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Nonuniform Random Recursive Trees with Bounded Degree

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ABSTRACT

In this paper we find exact and asymptotic formulae for the number of n vertex recursive 3-trees (no vertex of degree greater than 3). We also obtain the expected number of vertices of degrees 1, 2 and 3 as well as the expected degree of the root of such trees. This is done for both uniformly and nonuniformly distributed random recursive 3-trees.

1. Introduction

A *tree* is a connected graph which has no cycles (see [2] for definitions not given here). A tree with n vertices labelled $1, 2, \ldots, n$ is a recursive tree if, for each k such that $2 \leq k \leq n$, the labels of the vertices in the unique path from the root (the vertex with label 1) to the kth vertex form an increasing sequence. Such a tree can be also defined as a result of successively joining the ith vertex to one of the first $i-1$ vertices, for $i = 2, 3, \ldots, n$ in accordance with some deterministic or probabilistic rule.

A *planted recursive tree* is a recursive tree with root having degree 1. Let $\mathcal{R}_n$ and $\mathcal{P}_n$, respectively, denote the family of all recursive and planted recursive n vertex 3-trees (no vertex of degree greater then 3).

A *random* recursive (planted recursive) tree is one which is the outcome of a random process. A tree selected with equal probability from the set $\mathcal{R}_n$ ($\mathcal{P}_n$) is called a *uniform* random recursive (planted recursive) 3-tree of order n. If a tree is selected with a nonuniform probability distribution from some specified set of recursive trees it will be referred to as a *nonuniform* random recursive tree with the corresponding probability distribution and type of tree appropriately identified.

In this paper we find exact and asymptotic formulae for the number of recursive 3-trees of order n. We also obtain the expected number of vertices of degrees 1, 2 and 3 as well as the expected degree of the root of such trees. This is done for both uniform and nonuniform random recursive 3-trees.

2. Uniform recursive 3-trees

Our study of uniform random recursive 3-trees requires the enumeration of such trees. We proceed by defining $a_1 = 1$ and a_n $(n \geq 2)$ to be the number of planted recursive 3-trees having order n. Let the function y be defined as follows

$$y(x) = \sum_{i=0}^{\infty} \frac{a_{i+1}}{i!} x^i.$$

Then

$$y'(x) = \sum_{i=0}^{\infty} \frac{a_{i+2}}{i!} x^i$$

and

$$y''(x) = \sum_{i=0}^{\infty} \frac{a_{i+3}}{i!} x^i.$$

Lemma 2.1.

$$y(x) = \tan(\frac{1}{2}x + \frac{\pi}{4}) = \tan x + \sec x$$

Proof. For a planted recursive 3-tree, let $\deg(k)$ denote the degree of the vertex with label k. To find a_n we first observe that the number of planted recursive 3-trees such that $\deg(2) = 2$ is clearly equal to a_{n-1}; and second that for $0 \leq k \leq n-4$, $\binom{n-3}{k} a_{k+2}\, a_{n-k-2}$ is the number of n vertex planted 3-trees such that $\deg(2) = 3$ and $k+2$ is the order of the planted subtree containing vertex 3 and rooted at vertex 2.

So, we get

$$\begin{aligned} a_n &= a_{n-1} + \sum_{k=0}^{n-4} \binom{n-3}{k} a_{k+2}\, a_{n-k-2} \\ &= \sum_{k=0}^{n-3} \binom{n-3}{k} a_{k+2}\, a_{n-k-2} \end{aligned} \tag{1}$$

From (1) we can write the coefficient of x^t in y'' as

$$\begin{aligned} \frac{a_{t+3}}{t!} &= \sum_{k=0}^{t} \frac{a_{k+2}}{k!} \frac{a_{t-k+1}}{(t-k)!} \\ &= \sum_{k=0}^{t} \frac{a_{t-k+2}}{(t-k)!} \frac{a_{k+1}}{k!}. \end{aligned} \tag{2}$$

Let us compute

$$yy' = \sum_{t=0}^{\infty} x^t \sum_{k=0}^{t} \frac{a_{t-k+2}}{(t-k)!} \frac{a_{k+1}}{k!}.$$

Thus, by (2) we obtain

$$yy' = \sum_{t=0}^{\infty} \frac{a_{t+3}}{t!} x^t = y''.$$

Therefore,

$$y'' = yy'$$

with initial conditions

$$y(0) = y'(0) = 1.$$

Solving this initial value problem one can complete the proof. ■

Expanding tan and sec functions into power series we can find an explicit formula for a_n in terms of the well known Bernoulli numbers B_n and Eulerian numbers E_n (for definitions and properties of B_n and E_n see for example [6]).

