

Asymptotically normal distribution of some tree families relevant for phylogenetics, and of partitions without singletons

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Abstract

P.L. Erdős and L.A. Székely [*Adv. Appl. Math.* **10**(1989), 488–496] gave a bijection between rooted semilabeled trees and set partitions. L.H. Harper’s results [*Ann. Math. Stat.* **38**(1967), 410–414] on the asymptotic normality of the Stirling numbers of the second kind translates into asymptotic normality of rooted semilabeled trees with given number of vertices, when the number of internal vertices varies. The Erdős-Székely bijection specializes to a bijection between phylogenetic trees and set partitions with classes of size ≥ 2 . We consider modified Stirling numbers of the second kind that enumerate partitions of a fixed set into a given number of classes of size ≥ 2 , and obtain their asymptotic normality as the number of classes varies. The Erdős-Székely bijection translates this result into the asymptotic normality of the number of phylogenetic trees with given number of vertices, when the number of leaves varies. We also obtain asymptotic normality of the number of phylogenetic trees with given number of leaves and varying number of internal vertices, which make more sense to students of phylogeny. By the Erdős-Székely bijection this means the asymptotic normality of the number of partitions of $n + m$ elements into m classes of size ≥ 2 , when n is fixed and m varies. The proofs are adaptations of the techniques of L.H. Harper [ibid.]. We provide asymptotics for the relevant expectations and variances with error term $O(1/n)$.

1 Semilabeled trees and set partitions

Péter Erdős and László Székely [8] enumerated $F(n, k)$, the number of *rooted semilabeled trees* with k uniquely labeled leaves and n non-root vertices. Such trees have a root, which may or may not have degree one, and is not being counted as vertex or leaf; and have k leaves. Two such trees are identical, if there is a graph isomorphism between them that maps root to root and every leaf label to the same leaf label. The labels of the leaves come from the set $\{1, 2, \dots, k\}$ and labels are not repeated.

Erdős and Székely in [8] established a bijection between the trees counted by $F(n, k)$ and partitions of an n -element set into $n - k + 1$ classes, under which out-degrees of non-root vertices and the root correspond to class sizes in the partition. The cited result immediately implies that $F(n, k) = S(n, n - k + 1)$, where $S(a, b)$ denotes the *Stirling number of the second kind* that enumerates partitions of an a -element set into b non-empty classes; and

that $\sum_k F(n, k) = \sum_i S(n, i) = B_n$, the *Bell number* [18] A000110. Any information available on the Stirling numbers of the second kind translates for information on the F -numbers. For example, the recurrence relation

$$S(n, k) = S(n - 1, k - 1) + kS(n - 1, k) \quad (1)$$

translates to $F(n, k) = F(n - 1, k) + (n + 1 - k)F(n - 1, k - 1)$. However, phylogeneticists are not interested in semilabeled trees with internal vertices of degree 2 and with root degree 1. We use the term *phylogenetic tree* for semilabeled trees that do not fall into these degenerate categories. Let $F^*(n, k)$ denote the number of phylogenetic trees with k leaves and n non-root vertices, and let $S^*(n, k)$ denote the number of partitions of an n -element set into k classes, such that each contains at least 2 elements. The Erdős–Székely bijection still provides $F^*(n, k) = S^*(n, n - k + 1)$ and $S^*(n, i) = F^*(n, n - i + 1)$.

Felsenstein [10, 11], and also Foulds and Robinson [12] investigated the numbers $T_{n,m}$. $T_{n,m}$ is the number of rooted trees with n labeled leaves, m unlabeled internal vertices (the root is one of them), where the root has degree at least 2 and no other internal vertices have degree 2. Clearly

$$T_{n,m} = F^*(n + m - 1, n) = S^*(n + m - 1, m). \quad (2)$$

If we are interested only in evaluating certain $T_{n,m}$ numbers, formula (2) would suffice. However, the $T_{n,m}$ notation suggests that the distributions of $F(n, k)$ and $F^*(n, k)$ for large but fixed number of vertices n and varying number of leaves k , albeit is mathematically interesting, not relevant for phylogenetics. The relevant distribution for phylogenetics is large but fixed number of leaves n , and varying number of internal vertices, with which total number of vertices varies as well. Let $t_n = \sum_k T_{n,k}$ denote the number of all phylogenetic trees with n labeled leaves. This sequence is A000311 in [18], which is the solution to Schroeder’s fourth problem [17].

This paper proves central and local limit theorems for the arrays $S^*(n, k)$ and $T_{n,k}$, which translate into such results for $F^*(n, i)$ and $S(n - 1 + m, m)$. We compute the expectations and variances with $O(1/n)$ error term, to support the phylogeneticists who may use our results to approximate certain large numbers. The technique to be used is Harper’s method [13], and we heavily exploit far-reaching asymptotic results on Bell numbers.

