_0, y_0) = 0$ then $F(x, y)$ (and $y(x)$) would not depend on x. Furthermore, if $F_{yy}(x_0, y_0) = 0$ then F is linear in y:

$$F(x, y) = yF_1(x) + F_2(x), \tag{20}$$

and consequently

$$y(x) = \frac{F_2(x)}{1 - F_1(x)} \tag{21}$$

is explicit and surely not of the form (18). However, a representation of the form (21) (where $F_1(x) \not\equiv 0$) usually leads to almost the asymptotic expansions for the coefficients of $y(x)$ in the case covered by Theorem 10. Suppose that the radius r of convergence of $F_1(x)$ is large enough that there is $0 < x_0 < r$ with $F_1(x_0) = 1$ and that $[x^n]y(x) > 0$ for $n \geq n_0$ then x_0 is the only singularity on the circle of convergence $|x| = x_0$ of $y(x)$ and one gets

$$[x^n]y(x) = \frac{F_2(x_0)}{x_0 F'(x_0)} x_0^{-n} + \mathcal{O}\left((x_0 + \eta)^{-n}\right).$$

for some $\eta > 0$.

Proof. Firstly, we show that there exists a unique (analytic) solution $y = y(x)$ of $y = F(x, y)$ with $y(0) = 0$. Since $F(0, y) = 0$ it follows that the functional mapping

$$y(x) \mapsto F(x, y(x))$$

is a contraction for small x. Thus the iteratively defined functions $y_0(x) \equiv 0$ and

$$y_{m+1}(x) = F(x, y_m(x)) \qquad (n \geq 0)$$

converge uniformly to a limit function $y(x)$ which is the unique solution of (17). By definition it is clear that $y_m(x)$ is an analytic function around 0 and has real and non-negative Taylor coefficients. Consequently, the uniform limit $y(x)$ is analytic, too, with non-negative Taylor coefficients.

It is also possible to use the implicit function theorem. Since

$$F_y(0, 0) = 0 \neq 1.$$

there exists a solution $y = y(x)$ of (17) which is analytic around 0.

However, it is useful to know that all Taylor coefficients of $y(x)$ are non-negative. Namely, it follows that if $y(x)$ is regular at x' (which is real and positive) then $y(x)$ is regular for all x with $|x| \leq x'$.

Let x_0 denote the radius of convergence of $y(x)$. Then x_0 is a singularity of $y(x)$. The mapping

$$x \mapsto F_y(x, y(x))$$

is strictly increasing for real and non-negative x as long as $y(x)$ is regular. Note that $F_y(0, y(0)) = 0$. As long as $F_y(x, y(x)) < 1$ it follows from the implicit function theorem that $y(x)$ is regular even in a neighbourhood of x. Hence there exists a finite limit point x_0 such that $\lim_{x \to x_0-} y(x) = y_0$ is finite and satisfies $F_y(x_0, y_0) = 1$. If $y(x)$ were regular at $x = x_0$ then

$$y'(x_0) = F_x(x_0, y(x)) + F_y(x_0, y(x_0))y'(x_0)$$

would imply $F_x(x_0, y(x_0)) = 0$ which is surely not true. Thus, $y(x)$ is singular at $x = x_0$ (that is, x_0 is the radius of convergence) and $y(x_0)$ is finite.

Now, let us consider the equation $y - F(x, y) = 0$ around $x = x_0$ and $y = y_0$. We have $1 - F_y(x_0, y_0) = 0$ but $-F_{yy}(x_0, y_0) \neq 0$. Hence by the Weierstrass preparation theorem (see [11]) there exist functions $H(x, y)$, $p(x)$, $q(x)$ which are analytic around $x = x_0$ and $y = y_0$ and satisfy $H(x_0, y_0) \neq 1$, $p(x_0) = q(x_0) = 0$ and

$$y - F(x, y) = H(x, y)((y - y_0)^2 + p(x)(y - y_0) + q(x))$$

locally around $x = x_0$ and $y = y_0$. Since $F_x(x_0, y_0) \neq 0$ we also have $q_x(x_0) \neq 0$. This means that any analytic function $y = y(x)$ which satisfies $y(x) = F(x, y(x))$ in a subset of a neighbourhood of $x = x_0$ with x_0 on its boundary and is given by

$$y(x) = y_0 - \frac{p(x)}{2} \pm \sqrt{\frac{p(x)^2}{4} - q(x)}.$$

Since $p(x_0) = 0$ and $q_x(x_0) \neq 0$ we have

$$\frac{\partial}{\partial x} \left(\frac{p(x)^2}{4} - q(x) \right)_{x = x_0} \neq 0,$$

