TREE HEIGHT AND THE ASYMPTOTIC MEAN OF THE COLIJN–PLAZZOTTA RANK OF UNLABELED BINARY ROOTED TREES

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Abstract. The Colijn–Plazzotta ranking is a bijective encoding of the unlabeled binary rooted trees with positive integers. We show that the rank $f(t)$ of a tree t is closely related to its height h, the maximal path length from a leaf to the root. We consider the rank $f(\tau_n)$ of a random n-leaf tree τ_n under each of three models: (i) uniformly random unlabeled unordered binary rooted trees, or unlabeled topologies; (ii) uniformly random leaf-labeled binary trees, or labeled topologies under the uniform model; and (iii) random binary search trees, or labeled topologies under the Yule–Harding model. Relying on the close relationship between tree rank and tree height, we obtain results concerning the asymptotic properties of $\log\log f(\tau_n)$. In particular, we find $\mathbb{E}\{\log_2 \log f(\tau_n)\} \sim 2\sqrt{\pi n}$ for uniformly random unlabeled ordered binary rooted trees and uniformly random leaf-labeled binary trees, and for a constant $\alpha \approx 4.31107$, $\mathbb{E}\{\log_2 \log f(\tau_n)\} \sim \alpha \log n$ for leaf-labeled binary trees under the Yule–Harding model. We show that the mean of $f(\tau_n)$ itself under the three models is largely determined by the rank c_{n-1} of the highest-ranked tree—the caterpillar—obtaining an asymptotic relationship with $\pi_n c_{n-1}$, where π_n is a model-specific function of n. The results resolve open problems, providing a new class of results on an encoding useful in mathematical phylogenetics.

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1. Introduction

The Colijn–Plazzotta rank $f(t)$ of a binary rooted tree t is defined recursively as follows [7]: if $\ell(t)$ and $r(t)$ are the left and right subtree, respectively, arranged in such a way that $f\big(\ell(t)\big) \geq f\big(r(t)\big)$, then

$$f(t) = \frac{f\big(\ell(t)\big)\,\big(f(\ell(t)) - 1\big)}{2} + 1 + f\big(r(t)\big).$$

The rank 1 is assigned to a tree with a single leaf.

In the study of evolutionary trees, statistical summaries of trees are often used for characterizing the outcomes of evolutionary models and for statistical inference of the processes that have given rise to the trees [14]. Colijn–Plazzotta rank, or *CP rank*, has been used as a summary of tree shape in empirical scenarios in which trees of biological relationships are unconcerned with leaf labels, such as in examples with trees of sequences from the same pathogenic organism [7].

Informally, for a fixed number of leaves, the CP rank is lowest for balanced trees and greatest for unbalanced trees. It has therefore been proposed as a measure of tree balance [14, 26]. In a compilation of mathematical results for tree balance indices that capture many different features of rooted trees, Fischer et al. [14] have listed a set of basic properties that are of interest for any balance index. Among these are the minimal and maximal values of the index across all trees with a fixed number of leaves, and the mean and variance of the index under the two most frequently used probabilistic models in mathematical phylogenetics. One is the uniform model, also sometimes known as the proportional-to-distinguishable-arrangements or PDA model, which assigns equal probability to all binary rooted labeled trees with a fixed number of leaves. The other is the Yule–Harding model, also sometimes known as the equal-rates Markov or ERM model or simply as the Yule model, in which, conditional on the number of leaves, the probability of a binary rooted labeled tree is proportional to the number of sequences of bifurcations that can give rise to the tree. The mathematical properties of balance indices assist in characterizing the way that balance indices relate to one another and how they perform in empirical settings.

The trees of minimal and maximal CP rank for a fixed number of leaves have been characterized [26], and indeed the asymptotic CP ranks of these trees in terms of the number of leaves have also been obtained [11, 26]. The mean and variance under the uniform and Yule–Harding models have been listed as open problems [14, p. 243].

