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ON THE DISTRIBUTION OF THE NUMBER OF VERTICES IN LAYERS OF RANDOM TREES[1]

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ABSTRACT

Denote by S_n the set of all distinct rooted trees with n labeled vertices. A tree is chosen at random in the set S_n, assuming that all the possible n^{n-1} choices are equally probable. Define $\tau_n(m)$ as the number of vertices in layer m, that is, the number of vertices at a distance m from the root of the tree. The distance of a vertex from the root is the number of edges in the path from the vertex to the root. This paper is concerned with the distribution and the moments of $\tau_n(m)$ and their asymptotic behavior in the case where $m = [2\alpha\sqrt{n}], 0 < \alpha < \infty$ and $n \to \infty$. In addition, more random trees, branching processes, the Bernoulli excursion and the Brownian excursion are also considered.

Key words: Random trees, Branching processes, Bernoulli excursion, Brownian excursion, Local times, Limit theorems.

AMS (MOS) subject classifications: 60F05, 05C05, 60J55, 60J65, 60J80.

1. INTRODUCTION

In 1889, A. Cayley [3] observed that the number of distinct trees with n labeled vertices is n^{n-2}. Since then various proofs have been found for Cayley's formula. For a simple proof see L. Takács [23]. The number of distinct rooted trees with n labeled vertices is

$$R_n = n^{n-1} \tag{1}$$

for $n = 1, 2, \ldots$. Since among the n vertices we can choose a root in n ways, (1) immediately follows from Cayley's formula.

The number of vertices in layer m in a rooted tree is the number of vertices at a distance m from the root. The distance of a vertex from the root is the number of edges in the path from the vertex to the root.

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Let S_n be the set of all distinct rooted trees with n labeled vertices and denote by $t_n(j,m), j = 0,1,\ldots,n-m$, the number of trees in S_n having j vertices at a distance m from the root. Let us choose a tree at random in the set S_n, assuming that all the possible n^{n-1} choices are equally probable. Define $\tau_n(m)$ as the number of vertices in layer m, that is, the number of vertices at a distance m from the root of the tree chosen at random. If all the possible trees in S_n are equally probable, then

$$P\{\tau_n(m) = j\} = t_n(j,m)/n^{n-1} \tag{2}$$

for $j = 0,1,\ldots,n-m$.

In this paper we are concerned with the distribution and the moments of $\tau_n(m)$ and their asymptotic behavior in the case where $m = [2\alpha\sqrt{n}], 0 < \alpha < \infty$ and $n \to \infty$. The results derived for $\tau_n(m)$ are extended to other random trees, branching processes, the Bernoulli excursion and the Brownian excursion.

2. AUXILIARY THEOREMS

Let us define the generating functions

$$g_n(z,m) = \sum_{j=0}^{n-m} t_n(j,m) z^j \tag{3}$$

and

$$G_m(z,w) = \sum_{n=1}^{\infty} g_n(z,m) w^n/n! \tag{4}$$

for $n \geq 1$ and $m \geq 0$. If $|z| \leq 1$ and $|w| \leq 1/e$, then (4) is convergent.

Lemma 1: *If $|w| \leq 1/e$, then the equation*

$$ye^{-y} = w \tag{5}$$

has exactly one root in the unit disk $|y| \leq 1$ and

$$y^r = [y(w)]^r = r\sum_{n=r}^{\infty} \frac{n^{n-r} w^n}{n(n-r)!} \tag{6}$$

for $|w| \leq 1/e$ and $r = 1,2,\ldots$.

Proof: By Rouché's theorem it follows that (5) has exactly one root in the unit disk $|y| \leq 1$ and we obtain (6) by Lagrange's expansion. For $r = 1$ the expansion (6) was already known to L. Euler [7].

Lemma 2: *If $m \geq 1$, $|z| \leq 1$ and $|w| \leq 1/e$, then*

$$G_m(z,w) = we^{G_{m-1}(z,\omega)} \tag{7}$$

where $G_0(z,w) = zy(w)$, and $y = y(w)$ is given by (6) with $r = 1$.