too. Thus there exist an analytic function $K(x)$ such that $K(x_0) \neq 0$ and

$$\frac{p(x)^2}{4} - q(x) = K(x)(x - x_0)$$

locally around $x = x_0$. This finally leads to a local representation of $y = y(x)$ of the kind

$$y(x) = g(x) - h(x)\sqrt{1 - \frac{x}{x_0}}, \tag{22}$$

in which $g(x)$ and $h(x)$ are analytic around $x = x_0$ and satisfy $g(x_0) = y_0$ and $h(x_0) < 0$.

In order to calculate $h(x_0)$ we use Taylor's theorem

$$\begin{aligned} 0 &= F(x, y(x)) \\ &= F_x(x_0, y_0)(x - x_0) + \frac{1}{2}F_{yy}(x_0, y_0)(y(x) - y_0)^2 + \cdots \qquad (23) \\ &= F_x(x_0, y_0)(x - x_0) + \frac{1}{2}F_{yy}(x_0, y_0)h(x_0)^2(1 - x/x_0) + O(|x - x_0|^{3/2}). \end{aligned}$$

By comparing the coefficients of $(x - x_0)$ we immediately obtain

$$h(x_0) = \sqrt{\frac{2x_0 F_x(x_0, y_0)}{F_{yy}(x_0, y_0)}}.$$

We now want to apply the transfer lemma (Lemma 1). For this purpose we have to show that $y(x)$ can be analytically continued to a region of the form Δ. The representation (22) provides such an analytic continuation for x in a neighborhood of x_0. Now suppose that $|x_1| = x_0$ and $|\arg(x_1)| \geq \delta$. Then the assumption $y_n > 0$ for $n \geq n_0$ implies that $|y(x_1)| < y(|x_1|) = y(x_0)$ and consequently

$$|F_y(x_1, y(x_1))| \leq F_y(|x_1|, |y(x_1)|) < F_y(|x_1|, y(|x_1|)) = F_y(x_0, y_0) = 1.$$

Thus, $F_y(x_1, y(x_1)) \neq 1$ and the implicit function theorem shows that there exists an analytic solution $y = y(x)$ in a neighborhood of x_1. For $|x| < x_0$ this solution equals the power series $y(x)$ and for $|x| \geq x_0$ it provides an analytic continuation to a region of the form Δ (by compactness it is sufficient to consider finitely many x_1 with $|x_1| = x_0$ and $|\arg(x_1)| \geq \delta$). So finally we can apply Lemma 1 (resp. (16) with $\alpha = -1/2$ and $\beta = -3/2$; the analytic part of $g(x)$ provides exponentially smaller contributions.) This completes the proof of (19). $\square$

2. Parameters in Trees

2.1. **The Number of Leaves.**

In this section we will treat more involved enumeration problems. As an introductory example we consider the numbers $p_{n,k}$ of planted plane trees of size n with exactly k leaves. Again the concept of generating functions is a valuable tool for deriving explicit and asymptotic results.

Theorem 11. *The numbers $p_{n,k}$ of planted plane trees of size n with exactly k leaves are given by*

$$p_{n,k} = \frac{1}{n}\binom{n}{k}\binom{n-1}{k}.$$

Proof. Let $p(x,u) = \sum_{n,k} p_{n,k} x^n z^k$ denote the bivariate generating function of the numbers $p_{n,k}$. Then following the recursive description of planten plane trees one gets

$$p(x,u) = xu + x \sum_{k \geq 1} p(x,u)^k = xu + \frac{x\, p(x,u)}{1 - p(x,u)}.$$

For a moment, let x be considered as a *parameter*. Then we have

$$p(x,u) = \frac{u}{x\left(1 - \frac{x}{1-p(x,u)}\right)}$$

and consequently

$$[u^k]p(x,u) = \frac{1}{k}[v^{k-1}]\left(\frac{x}{1 - \frac{x}{1-v}}\right)^k$$

Finally this implies

$$\begin{aligned} p_{n,k} &= [x^n u^k] p(x,u) \\ &= \frac{1}{k}[x^n v^{k-1}] \left(\frac{x}{1-\frac{x}{1-v}}\right)^k \\ &= \frac{1}{k}\binom{n-1}{k-1}[v^{k-1}](1-v)^{-n+k} \\ &= \frac{1}{k}\binom{n-1}{k-1}\binom{n-1}{k} \\ &= \frac{1}{n}\binom{n}{k}\binom{n-1}{k}. \end{aligned}$$