We show here that the asymptotic mean and variance under the Yule–Harding model can be obtained by a connection between this model in the phylogenetics setting and the nearly equivalent formulation of random binary search trees in computer science. First, we show that the order of magnitude of the CP rank of a tree is determined by the height of the tree, the greatest distance from the root to a leaf. By connecting the CP rank to tree height and in turn to probabilistic results for the height, we obtain distributional properties of the CP rank under the Yule–Harding model. We also obtain related results on the closely related uniform model on labeled binary rooted trees and the uniform model on *un*labeled binary rooted trees.

2. TREE HEIGHT AND THE COLIJN–PLAZZOTTA RANK

We consider all trees to be binary and rooted. The *height* of a tree is the maximal path length in edges from the root to a leaf. Two special families of binary trees with n leaves play a key role in our analysis: the caterpillars, and the pseudocaterpillars (Figure 1). In a *caterpillar* with n leaves, $n \geq 1$, every non-leaf has at least one leaf child. This condition forces each caterpillar to consist of a chain of $n-1$ internal (i.e. non-leaf) nodes to which a layer of external nodes is added. The *pseudocaterpillars* [25] (or *4-pseudocaterpillars* in the terminology of [4]) can be constructed as follows for $n \geq 4$: start with a chain of $n-3$ internal nodes. Give the bottom node in the chain two children, and finally, complete the tree by adding a layer of n external nodes. Caterpillars have height $n-1$, and pseudocaterpillars have height $n-2$.

Among binary rooted trees with a fixed number of leaves, Rosenberg [26, Corollary 10] found that the tree with the largest CP rank was the caterpillar. The CP rank of the caterpillar tree with n leaves can be computed recursively via a sequence termed b_n by [26, Theorem 9]. It is convenient to shift the index of the sequence by 1 so that here, we will use c_k to correspond to the CP rank of the caterpillar with height

k and $k+1$ leaves. The sequence c_k begins 1, 2, 3, 5, 12, 68, 2280 starting at $k = 0$ (matching OEIS A108225 [22] for $k \geq 1$).

Lemma 1. *Let the sequence* c_k *be defined by* $c_0 = 1$ *and* $c_{k+1} = c_k(c_k - 1)/2 + 2$ *for* $k \geq 0$. *For every tree* t *of height* h, *we have*

$$c_h \leq f(t) < c_{h+1}.$$

Proof. The proof proceeds by induction on h. For $h = 0$, the tree consists of a single leaf, and we have $1 = c_0 = f(t) < c_1 = 2$. Thus, the statement holds in this case, and we can proceed with the induction step.

For a tree t of height h, suppose $h_\ell < h$ and $h_r < h$ are the heights of subtrees $\ell(t)$ and $r(t)$, respectively. From the induction hypothesis for trees of height less than h and the left–right arrangement so that $f\big(\ell(t)\big) \geq f\big(r(t)\big)$, it follows that

$$c_{h_r} \leq f(r(t)) \leq f(\ell(t)) < c_{h_\ell+1}.$$

The sequence c_k is increasing [26, Lemma 8], so that $h_r < h_\ell + 1$, and hence, $h_r \leq h_\ell$.

Because $h = \max(h_\ell, h_r) + 1$, it follows that $h_\ell = h - 1$. Thus, we have, again by the induction hypothesis,

$$\begin{aligned} f(t) &= \frac{f\big(\ell(t)\big)\,\big(f\big(\ell(t)\big) - 1\big)}{2} + 1 + f\big(r(t)\big) \\ &\geq \frac{f\big(\ell(t)\big)\,\big(f\big(\ell(t)\big) - 1\big)}{2} + 1 + 1 \\ &\geq \frac{c_{h-1}(c_{h-1} - 1)}{2} + 2 \\ &= c_h, \end{aligned}$$