2 Harper’s method

Harper [13] made a very elegant proof for the asymptotic normality of the array $S(n, k)$. We follow the interpretation of Canfield [2] and Clark [6],

who clarified and explained the details of [13], although our discussion is somewhat restrictive. Let $A(n, j)$ be an array of non-negative real numbers for $j = 0, 1, \dots, d_n$, and define $A_n(x) = \sum_j A(n, j)x^j$. Observe that $\sum_j A(n, j) = A_n(1)$. Let Z_n denote the random variable, for which the probability $\mathcal{P}(Z_n = j) = \frac{A(n, j)}{A_n(1)}$. In terms of $A_n(x)$, there is a well-known [6] and easy to verify expression for the expectation and variance of Z_n :

$$\mathcal{E}(Z_n) = \frac{A'_n(1)}{A_n(1)} \quad \text{and} \quad \mathcal{D}^2(Z_n) = \frac{A'_n(1)}{A_n(1)} + \left(\frac{A'_n(x)}{A_n(x)} \right)' \Big|_{x=1}. \quad (3)$$

As $\mathcal{E}(Z_n)$ and $\mathcal{D}(Z_n)$ are determined by the array $A(n, j)$, we will also write them as $\mathcal{E}(A(n, \cdot))$ and $\mathcal{D}(A(n, \cdot))$

The array $A(n, j)$ is called *asymptotically normal* in the sense of a *central limit theorem*, if

$$\frac{1}{A_n(1)} \sum_{j=1}^{\lfloor x_n \rfloor} A(n, j) \rightarrow \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt \quad (4)$$

as $n \rightarrow \infty$ uniformly in x , where

$$x_n = \mathcal{E}(Z_n) + x\mathcal{D}(Z_n). \quad (5)$$

Assume now that all the roots of the polynomial $A_n(x)$ are non-positive real numbers, say $\{-y_{nk} : k = 1, 2, \dots, d_n\}$. Define the independent random variables Y_{nk} by $\mathcal{P}(Y_{nk} = 0) = y_{nk}/(1 + y_{nk})$ and $\mathcal{P}(Y_{nk} = 1) = 1/(1 + y_{nk})$.

Observe that the probability generating function of the random variable Z_n is $A_n(x)/A_n(1)$; and the probability generating function of the random variable Y_{nk} is $\frac{x+y_{nk}}{1+y_{nk}}$. Since the probability generating function of a sum of independent random variables is the product of their probability generating functions, we have that the probability generating function of $\sum_k Y_{nk}$ is $\prod_{k=1}^{d_n} \frac{x+y_{nk}}{1+y_{nk}}$. However, as

$$\prod_{k=1}^{d_n} \frac{x+y_{nk}}{1+y_{nk}} = \frac{A_n(x)}{A_n(1)},$$

we conclude that Z_n and $\sum_k Y_{nk}$ have identical distribution. Let $G_{nj}(x) = \mathcal{P}\left(\frac{Y_{nj} - \mathcal{E}(Y_{nj})}{\mathcal{D}(Z_n)} \leq x\right)$ denote the cumulative distribution function of $\frac{Y_{nj} - \mathcal{E}(Y_{nj})}{\mathcal{D}(Z_n)}$ for $j = 1, \dots, d_n$. The Lindeberg–Feller Theorem ([7] pp. 98–101) to

the sequence $\frac{Z_n - \mathcal{E}(Z_n)}{\mathcal{D}_n(Z_n)} = \sum_j \frac{Y_{nj} - \mathcal{E}(Y_{nj})}{\mathcal{D}_n(Z_n)}$. The condition of the cited theorem, for all $\epsilon > 0$

$$\lim_{n \rightarrow \infty} \sum_{j=1}^{d_n} \int_{|y| > \epsilon} y^2 dG_{nj}(y) = 0$$

follows from

$$\lim_{n \rightarrow \infty} \mathcal{D}(Z_n) = \infty. \quad (6)$$

Therefore, the cited theorem proves the normal convergence (4), provided (6) holds and all the roots of the polynomials $A_n(x)$ have non-positive real numbers.

A sequence a_k is called *unimodal*, if first it increases, and then decreases. An array $A(n, k)$ is called *unimodal*, if for every n , the sequence $a_k = A(n, k)$ is such. A sequence a_k , which is 0 for $k < t$ and $\ell < k$, with $a_t \neq 0$ and $a_\ell \neq 0$, is called *strictly log-concave* (SLC) if $a_k^2 - a_{k-1}a_{k+1} > 0$ for $t+1 \leq k \leq \ell-1$. An array $A(n, k)$ is called *strictly log-concave* (SLC), if for every fixed n , the sequence $a_k = A(n, k)$ is such. It is well-known and easy to see that any SLC sequence is unimodal in the variable k . Using Newton's Inequality, Lieb [14] showed that if a polynomial $\sum_{k=1}^N C_k x^k$ has only real roots, then for $k = 2, \dots, N-1$

$$C_k^2 \geq C_{k+1}C_{k-1} \left(\frac{k}{k-1} \right) \left(\frac{N-k+1}{N-k} \right), \quad (7)$$

and hence the C_k sequence is SLC, and showed the SLC property of $S(n, k)$ through (7).