□

By using Stirling's formula we directly obtain bivariate asymptotic expansions for $p_{n,k}$ of the form

$$\begin{aligned} p_{n,k} &= \frac{1}{2\pi k n}\left(\frac{n}{k}\right)^{2k}\left(\frac{n}{n-k}\right)^{2(n-k)} \cdot \left(1 + \mathcal{O}\left(\frac{1}{k}\right) + \mathcal{O}\left(\frac{1}{n-k}\right)\right) \\ &= \frac{1}{2\pi n^2} \cdot \frac{n}{k} \cdot \left(\frac{1-\frac{k}{n}}{\frac{k}{n}}\right)^{2k} \cdot \left(\frac{1}{1-\frac{k}{n}}\right)^{2n} \cdot \left(1 + \mathcal{O}\left(\frac{1}{k}\right) + \mathcal{O}\left(\frac{1}{n-k}\right)\right). \quad (24) \end{aligned}$$

In particular, if we fix n then $p_{n,k}$ is maximal if $k \approx n/2$ and we *locally* get a behaviour of the kind

$$p_{n,k} \sim \frac{4^n}{\pi n^2} \exp\left(-\frac{(n-2k)^2}{n}\right). \quad (25)$$

This approximation has several implications. First, it shows that it is most likely that a *typical* tree of size n has approximately $n/2$ leaves and the *distribution* of the number of leaves around $n/2$ looks like a Gaussian distribution.

We can make this observation precisely. Let n be given and assume that each of the p_n planted plane trees of size n is equally likely. Then the number of leaves is a random variable on this set of trees which we will denote by X_n. More precisely, we have

$$\mathbf{Pr}[X_n = k] = \frac{p_{n,k}}{p_n}.$$

Then it turns out that $\mathbf{E}\, X_n = n/2 + \mathcal{O}(1)$ and $\mathbf{Var}\, X_n = n/8 + \mathcal{O}(1)$, and (25) can restated in a way that the normalized random variable

$$\frac{X_n - \mathbf{E}\, X_n}{\sqrt{\mathbf{Var}\, X_n}}$$

converges weakly to the normal distribution $N(0,1)$.

Interestingly, both observed properties, the bivariate asmyptotic expansion (24) and the Gaussian limiting distribution are intrinsic properties of a functional equation of the form $y = F(x,y,u)$ (for the unknown function $y = y(x,u)$), compare with Theorem 15, 16 and 17.)

In particular, we get the following general result for simply generated trees. For the sake of brevity we just state the central limit law and not the bivariate asymptotic expansion for $y_{n,k}$ (compare with the Remark following Theorem 12).

Theorem 12. *Let R denote the radius of convergence of $\varphi(t)$ and suppose that there exists τ with $0 < \tau < R$ that satisfies $\tau\varphi'(\tau) = \varphi(\tau)$. Let X_n be that random variables describing the number of leaves in trees of size n, that is*

$$\mathbf{Pr}[X_n = k] = \frac{y_{n,k}}{y_n},$$

where $y_{n,k} = \sum_{|T|=n, D_0(T)=k} \omega(T)$. Then $\mathbf{E}\, X_n = \mu n + \mathcal{O}(1)$ and $\mathbf{Var}\, X_n = \sigma^2 n + \mathcal{O}(1)$, where $\mu = \varphi_0/\varphi(\tau)$ and

$$\sigma^2 = \frac{\varphi_0}{\varphi(\tau)} - \frac{\varphi_0^2}{\varphi(\tau)^2} - \frac{\varphi_0^2}{\tau^2\varphi(\tau)\varphi''(\tau)}.$$

Furthermore, X_n satisfies a (weak) central limit theorem of the form

$$\frac{X_n - \mathbf{E}\, X_n}{\sqrt{\mathbf{Var}\, X_n}} \to N(0,1).$$

Proof. Set

$$y(x,u) = \sum_{n,k} y_{n,k} x^n u^k.$$

Then $y(x,u)$ satisfies the functional equation

$$y(x,u) = \varphi_0 x(u-1) + x\varphi(y(x,u)).$$

Thus, we just have to apply Theorem 15 and 16 of Appendix 2.A. □

Remark . Suppose that $d = \gcd\{j \ge 0 : \varphi_j > 0\} = 1$. Then we can apply Theorem 15 and 17 to get bivariate asymptotic expansions for $y_{n,k}$, too. We will demonstrate this for the case of planted plane trees, that is $\varphi(x) = 1/(1-x)$.