Theorem 2.1. *For $n \leq 1$,*

$$a_n = \begin{cases} 2^n(2^n-1)n^{-1}|B_n| & \text{if } n \text{ is even,} \\ |E_{n-1}| & \text{if } n \text{ is odd,} \end{cases}$$

where B_n are Bernoulli numbers and E_n are Eulerian numbers.

Corollary 2.1. *If $n \to \infty$ then*

$$a_n = 2^{n+1}\pi^{-n}(n-1)!(1+O(2^{-n})).$$

Proof. The proof is a simple consequence of known asymptotic formulae for Bernoulli and Eulerian numbers. ∎

For later use let us notice more precise estimations

$$\frac{2^{n+1}(n-1)!}{\pi^n}\frac{2^n-1}{2^n} \le a_n \le \frac{2^{n+1}(n-1)!}{\pi^n}\frac{2^n-1}{2^n-2} \tag{3}$$

Lemma 2.2. *Let r_n denote the number of recursive 3-trees of order n. Then*

$$\sum_{i=0}^{\infty}\frac{r_{i+1}}{i!}x^i = (y'(x))^2.$$

Proof. Let $r_{n,i}$ denote the number of recursive 3-trees having n vertices and root degree i. Then

$$r_n = a_n + r_{n,2} + r_{n,3}$$

and

$$a_{n+1} = a_n + r_{n,2}.$$

To evaluate $r_{n,3}$ let $k+1>0$, $l+1>0$ and $n-k-l-3>0$ be the numbers of vertices in the main branches. Then

$$r_{n,3} = \sum_{k=0}^{n-4}\binom{n-2}{k}a_{k+2}\sum_{i=0}^{n-k-4}\binom{n-k-3}{l}a_{l+2}a_{n-k-l-2}.$$

The inner sum of the above formula is equal to

$$\sum_{i=0}^{n-k-4}\binom{n-k-3}{l}a_{l+2}a_{n-k-l-2}$$

$$= \sum_{i=0}^{n-k-4}\binom{n-k-3}{l}a_{l+2}a_{n-k-l-2} - a_{n-k-1}$$

$$= a_{n-k} - a_{n-k-1}$$

because of (1). Hence we get

$$\begin{aligned} r_n &= a_{n+1} + \sum_{k=0}^{n-4} \binom{n-2}{k} a_{k+2} (a_{n-k} - a_{n-k-1}) \\ &= a_{n+1} + \sum_{k=0}^{n-4} \binom{n-2}{k} a_{k+2} a_{n-k} \\ &\qquad - \sum_{k=0}^{n-2} \binom{n-2}{k} a_{k+2} a_{n-k-1} + (n-2)a_{n-1} + a_n \\ &= \sum_{k=0}^{n-4} \binom{n-2}{k} a_{k+2} a_{n-k} + (n-2)a_{n-1} + a_n \end{aligned}$$

And finally we get

$$r_n = \sum_{k=0}^{n-2} \binom{n-2}{k} a_{k+2} a_{n-k}. \qquad \blacksquare \tag{4}$$

An alternative combinatorial proof of Lemma 2.2 can be obtained via an appropriate compounding of planted recursive 3-trees.

We make use of the following notation for limits concerning $I(n)$ and $J(n)$, two functions of the integer variable n:

if $\lim_{n\to\infty} \frac{I(n)}{J(n)} = 1$ we shall write $I(n) \sim J(n)$

and

if there is a constant K such that $|I(n)| \leq KJ(n)$, for sufficiently large n, we write $I(n) = O(J(n))$.

Theorem 2.2.

$$r_n \sim \frac{1}{3} 2^{n+3} \pi^{-n-2} (n+1)!$$

Proof. The assertion is a direct consequence of the formula (4) and estimations (3). ■

For the accuracy of the asymptotics of Corollary 2.1 and Theorem 2.2 see Table 1.