E.R. Canfield [2] noted that for asymptotically normal sequences (4), the SLC property and $\mathcal{D}(Z_n) \rightarrow \infty$ implies the following *local limit theorem*:

$$\lim_{n \rightarrow \infty} \frac{\mathcal{D}(Z_n)}{A_n(1)} A(n, \lfloor x_n \rfloor) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (8)$$

uniformly in x . Furthermore, from the fact that the convergence of the $A(n, j)$ numbers to the Gaussian function is actually uniform, he concluded that the number $k = J_n$ maximizing $A(n, k)$ satisfies

$$J_n - \mathcal{E}(Z_n) = o(\mathcal{D}(Z_n)); \quad (9)$$

and

$$A(n, J_n) \sim \frac{1}{\sqrt{2\pi}} \frac{A_n(1)}{\mathcal{D}_n(Z_n)}. \quad (10)$$

For the Stirling numbers of the second kind, $A(n, j) = S(n, j)$, $A_n(1) = B_n$, and one has

$$\mathcal{E}(S(n, \cdot)) = \frac{B_{n+1}}{B_n} - 1, \quad (11)$$

$$\mathcal{D}^2(S(n, \cdot)) = \frac{B_{n+2}}{B_n} - \left(\frac{B_{n+1}}{B_n}\right)^2 - 1. \quad (12)$$

Harper [13] showed that $\sum_k S(n, k)x^k$ has distinct nonpositive roots, that (12) goes to infinity, which is sufficient for the asymptotic normality of the Stirling numbers of the second kind. Harper [13] already observed (8) for $A(n, k) = S(n, k)$.

The SLC property of $S(n, k)$ implies the SLC property and unimodality of $F(n, k)$. Consequently, the $F(n, k)$ array is also asymptotically normal, in the sense of both the central and local limit theorems, with $\mathcal{E}(F(n, \cdot)) = n + 1 - \mathcal{E}(S(n, \cdot))$ and $\mathcal{D}(F(n, \cdot)) = \mathcal{D}(S(n, \cdot))$.

3 Asymptotics for Bell numbers

Asymptotic formula for the Bell numbers, in terms of the solution of the unique real solution of the equation $re^r = n$, was obtained by Moser and Wyman [15]: $B_n \sim (r+1)^{-\frac{1}{2}} \exp[n(r+r^{-1}-1)-1] \left(1 - \frac{r^2(2r^2+7r+10)}{24n(r+1)^3}\right)$. Iteration easily gives $r = r(n) = \ln n - \ln \ln n + O(1)$. The function $r(n)$ is also known as *LambertW*(n). The explicit form of their result is not convenient to obtain asymptotics for the expectation and the variance, as r will vary with n . Canfield and Harper [5], Canfield [3] made minor modifications on the proof of Moser and Wyman [15] to develop an estimate for B_{n+h} , which holds uniformly for $h = O(\ln n)$, using a *single* $r = r(n)$ value, as $n \rightarrow \infty$:

$$\begin{aligned} B_{n+h} &= \frac{(n+h)!}{r^{n+h}} \frac{e^{e^r-1}}{(2\pi B)^{1/2}} \\ &\times \left(1 + \frac{P_0 + hP_1 + h^2P_2}{e^r} + \frac{Q_0 + hQ_1 + h^2Q_2 + h^3Q_3 + h^4Q_4}{e^{2r}} \right. \\ &\left. + O(e^{-3r}) \right), \end{aligned} \quad (13)$$

where $B = (r^2 + r)e^r$, P_i and Q_i are explicitly known rational functions of r . We list and use in the Maple worksheet [19] their exact values from Canfield [4]. Using those, the formula (13) immediately provides asymptotics for

$\mathcal{E}(S(n, \cdot))$ and $\mathcal{D}(S(n, \cdot))$, as in [4] (note that [4] only claimed $O(r/n)$ error term in (15)):

$$\mathcal{E}(S(n, \cdot)) = \frac{n}{r} - 1 + \frac{r}{2(r+1)^2} + O\left(\frac{1}{n}\right). \quad (14)$$

$$\mathcal{D}^2(S(n, \cdot)) = \frac{n}{r(r+1)} + \frac{r(r-1)}{2(r+1)^4} - 1 + O\left(\frac{1}{n}\right). \quad (15)$$

With symbolic calculations Salvy and Shackell [16] obtained the following asymptotics *just* in terms of n , with a compromise at the error term:

$$\mathcal{E}(S(n, \cdot)) = \frac{n}{\ln n} + \frac{n(\ln \ln n + O(1/\ln n))}{\ln^2 n}, \quad (16)$$

$$\mathcal{D}^2(S(n, \cdot)) = \frac{n}{\ln^2 n} + \frac{n(2 \ln \ln n - 1 + O(1/\ln n))}{\ln^3 n}. \quad (17)$$

4 Phylogenetic trees and set partitions without singletons

Theorem 4.1. *For the sequence $A(n, j) = S^*(n, j)$ the central limit theorem (4) and the local limit theorem (8) hold with*

$$\mathcal{E}(S^*(n, \cdot)) = \frac{n}{r} - r - \frac{1}{2r} + \frac{1}{2r(r+1)^2} + O\left(\frac{1}{n}\right), \quad (18)$$

$$\begin{aligned} \mathcal{D}^2(S^*(n, \cdot)) &= \frac{n}{r(r+1)} - r + 1 - \frac{2}{r+1} - \frac{1}{2(r+1)^2} \\ &\quad - \frac{1}{2(r+1)^3} + \frac{1}{(r+1)^4} + O\left(\frac{1}{n}\right). \end{aligned} \quad (19)$$