Proof: If we take into consideration that the degree of the root of a tree may be $k = 0,1,2,\ldots$, then we obtain that

$$G_m(z,w) = w + w\sum_{k=1}^{\infty}[G_{m-1}(z,w)]^k/k! = we^{G_{m-1}(z,\omega)} \tag{8}$$

for $m = 1,2,\ldots$ and obviously

$$G_0(z,w) = z\sum_{n=1}^{\infty}\frac{n^{n-1}}{n!}w^n = zy(w) \tag{9}$$

for $|w| \leq 1/e$. Equation (7) appears also in A. Meir and J.W. Moon [19] and in A.M. Odlyzko and H.S. Wilf [20].

3. THE MOMENTS OF $\tau_n(m)$

The following theorem has been found by V.E. Stepanov [21]. In what follows we shall give a simple proof for it.

Theorem 1: *If $0 < \alpha < \infty$, then*

$$\lim_{n\to\infty} E\left\{\left(\frac{2\tau_n([2\alpha\sqrt{n}])}{\sqrt{n}}\right)^r\right\} = \mu_r(\alpha) \tag{10}$$

exists for $r = 0,1,2,\ldots$. We have $\mu_0(\alpha) = 1, \mu_1(\alpha) = 4\alpha e^{-2\alpha^2}$, and

$$\mu_r(\alpha) = 2^{r+1}r!\alpha^r\int_0^{r-1}(1+x)e^{-2\alpha^2(1+x)^2}g_{r-1}(x)dx \tag{11}$$

for $r \geq 2$, where

$$g_{r-1}(x) = \sum_{j=0}^{[x]}(-1)^j\binom{r-1}{j}\frac{(x-j)^{r-2}}{(r-2)!} \tag{12}$$

for $r \geq 2$ and $x \geq 0$.

Proof: Let us define

$$B_r(w,m) = \frac{1}{r!}\left(\frac{\partial^r G_m(z,w)}{\partial z^r}\right)_{z=1} = \sum_{n=1}^{\infty}E\left\{\binom{\tau_n(m)}{r}\right\}\frac{n^{n-1}w^n}{n!} \tag{13}$$

for $r \geq 0, m \geq 0$, and $|w| \leq 1/e$.

By forming the derivative of (7) with respect to z we obtain

$$\frac{\partial G_m(z,w)}{\partial z} = G_m(z,w)\,\frac{\partial G_{m-1}(z,w)}{\partial z} \tag{14}$$

for $m \geq 1$. Hence

$$B_1(w,m) = B_0(w,m)B_1(w,m-1) \tag{15}$$

for $m \geq 1$. Since

$$B_0(w,m) = y(w) \tag{16}$$

for $m \geq 0$, by (15) we obtain that

$$B_1(w,m) = [y(w)]^{m+1} \tag{17}$$

for $m \geq 0$, and thus by (6)

$$E\{\tau_n(m)\} = \gamma_n(m) = (m+1)\binom{n}{m+1}\frac{(m+1)!}{n^{m+1}}. \tag{18}$$

If $r \geq 2$, and $m \geq 1$, then the $(r-1)$st derivative of (14) with respect to z at $z = 1$ yields

$$r[B_r(w,m) - y(w)B_r(w,m-1)] = \sum_{j=1}^{r-1}(r-j)B_j(w,m)B_{r-j}(w,m-1), \tag{19}$$

whence for the determination of $B_r(w,m), (r = 2,3,\ldots)$, we get the following recurrence formula:

$$rB_r(w,m) = \sum_{j=1}^{r-1}(r-j)\sum_{0 \leq i < m}[y(w)]^{m-i-1}B_j(w,i+1)B_{r-j}(w,i). \tag{20}$$

If $r = 2$ in (20), then by (17)

$$B_2(w,m) = \frac{1}{2}\sum_{0 \leq i < m}[y(w)]^{m+i+2} \tag{21}$$

and thus by (6)

$$\begin{aligned} E\left\{\binom{\tau_n(m)}{2}\right\} &= \frac{1}{2}\sum_{0 \leq i < m}\gamma_n(m+i+1) \\ &= \frac{n!}{2n^{n-1}}\left(\frac{n^{n-m-2}}{(n-m-2)!} - \frac{n^{n-2m-2}}{(n-2m-2)!}\right). \end{aligned} \tag{22}$$