which proves the lower bound. On the other hand,

$$\begin{aligned} f(t) &= \frac{f\big(\ell(t)\big)\,\big(f(\ell(t)) - 1\big)}{2} + 1 + f\big(r(t)\big) \\ &\leq \frac{f\big(\ell(t)\big)\,\big(f(\ell(t)) - 1\big)}{2} + 1 + f\big(\ell(t)\big) \\ &= \frac{f\big(\ell(t)\big)\,\big(f\big(\ell(t)\big) + 1\big)}{2} + 1 \\ &\leq \frac{(c_h - 1)c_h}{2} + 1 \\ &= c_{h+1} - 1, \end{aligned}$$

proving the upper bound. This completes the induction. □

We conclude that the behavior of the height is to a great extent responsible for the behavior of the Colijn–Plazzotta rank of a tree. Indeed, because the CP rank is bijective with the positive integers [26, Proposition 2], the lemma implies that as the positive integers are traversed, for each $h \geq 0$, the ranking proceeds through trees with height h, then proceeds to those with height $h+1$, and so on. We immediately obtain the following corollaries (which are well known, see [19]).

Corollary 2. *For $h \geq 0$, the number of unlabeled binary rooted trees with height at most h is $c_{h+1} - 1$.*

Corollary 3. *For $h \geq 0$, the number of unlabeled binary rooted trees with height exactly h is $c_{h+1} - c_h$.*

The sequence $c_{h+1} - 1$ begins at $h = 0$ with values 1, 2, 4, 11, 67, 2279 (OEIS A006894 [22]). The sequence $c_{h+1} - c_h$ begins at $h = 0$ with values 1, 1, 2, 7, 56, 2212 (OEIS A002658 [22]).

According to [26, Corollary 14], $c_k \sim 2\gamma^{2^k}$ for a constant $\gamma \approx 1.11625$ as $k \to \infty$; note that $\gamma = \beta^2$ for the constant β in [26], owing to the shift by 1 in c_k relative to the indexing in [26]. We immediately obtain the following result.

Corollary 4. *Uniformly over all trees t with height h, we have,*

$$2^h + O(1) \leq \log_\gamma f(t) \leq 2^{h+1} + O(1),$$

and thus, for $h > 0$,

$$\log_2 \log_\gamma f(t) = \log_2 \log f(t) + O(1) = h + O(1).$$

In other words, the difference $|\log_2 \log_\gamma f(t) - h|$ is bounded by a universal constant.

We now analyze the behavior of the CP rank of random trees, which is mainly determined by the height. Indeed, we proceed by making use of extensive probabilistic results available on tree height under different sets of assumptions.

3. UNIFORMLY RANDOM UNLABELED BINARY TREES

Consider an unlabeled binary rooted tree on n leaves. Each node possesses either 0 offspring (leaves) or 2 offspring (internal nodes). Note that binary trees in which each node possesses either 0 or 2 (and not 1) offspring are sometimes termed *full* binary trees; here, all binary trees are "full" except where specified. A distinction exists between binary trees in which the left–right order of the children matters (*ordered* binary trees), and those in which the order is irrelevant (*unordered* binary trees, or *unlabeled topologies* in the terminology of mathematical phylogenetics, or *Otter trees* after [23]).

Let τ_n be a uniformly random ordered binary tree on $n \geq 1$ leaves, also called a random *Catalan tree* because the number of such trees is

$$k_{n-1} = \frac{1}{n}\binom{2n-2}{n-1},$$

where k_n is the n-th Catalan number [29, Exercise 5]. Catalan trees, viewed as ordered binary trees with n leaves, in which each node has 0 or 2 offspring, can be placed in bijection with trees with $n-1$ nodes in which the left–right order matters and each node has 0, 2, *or 1* offspring. For the bijection, we consider the latter type of tree, treating its $n-1$ nodes as internal nodes, and add descendant leaves so that each node that started with 0 or 1 offspring now has 2 offspring. Catalan trees are an example of a *simply generated family of trees*, and the random Catalan tree is also a special case of a *conditioned Galton–Watson tree*, with an offspring distribution whose support is $\{0, 2\}$. See, for example, [27, p. 224] and [13, Section 1.2.7]. We denote the CP rank of a random Catalan tree by C_n (C for Catalan).