Furthermore, the number $k = J_n$ that maximizes $S^*(n, k)$ satisfies

$$J_n = \frac{n}{r} + o\left(\frac{\sqrt{n}}{r}\right) \quad (20)$$

and

$$S^*(n, J_n) = \frac{rB_{n-1}}{\sqrt{2n\pi}}(1 + o(1)). \quad (21)$$

It is remarkable that making an asymptotic expansion in terms of r in (18), (19), after a few terms the error reduces to $O(1/n)$, as in the case of the Bell numbers in (14), (15). Using these asymptotic expansions we obtain that $\mathcal{E}(S^*(n, \cdot)) - \mathcal{E}(S(n, \cdot)) = O(r)$ and $\mathcal{D}^2(S^*(n, \cdot)) - \mathcal{D}^2(S(n, \cdot)) = O(r)$. Statement (i) below follows from these remarkably small differences.

Corollary 4.2. (i) (16) and (17) still hold when $S(n, \cdot)$ is changed to $S^*(n, \cdot)$.

(ii) $A(n, k) = F^*(n, k)$ satisfies (4) and (8) with $\mathcal{E}(F^*(n, \cdot)) = n + 1 - \mathcal{E}(S^*(n, \cdot)) = n - n/r + r + 1 + o(1/r)$ and $\mathcal{D}(F^*(n, \cdot)) = \mathcal{D}(S^*(n, \cdot))$.

Proof to Theorem 4.1. We start with some facts that we need. Set $B_n^* = \sum_k S^*(n, k)$, the number of all partitions of an n -element set not using singleton classes [18] A000296. Becker [1] observed that¹

$$B_n = B_{n+1}^* + B_n^*. \quad (22)$$

From $B_i = B_i^* + B_{i+1}^*$ for $i = 1, 2, \dots, n$, and $B_1^* = 0$, we obtain $B_{n+1}^* = \sum_{i=1}^n B_i (-1)^{n-i}$. As the B_n sequence is strictly increasing, we immediately obtain $B_t - B_{t-1} < B_{t+1}^* = \sum_{i=1}^t B_i (-1)^{t-i} < B_t$ for $t \geq 3$, and with $t = n - h$ the asymptotical formula

$$B_{n+1}^* = B_n - B_{n-1} + \dots + (-1)^h B_{n-h} + O(B_{n-h-1}). \quad (23)$$

In the special case $h = 0$, using (13), we obtain:

$$B_{n+1}^* = B_n - O(B_{n-1}) = B_n \left(1 - O\left(\frac{r}{n}\right)\right). \quad (24)$$

(It turns out, as a byproduct, that almost all set partitions contain a singleton.) We obtain the recurrence relation

$$S^*(n, k) = (n - 1)S^*(n - 2, k - 1) + kS^*(n - 1, k), \quad (25)$$

according to the case analysis whether the n^{th} element is in a doubleton class or not. We define the polynomial sequence $S_n(x) = \sum_k S^*(n, k)x^k$. It is easy to see that $S_1(x) = 0$, $S_2(x) = x$, and for $n \geq 3$ from (25),

$$S_n(x) = (n - 1)xS_{n-2}(x) + xS_{n-1}'(x). \quad (26)$$

For the proof, first we compute $\mathcal{E}(S^*(n, \cdot))$ and $\mathcal{D}(S^*(n, \cdot))$ exactly and then asymptotically. The central and local limit theorems hinge on $\mathcal{D}(S^*(n, \cdot)) \rightarrow \infty$. Formulae (20) and (21) follow from (9) and (10), where B_n^* is approximated with B_{n-1} by (24). Finally, Lemma 4.3 will provide the non-positive real roots of the generating polynomial.

¹Identity (22) can be proved by the following bijection from the partitions with at least one singleton class of an n -element set, $[n]$, to the partitions without singleton classes of an $n + 1$ -element set, $[n + 1]$: build a new class from the elements of all singletons and $n + 1$.

We obtain from (3), using (26) repeatedly,

$$\begin{aligned}\mathcal{E}(S^*(n, \cdot)) &= \frac{B_{n+1}^*}{B_n^*} - n \frac{B_{n-1}^*}{B_n^*}; \\ \mathcal{D}^2(S^*(n, \cdot)) &= \frac{B_{n+2}^*}{B_n^*} + 2n \frac{B_{n+1}^* B_{n-1}^*}{(B_n^*)^2} + n(n-1) \frac{B_{n-2}^*}{B_n^*} \\ &\quad - \left(\frac{B_{n+1}^*}{B_n^*} \right)^2 - n^2 \left(\frac{B_{n-1}^*}{B_n^*} \right)^2 - n \frac{B_{n-1}^*}{B_n^*} - (2n+1).\end{aligned}$$

To obtain (18) and (19), we started with the closed forms above, used (23) for the B^* numbers, and substituted the B numbers with (13), changed e^{-r} to r/n . For details, see the Maple worksheet [19].

Induction immediately gives from (26) that for $n \geq 2$

$$\deg(S_n(x)) = \left\lfloor \frac{n}{2} \right\rfloor \quad (27)$$

and the root $x = 0$ has multiplicity one. Hence $S'_n(0) > 0$ for $n \geq 2$.