If $r = 3$ in (20), then by (17) and (21)

$$B_3(w,m) = \frac{1}{2} \sum_{0 \le i < j < m} [y(w)]^{m+i+j+3} + \frac{1}{6} \sum_{0 \le i = j < m} [y(w)]^{m+i+j+3} \tag{23}$$

and hence

$$E\left\{\binom{\tau_n(m)}{3}\right\} = \frac{1}{2} \sum_{0 \le i < j < m} \gamma_n(m+i+j+2) + \frac{1}{6} \sum_{0 \le i = j < m} \gamma_n(m+i+j+2). \tag{24}$$

By continuing this procedure we obtain that for $r \ge 2$,

$$B_r(w,m) = \frac{(r-1)!}{2^{r-1}} \sum_{0 \le i_1 < i_2 < \ldots < i_{r-1} < m} [y(w)]^{m+i_1+\ldots+i_{r-1}+r+\ldots} \tag{25}$$

where the neglected terms are constant multiples of sums similar to the one displayed, except that in these sums $i_1, i_2, \ldots, i_{r-1}$ are not distinct; for at least one $\nu = 2, \ldots, r-1$ we have $i_{\nu-1} = i_\nu$. Formula (25) can be proved by mathematical induction. If we suppose that (25) is true for $B_2(w,m), \ldots, B_{r-1}(w,m)$ where $r = 3, 4, \ldots$, then by (20) it follows that (25) is true for $B_r(w,m)$ too. Accordingly, (25) is true for every $r \ge 2$.

It is easy to prove that

$$|\gamma_n(m) - me^{-m^2/(2n)}| < 4/3 \tag{26}$$

for $0 \le m < n$. If $r = 1$ and $m = [2\alpha\sqrt{n}]$, then by (18) we obtain that

$$E\{\tau_n(m)\} = \gamma_n(m) \sim 2\alpha\sqrt{n}e^{-2\alpha^2} \tag{27}$$

as $n \to \infty$, or

$$\lim_{n\to\infty} 2E\{\tau_n(m)\}/\sqrt{n} = 4\alpha e^{-2\alpha^2}. \tag{28}$$

This proves (10) for $r = 1$. If $r \ge 2, m = [2\alpha\sqrt{n}], 0 < \alpha < \infty$ and $n \to \infty$, then by (25)

$$E\left\{\binom{\tau_n(m)}{r}\right\} = \frac{(r-1)!}{2^{r-1}} \sum_{0 \le i_1 < i_2 < \ldots < i_{r-1} < m} \gamma_n(m+i_1+\ldots+i_{r-1}+r-1) + \ldots \tag{29}$$

where the neglected terms are of smaller order than the displayed one. If $r \ge 1$, $m = [2\alpha\sqrt{n}]$, $0 < \alpha < \infty$ and $n \to \infty$, then

$$E\{[\tau_n(m)]^r\} \sim r!E\left\{\binom{\tau_n(m)}{r}\right\}, \tag{30}$$

and by (26) and (29) we obtain that

$$\lim_{n\to\infty} 2^r E\{[\tau_n(m)]^r\}/n^{r/2} = \mu_r(\alpha) \tag{31}$$

exists and

$$\mu_r(\alpha) = (r-1)!\alpha_r$$

$$\int\cdots\int_{0<x_1<\ldots<x_{r-1}<1} (1+x_1+\ldots+x_{r-1})e^{-2\alpha^2(1+x_1+\ldots+x_{r-1})^2}dx_1\ldots dx_{r-1} \tag{32}$$

$$= \alpha_r \int_0^1 \cdots \int_0^1 (1+x_1+\ldots+x_{r-1})e^{-2\alpha^2(1+x_1+\ldots+x_{r-1})^2}dx_1\ldots dx_{r-1}$$

for $r \geq 2$, where $\alpha_r = 2^{r+1}r!\alpha^r$. We can write also that

$$\mu_r(\alpha) = 2^{r+1}r!\alpha^r \int_0^{r-1} (1+x)e^{-2\alpha^2(1+x)^2} g_{r-1}(x)dx \tag{33}$$

for $r \geq 2$ where $g_{r-1}(x)$ is the density function of $\xi_1+\xi_2+\ldots+\xi_{r-1}$ where $\xi_1, \xi_2, \ldots, \xi_{r-1}$ are independent random variables each having a uniform distribution over the interval $(0,1)$. For the density function $g_{r-1}(x)$, formula (12) has been found by P.S. Laplace [14], pp. 256-257. For a simple proof of (12) see L. Takács [22].