From Theorem 15 we get

$$y_n(u) = \sqrt{\frac{\sqrt{u}}{2\pi(\sqrt{u}+1)^2}} \cdot (\sqrt{u}+1)^{2n} \cdot n^{-3/2} \cdot \left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right).$$

Hence, in terms of Theorem 17 we have $\lambda(u) = (\sqrt{u}+1)^2$, $\mu(u) = \sqrt{u}/(\sqrt{u}+1)$, $\sigma^2(u) = \sqrt{u}/(2(\sqrt{u}+1)^2)$, $h(y) = (y/(1-y))^2$, and $\lambda(h(y)) = 1/(1-y)^2$. Consequently, Theorem 17 provides the same asymptotic expansion as (24).

2.2. **Additive Parameters.**

The above concept easily generalizes to so-called *additive parameters*. Let $v(T)$ denote the value of a parameter of a rooted trees T. We call it additive if

$$v(T) = v(\circ \times T_1 \times T_k \times \cdots \times T_k) = c_k + v(T_1) + v(T_2) + \cdots + v(T_k),$$

where $T_1, \ldots, T_k$ denote the subtrees of the root of T that are rooted at the successors of the root and c_k is a given sequence of real numbers. Equivalently

$$v(T) = \sum_{j\ge 0} c_j D_j(T).$$

For example, if $c_0 = 1$ and $c_j = 0$ for $j \ge 0$ then $v(T)$ is just the number of leaves. For $n \ge 1$ we now set

$$y_n(u) = \sum_{|T|=n} \omega(T) u^{v(T)}$$

and

$$y(x,u) = \sum_{n\ge 1} y_n(u) x^n.$$

Of course, the definition of $v(T)$ and the recursive structure of simply generated trees implies that $y(x,u)$ satisfies the functional equation

$$y(x,u) = x \sum_{k\ge 0} \varphi_k u^{c_k} y(x,u)^k.$$

If c_k are non-negative integers then $y_k(u)$ may be interpreted as

$$y_n(u) = \sum_{k\ge 0} y_{n,k} u^k,$$

where $y_{n,k}$ denotes the (weighted) number of trees T of size n with $v(T) = k$. It is convenient now to consider the random variables X_n defined by

$$\mathbf{E}\, u^{X_n} = \frac{y_n(u)}{y_n}, \tag{26}$$

that is, X_n describes the distribution of $v(T)$ on the set of trees of size n, where these trees are distributed according to their weights $\omega(T)$. In particular, if c_j are non-negative integers then

$$\mathbf{Pr}[X_n = k] = \frac{y_{n,k}}{y_n}.$$

As above, the distribution of X_n is (usually) Gaussian with mean value and variance of order n.

Theorem 13. *Let R denote the radius of convergence of $\varphi(t)$ and suppose that there exists τ with $0 < \tau < R$ that satisfies $\tau\varphi'(\tau) = \varphi(\tau)$. Furthermore, let c_k $(k \ge 0)$ be a sequence of real numbers such that the function*

$$F(x,y,u) = x \sum_{k\ge 0} \varphi_k u^{c_k} y^k$$

is analytic at $x = x_0 = 1/\varphi'(\tau)$, $y = y_0 = \tau$, $u = 1$. Then the random variable X_n defined by (26) has expected value $\mathbf{E}\, X_n = \mu n + \mathcal{O}(1)$ and variance $\mathbf{Var}\, X_n = \sigma^2 n + \mathcal{O}(1)$, where $\mu = \sum_{k\ge 0} c_k \varphi_k \tau^k / \varphi(\tau)$ and $\sigma^2 \ge 0$. Furthermore, if $\sigma^2 > 0$ then X_n satisfies a (weak) central limit theorem of the form

$$\frac{X_n - \mathbf{E}\, X_n}{\sqrt{\mathbf{Var}\, X_n}} \to N(0,1).$$

Proof. We just have to apply Theorem 15 and 16 of Appendix 2.A. □

Remark . With help of the Remark following Theorem 16 it would have been possible to provide an explicit formula for σ^2 that is not really elegant. Note also that there are cases with $\sigma^2 = 0$. For example, if $c_k = 1$ for all $k \ge 0$ then $v(T) = |T|$ and consequently X_n is concentrated at n.