Lemma 4.3. *Apart from $x = 0$, the roots of $S_{2n}(x)$ and $S_{2n+1}(x)$ are negative real numbers and every root occurs with multiplicity one. Furthermore, if the roots of $S_{2n}(x)$ are denoted by $\beta_i^{(2n)}$ in increasing order, and the roots of $S_{2n-1}(x)$, $S_{2n+1}(x)$ are denoted by $\alpha_i^{(2n-1)}$, $\alpha_i^{(2n+1)}$, both in increasing order, then the following interlacing properties hold:*

$$\begin{aligned}\beta_1^{(2n)} &< \alpha_1^{(2n-1)} < \beta_2^{(2n)} < \alpha_2^{(2n-1)} < \dots < \beta_{n-1}^{(2n)} < \alpha_{n-1}^{(2n-1)} = 0 = \beta_n^{(2n)}, \\ \beta_1^{(2n)} &< \alpha_1^{(2n+1)} < \beta_2^{(2n)} < \alpha_2^{(2n+1)} < \dots < \alpha_{n-2}^{(2n+1)} < \beta_{n-1}^{(2n)} < \alpha_{n-1}^{(2n+1)} < \beta_n^{(2n)} = 0 = \alpha_n^{(2n+1)}.\end{aligned}$$

Proof. We will use mathematical induction on n . The roots of $S_2(x) = S_3(x) = x$, $S_4(x) = 3x^2 + x$ (roots $\beta_1^{(4)} = -1/3$ and $\beta_2^{(4)} = 0$) and $S_5(x) = 10x^2 + x$ (roots $\alpha_1^{(5)} = -1/10$ and $\alpha_2^{(5)} = 0$) satisfy Lemma 4.3. The inductive step follows from the following two statements for $k \geq 2$:

- (i) If the roots of $S_{2n-2}(x)$ and $S_{2n-1}(x)$ occur with multiplicity one and satisfy

$$\beta_1^{(2n-2)} < \alpha_1^{(2n-1)} < \beta_2^{(2n-2)} < \alpha_2^{(2n-1)} < \dots < \alpha_{n-2}^{(2n-1)} < \beta_{n-1}^{(2n-2)} = 0 = \alpha_{n-1}^{(2n-1)},$$

then the roots $\beta_i^{(2n)}$ of $S_{2n}(x)$ satisfy

$$\beta_1^{(2n)} < \alpha_1^{(2n-1)} < \beta_2^{(2n)} < \alpha_2^{(2n-1)} < \dots < \beta_{n-1}^{(2n)} < \alpha_{n-1}^{(2n-1)} = 0 = \beta_n^{(2n)}.$$

(ii) If the roots of $S_{2n-1}(x)$ and $S_{2n}(x)$ occur with multiplicity one and satisfy

$$\beta_1^{(2n)} < \alpha_1^{(2n-1)} < \beta_2^{(2n)} < \alpha_2^{(2n-1)} < \dots < \beta_{n-1}^{(2n)} < \alpha_{n-1}^{(2n-1)} = 0 = \beta_n^{(2n)}$$

then the roots $\alpha_i^{(2n+1)}$ of $S_{2n+1}(x)$ satisfy

$$\beta_1^{(2n)} < \alpha_1^{(2n+1)} < \beta_2^{(2n)} < \alpha_2^{(2n+1)} < \dots < \alpha_{n-2}^{(2n+1)} < \beta_{n-1}^{(2n)} < \alpha_{n-1}^{(2n+1)} < \beta_n^{(2n)} = 0 = \alpha_n^{(2n+1)}.$$

First we prove (i). In our setting the identity (26) specifies to

$$S_{2n}(x)/x = (2n-1)S_{2n-2}(x) + S'_{2n-1}(x), \quad (28)$$

where the RHS is the sum of two polynomials of degree $n-1$ and $n-2$, respectively.

Set $\alpha_0^{(2n-1)} = -\infty$. The proof hinges on the following three claims:

- The sign of $S_{2n-2}(x)$ alternates on $\alpha_i^{(2n-1)}, \alpha_{i+1}^{(2n-1)}$ for $i = 0, 1, \dots, n-3$;
- The sign of $S'_{2n-1}(x)$ alternates on $\alpha_i^{(2n-1)}, \alpha_{i+1}^{(2n-1)}$ for $i = 1, \dots, n-2$; and
- $\text{sign}(S_{2n-2}(\alpha_1^{(2n-1)})) = \text{sign}(S'_{2n-1}(\alpha_1^{(2n-1)}))$.

The first claim follows from the hypotheses.

The second claim follows from the fact that $S'_{2n-1}(x)$ is a polynomial of degree $n-2$ and it has exactly one root in every interval $(\alpha_i^{(2n-1)}, \alpha_{i+1}^{(2n-1)})$ for $i = 1, 2, \dots, n-2$, as it must have a root between consecutive roots of $S_{2n-1}(x)$.