We note that

$$\mu_2(\alpha) = 4(e^{-2\alpha^2} - e^{-8\alpha^2}), \tag{34}$$

and

$$\mu_3(\alpha) = 12\sqrt{2\pi}[2\Phi(4\alpha) - \Phi(2\alpha) - \Phi(6\alpha)] \tag{35}$$

where

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-u^2/2}du \tag{36}$$

is the normal distribution function.

4. THE ASYMPTOTIC DISTRIBUTION OF $\tau_n(m)$

The asymptotic distribution of $\tau_n(m)$ has been found by V.E. Stepanov [21] in a different form.

Theorem 2: *If $0 < \alpha < \infty$, then*

$$\lim_{n\to\infty} P\left\{ \frac{2\tau_n([2\alpha\sqrt{n}])}{\sqrt{n}} \le x \right\} = G_\alpha(x) \tag{37}$$

for $x > 0$ where $G_\alpha(x)$ is the distribution function of a nonnegative random variable and is given by

$$G_\alpha(x) = 1 - 2\sum_{j=1}^{\infty} \sum_{k=0}^{j-1} \binom{j-1}{k} e^{-(x+2\alpha j)^2/2} (-x)^k H_{k+2}(x+2\alpha j)/k! \tag{38}$$

for $x \ge 0$ where $H_0(x), H_1(x), \ldots$ are the Hermite polynomials defined by

$$H_n(x) = n! \sum_{j=0}^{[n/2]} \frac{(-1)^j x^{n-2j}}{2^j j!(n-2j)!}. \tag{39}$$

We have

$$G_\alpha(0) = 1 - 2\sum_{j=1}^{\infty} (4\alpha^2 j^2 - 1) e^{-2\alpha^2 j^2} \tag{40}$$

and

$$\frac{dG_\alpha(x)}{dx} = 2\sum_{j=1}^{\infty} \sum_{k=1}^{j} \binom{j}{k} e^{-(x+2\alpha j)^2/2} (-x)^{k-1} H_{k+2}(x+2\alpha j)/(k-1)! \tag{41}$$

if $x > 0$.

Proof: Since

$$ue^{-u^2} \le (2e)^{-1/2} < 1/2 \tag{42}$$

if $u \ge 0$, it follows from (11) that

$$\mu_r(\alpha)/r! < (2\alpha)^r/\alpha^0 \tag{43}$$

for $r \ge 2$. Accordingly, there exists one and only one distribution function $G_\alpha(x)$ such that $G_\alpha(x) = 0$ for $x < 0$ and

$$\int_{-0}^{\infty} x^r dG_\alpha(x) = \mu_r(\alpha) \tag{44}$$

for $r \ge 0$. By the moment convergence theorem of M. Fréchet and J. Shohat [8] it follows from (10) that (37) holds in every continuity point of $G_\alpha(x)$. If $|s| < 1/(2\alpha)$, then the Laplace-Stieltjes transform

$$\Psi_\alpha(s) = \int_{-0}^{\infty} e^{-sx} dG_\alpha(x) \tag{45}$$

can be expressed as

$$\Psi_\alpha(s) = \sum_{r=0}^{\infty} (-1)^r \mu_r(\alpha) s^r / r!. \tag{46}$$

By (11) we obtain that

$$\Psi_\alpha(s) = 1 + 2\sum_{k=1}^{\infty} \frac{(2\alpha s)^k}{(k-1)!} \int_k^{\infty} (1 - 4\alpha^2 u^2)(u-k)^{k-1} e^{-2\alpha^2 u^2 - 2\alpha(u-k)s} du \tag{47}$$

for $|s| < 1/(2\alpha)$. Hence (38) and (41) follow by inversion.