2.3. Unrooted Trees.

It is also intersting to consider the class $\tilde{\mathcal{T}}$ of unrooted trees and define a *additive parameter* v by

$$v(\tilde{T}) = \sum_{j\ge 1} c_j \tilde{D}_j(\tilde{T}), \tag{27}$$

where $\tilde{D}_j(\tilde{T})$ denotes the number of nodes in $\tilde{T}$ of degree j. For example, if $c_k = 1$ for some $k \ge 1$ and $c_j = 0$ for $j \ne k$ then $v(\tilde{T})$ is just the number of nodes of degree k (see [6]).

In order to tackle $v(\tilde{T})$ we also have to consider the class $\mathcal{T}$ of rooted trees and use the two generating functions

$$t(x,u) = \sum_{T\in\mathcal{T}} x^{|T|} u^{v'(T)} = \sum_{n\ge 1} \left(\sum_{|T|=n} u^{v'(T)} \right) x^n$$

and

$$\tilde{t}(x,u) = \sum_{\tilde{T}\in\tilde{\mathcal{T}}} x^{|\tilde{T}|} u^{v(\tilde{T})} = \sum_{n\ge 1} \left(\sum_{|\tilde{T}|=n} u^{v(\tilde{T})} \right) x^n$$

where v' is the proper version of v for rooted trees T:

$$v'(T) = \sum_{j\ge 0} c_{j+1} D_j(T).$$

Following the combinatorial constructions of section 1.3 we obtain the following system of functional equations:

$$t(x,u) = x \sum_{k\ge 0} u^{c_{k+1}} Z_k(S_k; t(x,u), t(x^2,u^2), \ldots, t(x^k,u^k)), \tag{28}$$

$$\tilde{t}(x,u) = x + x \sum_{k\ge 1} u^{c_k} Z_k(S_k; t(x,u), t(x^2,u^2), \ldots, t(x^k,u^k)) - \frac{1}{2} t(x,u)^2 + \frac{1}{2} t(x^2,u^2). \tag{29}$$

Finally, we introduce the random variable X_n (describing the distribution of v on trees of size n) in the usual way:

$$\mathbf{E}\, u^{X_n} = \frac{1}{\tilde{t}_n} \sum_{|\tilde{T}|=n} u^{v(\tilde{T})}. \tag{30}$$

The following theorem is a generalization of [6].

Theorem 14. *Let $(c_k)_{k\ge 1}$ be a bounded sequence of real numbers, and let $v(T)$ and X_n be defined by (27) and (30). Then there exist μ and $\sigma^2 \ge 0$ with $\mathbf{E}\, X_n = \mu\, n + \mathcal{O}(1)$ and $\mathbf{Var}\, X_n = \sigma^2\, n + \mathcal{O}(1)$. Furthermore, if $\sigma^2 > 0$ then X_n satisfies a (weak) central limit theorem of the form*

$$\frac{X_n - \mathbf{E}\, X_n}{\sqrt{\mathbf{Var}\, X_n}} \to N(0,1).$$

Proof. The plan of the proof is the following one. First, we apply Theorem 15 to (28) which implies that $t(x,u)$ has a square root singularity of the kind (35). Second, we use this representation and (29) to get an expansion for $\tilde{t}(x,u)$ of the form

$$\tilde{t}(x,u) = \overline{g}(x,u) - \overline{h}(x,u)\left(1 - \frac{x}{f(u)}\right)^{3/2}. \tag{31}$$

Then we apply the transfer lemma (Lemma 1) to obtain an asymptotic expansion for $\tilde{t}_n(u)$, and finally we use the quasi power theorem (Theorem 16). The last two steps are direct applications. So we just have to look at the first two steps.

In order to apply Theorem 15 we just have to ensure that the functions $t(x^2,u^2), t(x^3,u^3), \ldots$ are analytic if x is close to ρ and u is close to 1. Since the sequence c_k is bounded we have $|c_k| \le M$ for some $M > 0$ and thus $|v'(T)| \le M\,|T|$. Hence, if $|u| > 1$ and $|xu^M| < \rho$ then we have

$$|t(x,u)| \le \sum_{n\ge 1} t_n |u|^{Mn}|x|^n = t(|xu^M|, 1).$$

In particular if $|x| \le \rho + \eta$ and $|u| \le (\sqrt{\rho}/(\rho+\eta))^{1/M}$ (where $\eta > 0$ is small enough that $(\sqrt{\rho}/(\rho+\eta))^{1/M} > 1$) we get for $k \ge 2$