The third claim follows from the facts that

$\text{sign}(S_{2n-2}(\alpha_1^{(2n-1)})) = -\text{sign}(S_{2n-2}(-\infty)) = -(-1)^{n-1}$, as $S_{2n-2}(x)$ has a single root, $\beta_1^{(2n-2)}$, which is less than $\alpha_1^{(2n-1)}$; and $\text{sign}(S'_{2n-1}(\alpha_1^{(2n-1)})) = \text{sign}(S'_{2n-1}(-\infty)) = (-1)^{n-2}$, as $S'_{2n-1}(x)$ has no root less than $\alpha_1^{(2n-1)}$.

From the three claims and (28) follows that the sign of $S_{2n}(x)/x$, and hence of $S_{2n}(x)$, alternates on $\alpha_i^{(2n-1)}, \alpha_{i+1}^{(2n-1)}$ for $i = 1, \dots, n-3$; and this fact provides the required $\beta_{i+1}^{(2n)}$ root between these numbers, $i = 1, \dots, n-3$.

From the proof of the third claim and (28) follows that $\text{sign}(S_{2n}(\alpha_1^{(2n-1)})/\alpha_1^{(2n-1)}) = (-1)^n$. If we show that $S_{2n}(x)/x$ has a different sign at $-\infty$, then we provided the required $\beta_1^{(2n)} < \alpha_1^{(2n-1)}$ root for $S_{2n}(x)/x$, and hence for $S_{2n}(x)$. Indeed, the degree of $S_{2n-2}(x)$ is greater than the degree of $S'_{2n-1}(x)$, and therefore the sign of $S_{2n}(x)/x$ at $-\infty$ is the sign of $S_{2n-2}(x)$ at $-\infty$, namely $(-1)^{n-1}$.

As $S_{2n-2}(\alpha_{n-1}^{(2n-1)}) = S_{2n-2}(0) = 0$, the second and the third claim, and (28) imply that $S_{2n}(x)/x$ alternates on $\alpha_{n-2}^{(2n-1)}, \alpha_{n-1}^{(2n-1)}$, providing the

required root $\beta_{n-1}^{(2n)}$ between these numbers, also for $S_{2n}(x)$. Finally, the last root to find is $\beta_n^{(2n)} = 0$.

Next we prove (ii). In our setting the identity (26) specifies to

$$S_{2n+1}(x)/x = 2nS_{2n-1}(x) + S'_{2n}(x), \quad (29)$$

where the RHS is the sum of two polynomials of degree $n - 1$. The proof hinges on the following three claims:

- The sign of $S_{2n-1}(x)$ alternates on $\beta_i^{(2n)}, \beta_{i+1}^{(2n)}$ for $i = 1, \dots, n - 2$;
- The sign of $S'_{2n}(x)$ alternates on $\beta_i^{(2n)}, \beta_{i+1}^{(2n)}$ for $i = 1, \dots, n - 1$; and
- $\text{sign}(S_{2n-1}(\beta_1^{(2n)})) = \text{sign}(S'_{2n}(\beta_1^{(2n)}))$.

The first claim follows from the hypotheses.

The second claim follows from the fact that $S'_{2n}(x)$ is a polynomial of degree $n - 1$ and it has exactly one root in every interval $\beta_i^{(2n)}, \beta_{i+1}^{(2n)}$ for $i = 1, 2, \dots, n - 1$, as it must have a root between consecutive roots of $S_{2n}(x)$.

The third claim follows from the facts that

$\text{sign}(S_{2n-1}(\beta_1^{(2n)})) = \text{sign}(S_{2n-1}(-\infty)) = (-1)^{n-1}$, and $\text{sign}(S'_{2n}(\beta_1^{(2n)})) = \text{sign}(S'_{2n}(-\infty)) = (-1)^{n-1}$, as neither $S'_{2n}(x)$ nor $S_{2n-1}(x)$ has a root less than $\beta_1^{(2n)}$.

From the three claims and (29) follows that the sign of $S_{2n+1}(x)/x$, and hence of $S_{2n+1}(x)$, alternates on $\beta_i^{(2n)}, \beta_{i+1}^{(2n)}$ for $i = 1, \dots, n - 2$; and this fact provides the required $\alpha_i^{(2n+1)}$ root between these numbers, $i = 1, \dots, n - 2$.

As $S_{2n-1}(\beta_n^{(2n)}) = S_{2n-1}(0) = 0$, the second and the third claim, and (29) imply that $S_{2n+1}(x)/x$ alternates on $\beta_{n-1}^{(2n)}, \beta_n^{(2n)}$, providing the required root $\alpha_{n-1}^{(2n+1)}$ between these numbers, also for $S_{2n}(x)$. Finally, the last root to find is $\alpha_n^{(2n+1)} = 0$. \square

5 Phylogenetic trees and set partitions in another distribution

Theorem 5.1. *For the array $A(n, j) = T_{n+1, j}$, the central limit theorem (4) and the local limit theorem (8) hold with*

$$\begin{aligned} \mathcal{E}(T_{n+1, \cdot}) &= \frac{1 - \rho}{2\rho}n + \frac{3/4 - \ln 2}{\rho} + O(1/n) \quad \text{and} \\ \mathcal{D}^2(T_{n+1, \cdot}) &= \frac{n}{4} \left(\frac{1}{\rho^2} - \frac{2}{\rho} - 1 \right) + \frac{1 + 4 \ln 2 - 8 \ln^2 2}{8\rho^2} + O(1/n), \end{aligned}$$

where $\rho = -1 + 2 \ln 2$. Furthermore, the number $k = J_n$ that maximizes $T_{n+1,k}$ satisfies

$$J_n = \frac{1 - \rho}{2\rho} n + o(\sqrt{n}), \quad (30)$$

and

$$T_{n+1, J_n} = \frac{n!(1 + o(1))}{\pi \sqrt{2n\rho^{n+\frac{1}{2}}} \sqrt{(\frac{1}{\rho^2} - \frac{2}{\rho} - 1)}}. \quad (31)$$