Let τ'_n be a uniformly random unordered binary tree, a uniformly random Otter tree. The number of such trees can be calculated recursively. The exact value u_n (Wedderburn–Etherington number, OEIS A001190 [22]) for the number of such trees on n leaves follows

$$u_n = \begin{cases} 1, & n = 1, \\ \sum_{j=1}^{(n-1)/2} u_j u_{n-j}, & \text{odd } n \geq 3, \\ \left(\sum_{j=1}^{n/2-1} u_j u_{n-j} \right) + \frac{u_{n/2}(u_{n/2}+1)}{2}, & \text{even } n \geq 2. \end{cases} \tag{1}$$

The asymptotic approximation follows [20, 23]

$$u_n \sim \big(1 + o(1)\big) \frac{1}{\kappa n^{3/2} \rho^n}, \tag{2}$$

where $\kappa \approx 3.13699$ and $\rho \approx 0.40270$. The CP rank of a random Otter tree is denoted by O_n (O for Otter).

To understand Theorem 5, we define a *theta random variable* as a random variable with distribution function [9]

$$F(x) = \frac{4\pi^{5/2}}{x^3} \sum_{j=1}^{\infty} j^2 e^{-\pi^2 j^2 / x^2} = \sum_{j=-\infty}^{\infty} (1 - 2j^2 x^2) e^{-j^2 x^2} \ , x > 0. \tag{3}$$

CP rank is defined for unordered binary trees. To extend the CP rank to ordered binary trees, we compute the CP rank of the unordered binary tree associated with an ordered binary tree.

Theorem 5. *(i) Let τ_n be a uniformly random unlabeled binary tree with n leaves, with CP rank $C_n = f(\tau_n)$. Then*

$$\mathbb{E}\{\log_2 \log C_n\} \sim 2\sqrt{\pi n},$$

and

$$\frac{\log_2 \log C_n}{2\sqrt{n}}$$

converges in distribution to a theta random variable as defined by (3).

(ii) Let τ'_n be a uniformly random unlabeled unordered binary tree with n leaves, with CP rank $O_n = f(\tau'_n)$. Then, with κ as in (2)*,*

$$\mathbb{E}\{\log_2 \log O_n\} \sim \kappa\sqrt{n},$$

and

$$\frac{\log_2 \log O_n}{\kappa\sqrt{n/\pi}}$$

converges in distribution to a theta random variable as defined by (3)*.*

Proof. (i) The statement on τ_n is a consequence of a result of Flajolet and Odlyzko [15, Theorem B] about the height H_n of τ_n: $\mathbb{E}\{H_n\}/\sqrt{n} \to 2\sqrt{\pi}$ as $n \to \infty$, and $H_n/(2\sqrt{n})$ tends in distribution to a theta random variable. By Corollary 4, the difference $|\log_2 \log C_n - H_n|$ is (deterministically, thus almost surely) bounded by a universal constant, so that

$$\frac{\log_2 \log C_n - H_n}{2\sqrt{n}}$$

is $O(n^{-1/2})$; for any sequence of random trees of increasing size, this quantity goes to 0 (almost sure convergence, and hence, convergence in probability). The statement on the expected value now follows from the linearity of expectation and the statement on convergence in distribution follows from Slutsky's theorem applied to the convergence in distribution of $H_n/(2\sqrt{n})$ and the convergence in probability to 0 of $(\log_2 \log C_n - H_n)/(2\sqrt{n})$.