$$|t(x^k,u^k)| \le t(|xu^M|^k, 1) \le t(\rho^{k/2}, 1) \le C\rho^{k/2}.$$

Thus, we can apply Theorem 15 with

$$F(x,y,u) = x\sum_{k\ge 0} u^{c_{k+1}} Z_k(S_k; y, t(x^2,u^2), \ldots, t(x^k,u^k))$$

and obtain an representation of the form

$$t(x,u) = g(x,u) - h(x,u)\sqrt{1 - \frac{x}{f(u)}}, \tag{32}$$

where $g_1 = g(f(u),u)$ satisfies the relation

$$g_1 = f(u)\sum_{k\ge 0} u^{c_{k+1}} Z_k(S_k; g_1, t(f(u)^2,u^2), \ldots, t(f(u)^k,u^k)).$$

Consequently, from (33) and (29) we obtain a representation for $\tilde{t}(x,u)$ of the form

$$\tilde{t}(x,u) = g_2(x,u) - h_2(x,u)\sqrt{1 - \frac{x}{f(u)}}, \tag{33}$$

where

$$h_2(x,u) = h(x,u)\Bigg(x\sum_{k\ge 1} u^{c_k}\frac{\partial}{\partial x_1} Z_k(S_k; g(x,u), t(x^2,u^2), \ldots, t(x^k,u^k)) \\ - g(x,u) + (x - f(u))H(x,u)\Bigg)$$

in which $H(x,u)$ denotes an analytic function in x and u. Note that

$$\frac{\partial}{\partial x_1} Z_k(S_k; x_1, \ldots, x_k) = Z_{k-1}(S_{k-1}, x_1, \ldots, x_{k-1})$$

This implies that

$$h_2(f(u),u) = h(f(u),u)f(u)\left(\sum_{k\ge 1} u^{c_k}\frac{\partial}{\partial x_1}Z_k(S_k;g_1,\ldots) - \sum_{k\ge 0} u^{c_k+1}Z_k(S_k;g_1,\ldots)\right)$$
$$= 0.$$

Hence, $h_2(x,u)$ can be represented as

$$h_2(x,u) = \overline{h}(x,u)\left(1-\frac{x}{f(u)}\right)$$

Of course, this implies (31) and completes the proof of Theorem 14. □

Appendix 2.A: Asymptotic Normality.

We start with a slight extension of Theorem 10, where we add an additional parameter u (see [5]).

Theorem 15. *Suppose that $F(x,y,u) = \sum_{n,m} F_{n,m}(u)x^n y^m$ is an analytic function in x, y around 0 and u around 0 such that $F(0,y,u) \equiv 0$, that $F(x,0,u) \not\equiv 0$, and that all coefficients $F_{n,m}(1)$ of $F(x,y,1)$ are real and non-negative. Then the unique solution $y = y(x,u) = \sum_n y_n(u)x^n$ of the functional equation*

$$y = F(x,y,u) \tag{34}$$

with $y(0,u) = 0$ is analytic around 0 and has non-negative coefficients $y_n(1)$ for $u = 1$.

Furthermore, if the region of convergence of $F(x,y,u)$ is large enough such that there exist non-negative solutions $x = x_0$ and $y = y_0$ of the system of equations

$$y = F(x,y,1),$$
$$1 = F_y(x,y,1).$$

with $F_x(x_0,y_0,1) \ne 0$ and $F_{yy}(x_0,y_0,1) \ne 0$ then there exist functions $f(u)$, $g(x,u)$, $h(x,u)$ which are analytic around $x = x_0$, $u = 1$ such that $y(x,u)$ is analytic for $|x| < x_0$ and $|u-1| \le \varepsilon$ (for some $\varepsilon < 0$) and has a representation of the form

$$y(x,u) = g(x,u) - h(x,u)\sqrt{1-\frac{x}{f(u)}} \tag{35}$$

locally around $x = x_0$, $u = 1$.

If $y_n(1) > 0$ for $n \ge 0$ then we also get

$$y_n(u) = \sqrt{\frac{f(u)F_x(f(u),y(f(u),u),u)}{2\pi F_{yy}(f(u),y(f(u),u),u)}}\, f(u)^{-n} n^{-3/2}\left(1+\mathcal{O}\left(n^{-1}\right)\right). \tag{36}$$

uniformly for $|u-1| < \varepsilon$.