Identity (2) immediately implies the following central and local limit theorems as corollaries:

$$\frac{1}{t_{n+1}} \sum_{j=1}^{\lfloor x_n \rfloor} S^*(n+j, j) \rightarrow \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt \quad (32)$$

and

$$\lim_{n \rightarrow \infty} \frac{\mathcal{D}(T_{n+1, \cdot})}{t_{n+1}} S^*(n + \lfloor x_n \rfloor, \lfloor x_n \rfloor) \rightarrow \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (33)$$

as $n \rightarrow \infty$, uniformly in x , with $x_n = \mathcal{E}(T_{n+1, \cdot}) + x\mathcal{D}(T_{n+1, \cdot})$.

Proof to Theorem 5.1. Felsenstein [10, 11] proved the recurrence relation²

$$T_{n,k} = (n+k-2)T_{n-1,k-1} + kT_{n-1,k} \quad (34)$$

for $k > 1$ with the initial condition $T_{n,1} = 1$ for $n > 1$. Consider the polynomials $P_n(x) = \sum_k T_{n+1,k} x^k$. Then $P_n(1) = t_{n+1}$ and the degree of $P_n(x)$ is n . Felsenstein's recurrence relation (34) implies the identity

$$P_n(x) = nxP_{n-1}(x) + (x+x^2)P'_{n-1}(x) \quad (35)$$

with initial term $P_0(x) = 1$, $P_1(x) = T_{2,1}x = x$. We have for the expectation and variance, from (3), using (35) repeatedly,

$$\mathcal{E}(T_{n+1, \cdot}) = \frac{t_{n+2}}{2t_{n+1}} - \frac{n+1}{2}; \quad (36)$$

$$\mathcal{D}^2(T_{n+1, \cdot}) = \frac{t_{n+3}}{4t_{n+1}} - \frac{t_{n+2}^2}{4t_{n+1}^2} - \frac{t_{n+2}}{2t_{n+1}} - \frac{n+1}{4}. \quad (37)$$

Consider the following bivariate generating function for $T_{n,k}$:

$$H(x, z) = \sum_{n \geq 1} \sum_k T_{n,k} x^k \frac{z^n}{n!} = \sum_{n \geq 1} P_{n-1}(x) \frac{z^n}{n!}, \quad (38)$$

²The recurrence is based on a case analysis whether the n^{th} leaf is to be grafted into an edge or to be joined to an internal vertex of an already existing tree with $n-1$ leaves.

in particular, $H(1, z) = \frac{z}{1!} + \frac{z^2}{2!} + \frac{4z^3}{3!} + \frac{26z^4}{4!} + \dots$. Flajolet [9] observed the functional equation

$$H(x, z) = z + x \left(e^{H(x, z)} - 1 - H(x, z) \right), \quad (39)$$

which immediately follows from the Exponential Formula, and obtained from this equation an expression for $H(1, z)$ in terms of the Lambert function:

$$H(1, z) = -\text{LambertW} \left(-\frac{1}{2} e^{\frac{z-1}{2}} \right) + \frac{z-1}{2}.$$

He also observed that $H(1, z)$, the EGF of the t_n sequence, has a singularity at $\rho = -1 + 2 \ln 2$, and it is the only singularity at this radius; and furthermore, for $|z| < \rho$, there is a singular expansion of $H(1, z)$ in terms of $\Delta = \sqrt{1 - z/\rho}$, of which the first few terms are

$$H(1, z) = \ln 2 - \sqrt{\rho} \Delta + \left(\frac{1}{6} - \frac{1}{3} \ln 2 \right) \Delta^2 - \frac{\rho^{3/2}}{36} \Delta^3 + O(\Delta^4). \quad (40)$$

Flajolet [9] used (40) to obtain asymptotic formula for t_n and noted that asymptotic expansion can be obtained by this method. Using Maple, we went further and obtained the following asymptotic expansion:

$$t_n \sim \frac{n!}{\sqrt{\pi} \rho^{n-\frac{1}{2}}} \left(\frac{1}{2n^{3/2}} + \frac{3}{16n^{5/2}} + \frac{25}{256n^{7/2}} + O\left(\frac{1}{n^{9/2}}\right) \right). \quad (41)$$

Combining (36) and (37) with (41), one obtains the asymptotics for the expectation and the variance in Theorem 5.1. The details are on a Maple worksheet [20].