5. VARIOUS EXTENSIONS

By using the same method which we used in proving Theorems 1 and 2 we can demonstrate that the distribution function $G_\alpha(x)$ appears also in the solutions of various other problems in probability theory. Apparently, the interesting interrelation among these problems has not been noticed before, and $G_\alpha(x)$ has appeared in various disguises. Here are some examples.

(*i*) *Random trees.* Denote by T_{n+1} the set of distinct rooted ordered trees with $n+1$ unlabeled vertices. There are

$$C_n = \binom{2n}{n} \frac{1}{n+1} \tag{48}$$

distinct trees in T_{n+1}. This follows from the obvious recurrence formula

$$C_n = \sum_{i=1}^{n} C_{i-1} C_{n-i} \tag{49}$$

for $n = 1, 2, \ldots$ where $C_0 = 1$. In (48) C_n is the nth Catalan number. Let us choose a tree at random, assuming that all the possible C_n trees are equally probable. Denote by $\tau_{n+1}(m)$ the number of vertices at a distance m from the root of a tree chosen at random. If $0 < \alpha < \infty$, then we have

$$\lim_{n\to\infty} P\left\{ \frac{2\tau_{n+1}([\alpha\sqrt{2n}])}{\sqrt{2n}} \le x \right\} = G_\alpha(x) \tag{50}$$

for $x > 0$.

Denote by T^*_{2n+2} the set of distinct planted trivalent trees with $2n+2$ unlabeled vertices. A planted tree is rooted at an end vertex. In a trivalent tree every vertex has degree 3 except the end vertices which have degree 1. In 1859, A. Cayley [2] demonstrated that there

are C_n distinct trees in T^*_{2n+2} where C_n is given by (48). Let us choose a tree at random in T^*_{2n+2} assuming that all the possible C_n choices are equally probable. Denote by $\tau_{2n+2}(m)$ the number of vertices at a distance m from the root of a tree chosen at random. If $0 < \alpha < \infty$, then we have

$$\lim_{n\to\infty} P\left\{ \frac{2\tau_{2n+2}([\alpha\sqrt{8n}])}{\sqrt{2n}} \le x \right\} = G_\alpha(x) \tag{51}$$

for $x > 0$.

(*ii*) *Branching processes.* Let us suppose that in a population initially we have a progenitor and in each generation each individual reproduces, independently of the others, and has probability p_j, $(j = 0,1,\ldots)$, of giving rise to j descendants in the following generation. Denote by $\xi(m)$, $(m = 0,1,\ldots)$, the number of individuals in the mth generation; $\xi(0) = 1$. Define

$$\rho = \sum_{m \ge 0} \xi(m), \tag{52}$$

that is, ρ is the total number of individuals (total progeny) in the process (possibly $\rho = \infty$). Let

$$f(z) = \sum_{j=0}^{\infty} p_j z^j, \tag{53}$$

and

$$gcd\{j: p_j > 0\} = d. \tag{54}$$

If $f(1) = 1$, $f'(1) = 1$, $f''(1) = \sigma^2$ where $0 < \sigma < \infty$, $f^{(r)}(1) < \infty$ for $r \ge 2$, and $0 < \alpha < \infty$, then

$$\lim_{n\to\infty} P\left\{ \frac{2\xi([2\alpha\sqrt{nd}/\sigma])}{\sigma\sqrt{nd}} \le x \mid \rho = nd+1 \right\} = G_\alpha(x) \tag{55}$$

for $x > 0$ where $G_\alpha(x)$ is defined by (38).

If $p_j = e^{-1}/j!$ for $j = 0,1,2,\ldots$, then $\sigma^2 = 1$ and $d = 1$ and (55) reduces to (37). If $p_j = 1/2^{j+1}$ for $j = 0,1,2,\ldots$, then $\sigma^2 = 2$ and $d = 1$ and (55) reduces to (50). If $p_0 = p_2 = 1/2$ and $p_j = 0$ otherwise, then $\sigma^2 = 1$ and $d = 2$ and (55) reduces to (51).