(ii) The statement on τ'_n follows in the same fashion from the results of Broutin and Flajolet ([5, Theorem 1 and Theorem 5], [6, Theorem 1 and Theorem 3]) on the height of unlabeled unordered binary trees. These state that the height H'_n of a random unlabeled unordered binary tree with n leaves satisfies $\mathbb{E}\{H'_n\}/\sqrt{n} \to \kappa$, and that $H'_n/(\kappa\sqrt{n/\pi})$ tends in distribution to a theta random variable. We remark here that our notation differs slightly from Broutin and Flajolet [6]: our constant $\kappa \approx 3.13699$ corresponds to the constant denoted $2\sqrt{\pi}/\lambda$ in [6], and our distribution function $F(x)$ in (3) is $1 - \Theta(2x)$ in the notation of Broutin and Flajolet. □

4. Uniformly random leaf-labeled binary trees

A leaf-labeled binary tree with n leaves is a binary tree in which the leaves are bijectively labeled from 1 to n, and in which each internal node has two children. The children are unordered. Such trees are also called *labeled topologies* or *cladograms*.

We consider a uniformly random cladogram τ_n. The number of such trees is

$$(2n-3)\cdot(2n-5)\cdots 3\cdot 1 = \frac{1}{2^{n-1}}\,\frac{(2n-2)!}{(n-1)!}, \tag{4}$$

all of which are equally likely under this model of randomness (OEIS A001147 [22]). The CP rank of a random cladogram is denoted by L_n (L for labeled).

A model of uniformly random cladograms is a special case of more general models on the cladograms, such as Ford's alpha-splitting model [16, 17] and Aldous's beta-splitting model [1, 3]. In particular, Aldous [1, Proposition 4, $\beta = -\frac{3}{2}$ case] showed that the expected height of a random cladogram satisfies

$$\mathbb{E}\left\{H_n\right\} \sim 2\sqrt{\pi n}.$$

It is worth pointing out that this result (including the constant $2\sqrt{\pi}$) is the same as for uniformly random unlabeled ordered binary trees (compare to Theorem 5i). This is no coincidence: for every unlabeled ordered binary tree on n leaves, there are $n!$ possibilities to label the leaves and turn it into a leaf-labeled ordered binary tree. Likewise, precisely 2^{n-1} possibilities turn a labeled unordered binary tree on n leaves into a labeled ordered binary tree (by switching the order of the children at the internal nodes). For this reason, the distribution of the height and any other parameters that do not depend on labels or order is the same for three uniform models: unlabeled ordered, labeled unordered, and labeled ordered binary trees [10, Section 3.1]. In particular, the following result is equivalent to part (i) of Theorem 5.

Theorem 6. *Let τ_n be a uniformly random leaf-labeled binary tree with n leaves, with CP rank $L_n = f(\tau_n)$. Then*

$$\mathbb{E}\{\log_2 \log L_n\} \sim 2\sqrt{\pi n},$$

and

$$\frac{\log_2 \log L_n}{2\sqrt{n}}$$

converges to a theta distribution.

Aldous's beta-splitting model for random binary trees has a shape parameter $\beta \in [-2, \infty]$, encompassing a limiting unbalanced model ($\beta = -2$), a limiting balanced model ($\beta = \infty$), the Yule model ($\beta = 0$), and the uniform model in Theorem 6 ($\beta = -\frac{3}{2}$). Generally, in [1, Proposition 4], Aldous proved the following results on the height H_n:

- For $\beta > -1$, the ratio $H_n / \log n$ tends in probability and in expectation to a constant $g(\beta)$. There is no explicit expression for this constant, but numerical values can be determined from an implicit equation given in [1, Proposition 4].

  To mention some examples, $g(\infty) = 1/\log 2 \approx 1.44270$, and we obtain $g(1) \approx 3.19258$, $g(0) \approx 4.31107$, and $g(-\frac{1}{2}) \approx 6.38090$ from the implicit equation (note that [1] only gives two digits each).