n	a_n	α_n	r_n	ρ_n
1	1	1.3	1	0.3
2	1	0.8	1	0.7
3	1	1.0	2	1.7
4	2	2.0	6	5.3
5	5	5.0	22	20.3
6	16	16.0	96	90.7
7	61	61.0	482	461.7
8	272	272.0	2736	2645.3
9	1385	1385.1	17302	16840.4
10	7936	7935.9	120576	117930.4
11	50521	50521.3	917762	900922.2
12	353792	353791.3	7574016	7456083.8
13	2702765	2702766.7	67354582	66453665.0
14	22368256	22368251.3	642041856	634585755.9
15	199360981	199360994.9	6530291042	6463837431.7
16	1903757312	1903757267.8	70589700096	69955114144.7
17	19391512145	19391512295.1	808090395862	801626559170.0
18	209865342976	209865342434.2	9766250151936	9696295034829.7
19	2404879675441	2404879677510.0	124258689304322	123457062757644.0
20	29088885112832	29088885104489.1	1660195646078976	1650499350988771.5

Table 1. *The number of planted recursive* 3*-trees* a_n*, recursive* 3*-trees* r_n*, and asymptotics* $\alpha_n = 2^{n+1}\pi^{-n}(n-1)!$ *and* $\rho_n = \frac{1}{3}2^{n+3}\pi^{-n-2}(n+1)!$.

Theorem 2.3. *Let D_n denote the degree of the root of a uniform random recursive 3-tree of order n, then*

$$P(D_n = 1) \sim \frac{3}{4}\pi^2 n^{-2},$$
$$P(D_n = 2) \sim \frac{3}{2}\pi n^{-1},$$
$$P(D_n = 3) = 1 + O(n^{-1}).$$

The expected value and variance of D_n are:

$$E(D_n) = 3 + O(n^{-1}),$$
$$\text{Var}\,(D_n) \sim \frac{3}{2}\pi n^{-1}.$$

Proof. First note that

$$P(D_n = 1) = \frac{a_n}{r_n},$$
$$P(D_n = 2) = \frac{a_{n+1} - a_n}{r_n},$$
$$P(D_n = 3) = 1 - \frac{a_{n+1}}{r_n}$$

then apply Corollary 2.1 and Theorem 2.2. ■

3. Nonuniform recursive 3-trees

Let p_{nd} denote the probability that the vertex labelled $n+1$ is joined to a given vertex of degree d in a random recursive 3-tree of order n. In the uniform case p_{nd} is independent of the degree of a vertex and is equal to $\frac{1}{n}$. In [9], the model with $p_{nd} = \frac{d}{2n-2}$ was studied. In this case the probability that a vertex is joined to a specified vertex is directly proportional to the degree of that vertex. The consequence is that the higher the degree the greater the attraction of obtaining a new neighbor. Here we study the probability function $p_{nd} = \frac{f-d}{(f-2)n+2}$ for fixed $f \geq 2$. This function implies that higher degree vertices possess a lower attraction for new neighbors and no vertex of degree greater then f is introduced. These are two properties of interest in chemical applications [1], [4]. The former corresponds to the fact that the fewer chemical sites that are available for bonding (edge formation) the lower the probability of a bond being formed. The bounded degree condition corresponds to the natural limit on the number of bonds that can be incident to a chemical species. A tree with no vertex of degree greater than f is called an f-tree. In what follows we obtain results about nonuniform random recursive f-trees.

Theorem 3.1. *Let T denote a random recursive f-tree ($f \geq 2$) of order $n \geq 3$ such that T has t_i vertices of degree i ($i = 1, 2, \ldots, f$). Then, in the model defined by*

$$p_{nd} = \frac{f-d}{(f-2)n+2}$$

it follows that T will be generated with probability

$$P(T) = \frac{\prod_{d=1}^{f-1} (f-d)^{t_{d+1}+t_{d+2}+\ldots+t_f}}{(f-2)^{n-2} \left(n - \frac{f-4}{f-2}\right)_{n-2}},$$

where $(x)_k = x(x-1)(x-2)\ldots(x-k+1)$ for $x \in \mathbb{R}$, $k \in \mathbb{N}$.

Proof. The proof is obtained by induction on the number of vertices. ■

Corollary 3.1.

$$\text{For } f=2, \qquad P(T) = 2^{2-n}$$

$$\text{For } f=3, \qquad P(T) = \frac{6\cdot 2^{n-t_1}}{(n+1)!}$$

$$\text{For } f=4, \qquad P(T) = \frac{3^{n-t_1}2^{n-t_1-t_2}}{n!}$$

Theorem 3.2. *Let $X_{n,k}$ denote the number of vertices of degree k in a random recursive 3-tree with n vertices. Then in the model defined by $p_{nd} = \frac{3-d}{n+2}$ we have*

$$E(X_{n,1}) = \frac{1}{3}n + \frac{2}{3} + \frac{4}{n(n+1)},$$
$$E(X_{n,2}) = \frac{1}{3}n + \frac{2}{3} - \frac{8}{n(n+1)},$$
$$E(X_{n,3}) = \frac{1}{3}n - \frac{4}{3} + \frac{4}{n(n+1)}.$$