The limit distribution (55) has already been determined by D.P. Kennedy [12] in a different form. By his results we can conclude that

$$G_\alpha(x) - G_\alpha(0) = \iint\limits_{\substack{0 < u < x/(2\alpha) \\ 0 < v < 1/(4\alpha^2)}} e^{-\alpha^2 u^2/(2(1-4\alpha^2 v))}(1-4\alpha^2 v)^{-3/2} u f(u,v)\,du\,dv \tag{56}$$

for $x > 0$ and

$$\int_0^\infty \int_0^\infty e^{-su-wv} f(u,v)\,du\,dv = \left\{ \frac{sinh(\sqrt{2w})}{\sqrt{2w}} + s\left(\frac{sinh(\sqrt{w/2})}{\sqrt{w/2}} \right)^2 \right\}^{-1} \tag{57}$$

for $Re(s) \geq 0$ and $Re(w) \geq 0$.

(*iii*) *Bernoulli excursion.* Let us arrange n white balls and n black balls in a row in such a way that for every $i = 1, 2, \ldots, 2n$ among the first i balls there are at least as many white balls as black. The total number of such arrangements is given by the nth Catalan number C_n, defined by (48). Let us suppose that all the possible C_n sequences are equally probable and choose a sequence at random. We associate a random walk with the random sequence chosen by assuming that a particle starts at time $t = 0$ at the origin of the x-axis and in the time interval $(i-1, i]$, $i = 1, 2, \ldots, 2n$, it moves with a unit velocity to the right or to the left according to whether the ith ball in the row is white or black respectively. Denote by $x = \eta_n^+(t)$ the position of the particle at time $2nt$ where $0 \leq t \leq 1$. The process $\{\eta_n^+(t), 0 \leq t \leq 1\}$ is called a Bernoulli excursion. Denote by $2\tau_n^+(m)(m = 1, 2, \ldots, n)$ the number of crossings of the sample function of the process $\{\eta_n^+(t), 0 \leq t \leq 1\}$ through the line $x = m - 1/2$. In other words, $\tau_n^+(m)/n$ is the total time spent in the interval $(m-1, m)$ by the process $\{\eta_n^+(t), 0 \leq t \leq 1\}$. If $0 < \alpha < \infty$, then

$$\lim_{n\to\infty} P\left\{ \frac{2\tau_n^+([\alpha\sqrt{2n}])}{\sqrt{2n}} \leq x \right\} = G_\alpha(x) \tag{58}$$

for $x > 0$. Since $\tau_n^+(m)$ has exactly the same distribution as $\tau_{n+1}(m)$ in (50), the two results, (50) and (58), imply each other.

(*iv*) *Brownian excursion.* The process $\{\eta_n^+(t)/\sqrt{2n}, 0 \leq t \leq 1\}$, where $\eta_n^+(t)$ is defined under (*iii*), converges weakly to the Brownian excursion $\{\eta^+(t), 0 \leq t \leq 1\}$. For the definition and properties of the Brownian excursion we refer to P. Lévy [15], [16], K. Itô and H.P. McKean, Jr. [11] and K.L. Chung [4]. For the process $\{\eta^+(t), 0 \leq t \leq 1\}$ define $\tau^+(\alpha)$ as the local time at the level α for $\alpha \geq 0$. From (58) we can conclude that

$$P\{\tau^+(\alpha) \leq x\} = G_\alpha(x) \tag{59}$$

for $x > 0$, and also

$$E\{[\tau^+(\alpha)]^r\} = \mu_r(\alpha) \tag{60}$$

for $r = 0, 1, 2, \ldots$ where $\mu_r(\alpha)$ is defined by (10).

The distribution function (59) has attracted considerable interest. In the articles by R.K. Getoor and M.J. Sharpe [9], J.W. Cohen and G. Hooghiemstra [5], G. Louchard [17], [18], E. Csáki and S.G. Mohanty [6], and Ph. Biane and M. Yor [1], $P\{\tau^+(\alpha) \leq x\}$ is expressed in the form of a complex integral. F.B. Knight [13] and G. Hooghiemstra [10] expressed $P\{\tau^+(\alpha) \leq x\}$ in explicit forms, but their formulas are hardly suitable for numerical calculations. We can easily produce tables and graphs for $G_\alpha(x)$ and $G'_\alpha(x)$ by using formulas (38) and (41) and the remarkable program MATHEMATICA by S. Wolfram [24].

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