  The case $\beta = 0$ corresponds to the Yule model (see Section 5 below for more information). For $\beta = \infty$, all internal nodes split their subtrees (almost) precisely in half: the difference of the subtree sizes is at most 1.
- For $\beta = -1$, $\mathbb{E}\{H_n\} \geq \big(6/\pi^2 + o(1)\big)(\log n)^2$ Aldous's proposition did not report a result for $\mathbb{E}\{H_n\}$ with $\beta = -1$, but this inequality follows quickly from Aldous's results reported in the proposition for related quantities. Recently, Aldous and Pittel [2, Theorem 1.5] showed that $H_n \leq (\gamma + \epsilon)(\log n)^2$ with probability approaching 1 with increasing n, where $\epsilon > 0$ and $\gamma \approx 42.9$.
- For $\beta \in (-2, -1)$, $n^{1+\beta}\mathbb{E}\{H_n\} \to g(\beta)$, and $n^{1+\beta} H_n$ has a non-degenerate limit distribution.

These results on tree height for cladograms under the beta-splitting model directly impact the Colijn–Plazzotta rank. For example, for $\beta \in (-2, -1)$, we have for Aldous's beta-splitting tree τ_n with n leaves

$$\mathbb{E}\{\log_2 \log f(\tau_n)\} \sim \frac{g(\beta)}{n^{1+\beta}}.$$

5. YULE–HARDING TREES, RANDOM BINARY SEARCH TREES

Among the probability distributions that could be placed on the leaf-labeled binary trees with n leaves, perhaps the most frequently considered, along with the uniform distribution of Section 4, is the $\beta = 0$ case of the beta-splitting model. This model corresponds to the random binary search trees, which are identical to Yule or Yule–Harding trees in phylogenetics [18], except for the convention that random binary search trees are typically indexed by the number of internal nodes and Yule–Harding trees are indexed by the number of leaves. We index trees by the number of leaves, considering random binary search trees in which all internal nodes have two children so that the total number of internal nodes is $n-1$ when the number of leaves is n.

To be precise, we start with a standard random binary search tree on $n-1$ (internal) nodes and attach a layer of n external nodes, i.e., we give a second child to all (internal) nodes having one child, and give two children to all leaves. The random CP rank of a tree under this model is denoted by S_n (S for $\underline{\text{s}}$earch tree).

For these trees, the height H_n satisfies [8, Theorem 5.1]

$$\frac{H_n}{\log n} \xrightarrow{p} \alpha,$$

where $\alpha \approx 4.31107$ is the unique solution in $(2, \infty)$ of the equation

$$\alpha \log(2e/\alpha) = 1.$$

Setting

$$\beta = \frac{3\alpha}{2\alpha - 2} \approx 1.95303,$$

Reed [24] and Drmota [12] showed that $H_n - \alpha \log n + \beta \log\log n$ is tight, i.e.,

$$\limsup_{x \uparrow \infty} \Big[\sup_n \mathbb{P}\left\{ |H_n - \alpha \log n + \beta \log\log n| \geq x \right\} \Big] = 0. \tag{5}$$

One way to see this result is as follows: Reed [24, Theorem 1] states that

$$\mathbb{E}\{H_n - \alpha \log n + \beta \log\log n\} = O(1)$$

and

$$\mathbb{V}\{H_n - \alpha \log n + \beta \log\log n\} = \mathbb{V}\{H_n\} = O(1),$$

from which tightness follows by a standard application of the Chebyshev inequality. Alternatively, one can use Lemmas 8 and 10 of [24], which provide explicit tail bounds.

Theorem 7. *Let τ_n be a random leaf-labeled binary tree with n leaves following the Yule–Harding distribution, with CP rank $S_n = f(\tau_n)$. Then*

$$\mathbb{E}\{\log_2 \log S_n\} \sim \alpha \log n,$$

and

$$\frac{\log_2 \log S_n}{\log n} \xrightarrow{p} \alpha.$$

Proof. The proof is similar to Theorem 5. By Corollary 4, the difference between $\log_2 \log S_n$ and the height H_n is bounded, so

$$\frac{\log_2 \log S_n - H_n}{\log n}$$

goes to 0 (almost surely, thus also in probability). The second part of the result follows immediately via Slutsky's theorem from the fact that $H_n/\log n \xrightarrow{p} \alpha$; the first part follows from the fact that $\mathbb{E}\{H_n/\log n\} \to \alpha$ as $n \to \infty$ [8]. □

Theorem 8. *Let τ_n be a random leaf-labeled binary tree with n leaves following the Yule–Harding distribution, with CP rank $S_n = f(\tau_n)$. Then*

$$\frac{(\log n)^{\beta \log 2} \log S_n}{n^{\alpha \log 2}}$$

is a tight sequence of random variables.