Proof. It has been shown (see proof of Theorem 1 in [9]) that

$$E(X_{n+1,1}) = (1-p_{n,1})E(X_{n,1}) + 1.$$

Thus, here we obtain

$$E(X_{n+1,1}) = \frac{n}{n+2}E(X_{n,1}) + 1.$$

Solving this recurrence equation with the initial condition $E(X_{2,1}) = 2$ we obtain required formula. Adopting formula (3) from [9] to our case we get

$$E(X_{n+1,2}) = \frac{n+1}{n+2}E(X_{n,2}) + \frac{2}{n+2}E(X_{n,1})$$

and

$$E(X_{n+1,3}) = E(X_{n,3}) + \frac{1}{n+2}E(X_{n,2}).$$

Using standard methods for solving linear recurrence equations one can complete the proof. ■

We mention here that in the uniform case without restrictions on vertex degrees, $E(X_{n,k}) \sim n2^{-k}$ (see [3], [5], [7] and [8]).

Theorem 3.3. *Let D_n denote the degree of the root of a random recursive 3-tree having order n. Then, in the model defined by $p_{n,d} = \frac{3-d}{n+2}$ we have*

$$P(D_n = 1) = \frac{6}{n(n+1)},$$
$$P(D_n = 2) = \frac{6(n-2)}{n(n+1)},$$
$$P(D_n = 3) = 1 - \frac{6(n-1)}{n(n+1)}$$

and

$$E(D_n) = 3 - \frac{6}{n+1},$$
$$\mathrm{Var}\,(D_n) = \frac{6n^2 - 18n + 12}{n(n+1)^2} = O\left(n^{-1}\right).$$

Proof. It is easily seen that

$$P(D_n = 1) = \prod_{k=2}^{n-1}(1 - p_{k,1}) = \prod_{k=2}^{n-1}\frac{k}{k+2} = \frac{6}{n(n+1)}.$$

The way of adding a new vertex to a recursive tree implies that (compare the proof of Theorem 7 in [9])

$$P(D_{n+1} = 2) = (1 - p_{n,2})P(D_n = 2) + p_{n,1}P(D_n = 1).$$

In the case $p_{nd} = \frac{3-d}{n+2}$ we get

$$P(D_{n+1} = 2) = \frac{n+1}{n+2}P(D_n = 2) + \frac{2}{n+2}\frac{6}{n(n+1)}.$$

Solving this recurrence equation one can get the formula for $P(D_n = 2)$. The formula for $P(D_n = 3)$ one can be obtained using

$$P(D_n = 3) = 1 - P(D_n = 1) - P(D_n = 2). \quad \blacksquare$$

Here we observe that the degree of the root in the above type of nonuniform random recursive 3-tree is almost surely 3, just as it is in the uniform distribution case.

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References

[1] K. T. Balińska and L. V. Quintas, The sequential generation of random f-graphs. Line maximal 2-, 3-, and 4-graphs, *Computers & Chemistry* **14**(1990), 323–328.

[2] C. Berge, *Graphs and Hypergraphs,* North-Holland, Amsterdam, 1973.

[3] M. Dondajewski and J. Szymański, On the distribution of vertex degrees in strata of a random recursive tree, *Bull. Acad. Sci. Ser. Sci. Math.* **30**(1982), 205–209.

[4] H. Galina and A. Szustalewicz, A kinetic theory of stepwise crosslinking polymerization with substitution effect, *Macromolecules* **22**(1989), 3124–3129.

[5] J. L. Gastwirth, A probability model of a pyramid scheme, *Amer. Statist.* **31**(1977), 79–82.

[6] D. Knuth, *The art of computer programming, Volume 3: sorting and searching,* Addison-Wesley, Reading, 1973.

[7] A. Meir and J. W. Moon, Path edge-covering constants for certain families of trees, *Util. Math.* **14**(1978), 313–333.

[8] H. S. Na and A. Rapoport, Distribution of nodes of a tree by degree, *Math. Biosci.* **6**(1970), 313–329.

[9] J. Szymański, On a nonuniform random recursive tree, *Annals of Discrete Math.* **33**(1987), 297–306.

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