Proof. The proof is completely the same as that of Theorem 10. We just have to take care of the additional analytic parameter u. □

Interestingly there is a strong relation to random variables that are asymptotically Gaussian. We state here a slightly modified version of a quite general theorem due to H.-K. Hwang [10] that usually referred as the *Quasi Power Theorem.* (Similar theorems can be found in [1, 2]).

Theorem 16. *Let X_n be a random variable with the property that*

$$\mathbf{E}\, u^{X_n} = e^{\lambda_n \cdot a(u)+b(u)} \left(1+\mathcal{O}\left(\frac{1}{\phi_n}\right)\right),$$

holds uniformly in a complex neighborhoud of $u=1$where λ_n and ϕ_n are sequences of positive real numbers with $\lambda_n\to\infty$ and $\phi_n\to\infty$, and $a(u)$ and $b(u)$ are analytic functions in this neighborhood of $u=1$ with $a(1)=b(1)=0$. Then $\mathbf{E}\, X_n = \mu\lambda_n+\mathcal{O}\left(1+\lambda_n/\phi_n\right)$ and $\mathbf{Var}\, X_n = \sigma^2\lambda_n+\mathcal{O}\left(1+\lambda_n/\phi_n\right)$, where $\mu=a'(1)$ and $\sigma^2 = a'(1)+a''(1)$. Furthermore, if $\sigma^2>0$ then X_n satisfies a central limit theorem of the form

$$\frac{X_n-\mathbf{E}\, X_n}{\sqrt{\mathbf{Var}\, X_n}} \to N(0,1).$$

Proof. By assumption we obtain for t in a neighborhood of $t=0$

$$\mathbf{E}\, e^{itX_n} = e^{it\lambda_n\mu-\frac12 t^2\lambda_n\sigma^2+\mathcal{O}\left(\lambda_n t^3\right)+\mathcal{O}(t)}\left(1+\mathcal{O}\left(\frac{1}{\phi_n}\right)\right).$$

Set $Y_n=(X_n-\lambda_n\mu)/\sqrt{\lambda_n\sigma^2}$ when $\sigma^2>0$. Then by replacing t by $t/\sqrt{\lambda_n\sigma^2}$ one directly gets

$$\mathbf{E}\, e^{itY_n} = e^{-\frac12 t^2+\mathcal{O}\left(t^3/\sqrt{\lambda_n}\right)+\mathcal{O}\left(t/\sqrt{\lambda_n}\right)}\left(1+\mathcal{O}\left(\frac{1}{\phi_n}\right)\right).$$

Thus, Y_n is asymptotically normal since $\lambda_n\to\infty$ and $\phi_n\to\infty$.

Next set $f_n(u)=\mathbf{E}\, u^{X_n}$. Then $f_n'(1)=\mathbf{E}\, X_n$. One the other hand, by Cauchy's formula we also have

$$f_n'(1) = \frac{1}{2\pi i}\int\limits_{|u-1|=\rho}\frac{f_n(u)}{(u-1)^2}\,du.$$

In particular, we use the circle $|u-1|=1/\lambda_n$ as the path of integration and get

$$\begin{aligned}&\mathbf{E}\, X_n = \\ &\frac{1}{2\pi i}\int\limits_{|u-1|=1/\lambda_n}\frac{1+(\lambda_n a'(1)+b'(1))(u-1)+\mathcal{O}\left(\lambda_n(u-1)^2\right)}{(u-1)^2}\left(1+\mathcal{O}\left(\frac{1}{\phi_n}\right)\right)du\\ &\quad = \lambda_n a'(1)+\mathcal{O}\left(1+\frac{\lambda_n}{\phi_n}\right).\end{aligned}$$

Similarly, we can treat the variance. Set $g_n(u) = f_n(u)u^{-\lambda_n a'(1)-b'(1)}$. Then $\mathbf{Var}\, X_n = g'(1)+g''(1)+\mathcal{O}\left(1+\lambda_n/\phi_n\right)$. By using the same kind of complex integration on the circle $|u-1|=1/\lambda_n$ and the approximation

$$\begin{aligned}&\exp\left(\lambda_n(a(u)-a'(1)\log u)+(b(u)-b'(1)\log u\right)\\ &\qquad = 1+(\lambda_n(a''(1)+a'(1))+(b''(1)+b'(1)))\frac{(u-1)^2}{2}+\mathcal{O}\left(\lambda_n(u-1)^3\right)\end{aligned}$$

one obtains

$$\mathbf{Var}\, X_n = \lambda_n(a''(1)+a'(1))+\mathcal{O}\left(1+\frac{\lambda_n}{\phi_n}\right).$$