Proof. By Corollary 4, there exists an absolute positive constant K such that $K \cdot 2^{H_n} \geq \log S_n$. Thus,

$$\frac{(\log n)^{\beta \log 2} \log S_n}{n^{\alpha \log 2}} \geq x$$

implies

$$2^{H_n} \geq \frac{x n^{\alpha \log 2}}{K (\log n)^{\beta \log 2}},$$

or

$$H_n - \alpha \log n + \beta \log \log n \geq \frac{\log(x/K)}{\log 2}.$$

This means that

$$\begin{aligned}\mathbb{P}\Big\{\Big|\frac{(\log n)^{\beta\log 2}\log S_n}{n^{\alpha\log 2}}\Big|\geq x\Big\} &= \mathbb{P}\Big\{\frac{(\log n)^{\beta\log 2}\log S_n}{n^{\alpha\log 2}}\geq x\Big\}\\ &\leq \mathbb{P}\Big\{H_n-\alpha\log n+\beta\log\log n\geq\frac{\log(x/K)}{\log 2}\Big\}\\ &\leq \mathbb{P}\Big\{|H_n-\alpha\log n+\beta\log\log n|\geq\frac{\log(x/K)}{\log 2}\Big\}.\end{aligned}$$

By (5), this expression goes to 0 if we take $\sup_n$ and then $\limsup_{x\uparrow\infty}$, showing that the sequence is indeed tight. □

6. MEAN AND VARIANCE OF THE COLIJN–PLAZZOTTA RANK

Sections 3–5 focus on properties of the distribution of $\log\log f(\tau_n)$ under various models of randomness; in this section, we focus on the distribution of the random CP rank $f(\tau_n)$ itself. In particular, we study the first-order asymptotics of the mean and variance of the Colijn–Plazzotta rank under the models of randomness from Sections 3–5, investigating C_n, O_n, L_n, and S_n. As pointed out in Section 4, the models of uniformly random unlabeled ordered binary trees (Catalan trees) and uniformly random labeled unordered binary trees are equivalent for our purposes, so that the distributions of C_n and L_n are the same.

We give a general theorem on the mean and variance of the Colijn–Plazzotta rank applicable to all random tree models specifying a certain condition. We then obtain first-order asymptotics for the means and variances of C_n, O_n, L_n and S_n as simple corollaries. The desired means and variances are determined mainly by the extreme cases for Colijn–Plazzotta ranks.

Lemma 9. *(i) Among all unlabeled binary rooted trees with n leaves, $n\geq 1$, the Colijn–Plazzotta rank is maximized by the caterpillar. (ii) Among all unlabeled binary rooted trees with n leaves and height $n-2$ or less, $n\geq 4$, the Colijn–Plazzotta rank is maximized by the pseudocaterpillar.*

Proof. (i) This result was proven in Corollary 20 of [26]. (ii) This result follows by induction and Lemma 1. For $n=4$, the pseudocaterpillar is the only tree with height at most $n-2=2$. Suppose for induction that for all k, $4 \leq k \leq n-1$, the pseudocaterpillar has the maximal Colijn–Plazzotta rank among trees with k leaves and height $k-2$.