Lemma 5.2. *For $n \geq 1$, the polynomial $P_n(x)$ has n distinct real roots, one of them is zero, and the other $n - 1$ roots are in the open interval $(-1, 0)$.*

Proof. We prove the theorem with mathematical induction on n . The small cases above are easy to verify. It is easy to see (by a different induction) that $P_1(-1) = -1$ and from (35), $P_n(-1) = (-n)P_{n-1}(-1)$, thus

$$\text{sign}(P_n(-1)) = (-1)^n. \quad (42)$$

Using the induction hypothesis, let the roots of $P_n(x)$ be

$$-1 < \alpha_1 < \dots < \alpha_{n-2} < \alpha_{n-1} < \alpha_n = 0.$$

By Rolle's theorem, $P'_n(x)$ has a root β_i in (α_i, α_{i+1}) for $i = 1, 2, \dots, n - 1$. From (35), observe that $\text{sign}(P_{n+1}(\beta_i)) = -\text{sign}(P_n(\beta_i))$. As the sign of $P_n(x)$ must alternate on the β_i , so does $P_{n+1}(x)$, and therefore $P_{n+1}(x)$ has a root in (β_i, β_{i+1}) for $i = 1, 2, \dots, n - 2$. We have to find 3 more roots: one is $x = 0$, and we will show that the other two are in the intervals $(-1, \beta_1)$ and $(\beta_{n-1}, 0)$, respectively.

Indeed, $\text{sign}(P_n(x))$ differs in -1 and β_1 , since $P_n(x)$ has a single root α_1 between. Also, $\text{sign}(P_{n+1}(-1)) = -\text{sign}(P_n(-1))$ by (42) and $\text{sign}(P_{n+1}(\beta_1)) = -\text{sign}(P_n(\beta_1))$ from our earlier observation. Hence, $\text{sign}(P_{n+1}(x))$ differs in -1 and β_1 , and therefore $P_{n+1}(x)$ has a root in $(-1, \beta_1)$.

Observe (35) with induction implies that for $n \geq 1$ the coefficient of x^n in $P_n(x)$ is positive. On one hand, we have that for $x < 0$ but x sufficiently close to zero, $\text{sign}(P_{n+1}(x)) = -1$. On the other hand, $\text{sign}(P_{n+1}(\beta_1)) = -\text{sign}(P_{n+1}(-1)) = (-1)^n$, $\text{sign}(P_{n+1}(\beta_i)) = (-1)^{n+i-1}$, and $\text{sign}(P_{n+1}(\beta_{n-1})) = 1$. Therefore $P_{n+1}(x)$ has a root in $(\beta_{n-1}, 0)$. \square

References

- [1] H.D. Becker, Solution to problem E 461, *Amer. Math. Monthly*, **48**(1941), 701–702.
- [2] E.R. Canfield, Central and local limit theorems for the coefficients of polynomials of binomial type, *J. Combin. Theory Ser. A* **23**(1977), no. 3, 275–290.
- [3] E.R. Canfield, Engel's inequality for Bell numbers, *J. Comb. Theory A* **72**(1995), 184–187.
- [4] E.R. Canfield, bellMoser.pdf, 6 pages manuscript.
- [5] E.R. Canfield, L.H. Harper, A simplified guide to large antichains in the partition lattice, *Congr. Numer.* **100**(1994), 81–88.
- [6] L. Clark, Central and local limit theorems for excedances by conjugacy class and by derangement, *Integers* **2**(2002), Paper A3, 9 pp. (electronic).
- [7] R. Durrett, *Probability: Theory and Examples*, Wadsworth and Brooks/Cole, Pacific Grove, CA, 1991.
- [8] P.L. Erdős, L.A. Székely, Applications of antilexicographic order I: An enumerative theory of trees, *Adv. Appl. Math.* **10**(1989), 488–496.

- [9] P. Flajolet, A problem in statistical classification theory, <http://algo.inria.fr/libraries/autocomb/schroeder-html/schroeder.html>
- [10] J. Felsenstein, The number of evolutionary trees, *Syst. Zool.* **27**(1)(1978), 27–33. Corrigendum *Syst. Zool.* **30**(1981), 122.
- [11] J. Felsenstein, *Inferring Phylogenies*, Sinauer Associates, Sunderland, Massachusetts, 2004.
- [12] L.R. Foulds, R.W. Robinson, Enumeration of phylogenetic trees without points of degree two. *Ars Combin.* **17**(1984), A, 169–183.
- [13] L.H. Harper, Stirling behaviour is asymptotically normal, *Ann. Math. Stat.* **38**(1967), 410–414.
- [14] E.H. Lieb, Concavity properties and a generating function for Stirling numbers, *J. Comb. Theory* **5**(1968), 203–206.
- [15] L. Moser, M. Wyman, An asymptotic formula for the Bell numbers, *Trans. Roy. Soc. Canada III* **49**(1955), 49–53.
- [16] B. Salvy, J. Shackell, Asymptotics of the Stirling numbers of the second kind, *Studies in Automatic Combinatorics II* (1997). Published electronically.
- [17] E. Schroeder, Vier combinatorische Probleme, *Z. f. Math. Phys.* **15**(1870), 361–376.
- [18] N.J.A. Sloane, *The On-Line Encyclopedia of Integer Sequences* <http://www.research.att.com/~njas/sequences/>
- [19] <http://www.math.sc.edu/~szekely/Aprilattemptformal.pdf>
- [20] <http://www.math.sc.edu/~szekely/copykiserletformal.pdf>