Finally note that Y_n and $(X_n-\mathbf{E}\, X_n)/\sqrt{\mathbf{Var}\, X_n}$ have the same limiting distribution (if $\sigma^2>0$). This completes the proof of Theorem 16. □

Remark . In particular, if $F(x,y,u)$ satisfies the assumptions of Theorem 15 and $y(x,u)$ is the solution of $y = F(x,y,u)$. Then X_n, defined by $\mathbf{E}\, u^{X_n} = [x^n]y(x,u)/[x^n]y(x,1)$, is asymptotically normal. We have $a(u) = -\log(f(u)/x_0)$, where $f(u) = x(u)$ (and $y(u)$) are the solutions of the system

$$y = F(x,y,u),$$
$$1 = F_y(x,y,u).$$

μ and σ^2 are then given by

$$\mu = -\frac{x'(1)}{x_0} \quad \text{and} \quad \sigma^2 = \mu + \mu^2 - \frac{x''(1)}{x_0}.$$

By implicit differentiation one gets (after some algebra)

$$x'(1) = -\frac{F_u(x_0,y_0,1)}{F_x(x_0,y_0,1)} = -\frac{F_u}{F_x}$$

and

$$x''(1) = -\frac{1}{F_x}\left(F_{xx}x'(1)^2 + 2F_{xy}x'(1)y'(1) + F_{yy}y'(1)^2 + 2F_{ux}x'(1) + 2F_{uy}y'(1) + F_{uu}\right),$$

where

$$y'(1) = -\frac{F_{xy}x'(1) + F_{uy}}{F_{yy}}.$$

Thus, it is possible to calculate μ and σ^2 explicitly.

Appendix 2.B: Bivariate Asymptotic Expansions.

The next theorem shows how the k-th coefficient of the n-th powers of functions behaves if n and k are proportional (see [3, 4]).

Theorem 17. *Suppose that a sequence of generating function $y_n(u)$ is asymptotically given by*

$$y_n(u) = g(u)\,\lambda(u)^n \cdot \left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right)$$

uniformly for $a \le |u| \le b$ and $|\arg(u)| \le \theta$ (for some $0 < a < b$ and $0 < \theta < \pi/2$) and bounded by

$$|y_n(u)| \le C\,\lambda(|u|)^{(1-\eta)n}$$

for $a \le |u| \le b$ and $\theta \le |\arg(u)| \le \pi$ and some $\eta > 0$, where $g(u)$ and $\lambda(u)$ are analytic in a region containing the range $a \le |u| \le b$, $|\arg(u)| \le \theta$.

Set

$$\mu(r) = \frac{r\lambda'(r)}{\lambda(r)}$$

and suppose that

$$\sigma^2(r) = r\mu'(r) = \frac{r\lambda'(r)}{\lambda(r)} + \frac{r^2\lambda''(r)}{\lambda(r)} - \frac{r^2\lambda'(r)^2}{\lambda(r)^2} > 0$$

for $a \le r \le b$. Let $h(y)$ denote the inverse function of $\mu(r)$.

Then we have

$$[u^k]\,y_n(u) = \frac{1}{\sqrt{2\pi n}}\frac{g\left(h\left(\frac{k}{n}\right)\right)}{\sigma\left(h\left(\frac{k}{n}\right)\right)}\frac{\lambda\left(h\left(\frac{k}{n}\right)\right)^n}{h\left(\frac{k}{n}\right)^k} \cdot \left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right)$$

uniformly for n, k with $\mu(a) \leq k/n \leq \mu(b)$.

Proof. We use Cauchy's formula

$$[u^k]\, y_n(u) = \frac{1}{2\pi i} \int_{|u|=r} \frac{y_n(u)}{u^{k+1}}\, du$$

where r is defined by

$$\frac{r\lambda'(r)}{\lambda(r)} = \frac{k}{n},$$

that is, $r = h\left(\frac{k}{n}\right)$. Note that r is exactly the saddle point of the function

$$\lambda(u)^n u^{-k} = e^{n \log \lambda(u) - k \log u}.$$

Now a standard saddle point method (see [4] or [14]) yields

$$[u^k]\, y_n(u) = \frac{1}{\sqrt{2\pi n \sigma^2(r)}} g(r)\lambda(r)^n r^{-k} \cdot \left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right).$$

□

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