Among trees t with n leaves and height at most $n-2$, by definition of the Colijn–Plazzotta rank, the rank $f(t)$ is maximized by choosing its left subtree $\ell(t)$ to have $f\big(\ell(t)\big)$ as large as possible. The left subtree $\ell(t)$ has at most $n-1$ leaves and height at most $n-3$, so that the inductive hypothesis applies: $\ell(t)$ is the pseudocaterpillar with $n-1$ leaves, the right subtree $r(t)$ is a single leaf, and t is the pseudocaterpillar with n leaves. □

For the following theorem, we recall Rosenberg's [26] sequence for the maximal Colijn–Plazzotta rank c_h among trees with height $h \geq 0$ and $h+1$ leaves: $c_0 = 1$, and

$$c_{h+1} = \binom{c_h}{2} + 2,\ h \geq 0. \tag{6}$$

Equivalently, c_h is the Colijn–Plazzotta rank of a caterpillar of height h. Recall that $c_2 = 3$, $c_3 = 5$, $c_4 = 12$, and $c_5 = 68$.

We also let d_h be the corresponding rank of a pseudocaterpillar of height h. Then $d_2 = 4$, and

$$d_{h+1} = \binom{d_h}{2} + 2,\ h \geq 2. \tag{7}$$

The sequences c_h and d_h obey identical recursions, only with different starting points. Sequence d_h begins with $d_2 = 4$, $d_3 = 8$, $d_4 = 30$, and $d_5 = 437$.

Theorem 10. *For a given probability model for random binary rooted trees T_n with n leaves, let*

$$\pi_n = \mathbb{P}\left\{T_n \textit{ is a caterpillar}\right\},$$

and let P_n be the Colijn–Plazzotta rank of T_n. If $\pi_n = o(1)$ and

$$\log(1/\pi_n) = o(2^n), \tag{8}$$

then

$$\begin{aligned}\mathbb{E}\left\{P_n\right\} &\sim \pi_n c_{n-1},\\ \mathbb{V}\left\{P_n\right\} \sim \mathbb{E}\left\{P_n^2\right\} &\sim \pi_n c_{n-1}^2.\end{aligned}$$

The idea of the result is that under the conditions specified, the CP rank of the n-leaf pseudocaterpillar—the tree of second-largest CP rank among those with n leaves—grows sufficiently slowly that the CP ranks of this tree and all other non-caterpillar trees are negligible in relation to that of the n-leaf caterpillar. The mean and variance of the CP rank of a random tree then depend only on the probability that a tree is a caterpillar and the CP rank of the caterpillar.

Proof. We distinguish two events. If T_n is a caterpillar of height $n-1$, then $P_n = c_{n-1}$. Otherwise, if T_n is some other tree, then its CP rank P_n has upper bound d_{n-2}, the CP rank of a pseudocaterpillar of height $n-2$. These values yield the trivial bounds

$$\pi_n c_{n-1} \leq \mathbb{E}\left\{P_n\right\} \leq \pi_n c_{n-1} + d_{n-2}, \tag{9}$$

$$\pi_n c_{n-1}^2 \leq \mathbb{E}\left\{P_n^2\right\} \leq \pi_n c_{n-1}^2 + d_{n-2}^2. \tag{10}$$

By taking the ratio of (9) with $\pi_n c_{n-1}$, to verify $\mathbb{E}\left\{P_n\right\} \sim \pi_n c_{n-1}$, it suffices to show

$$\lim_{n\to\infty} \frac{d_{n-2}}{\pi_n c_{n-1}} = 0. \tag{11}$$

Similarly, because $d_{n-2} < c_{n-1}$ so that $(d_{n-2}/c_{n-1})^2 < d_{n-2}/c_{n-1}$, by taking the ratio of (10) and $\pi_n c_{n-1}^2$, verifying condition (11) suffices for verifying $\mathbb{V}\left\{P_n\right\} \sim \mathbb{E}\left\{P_n^2\right\} \sim \pi_n c_{n-1}^2$; we see first that $\mathbb{E}\left\{P_n^2\right\} \sim \pi_n c_{n-1}^2$, and then $\mathbb{V}\left\{P_n\right\} = \mathbb{E}\left\{P_n^2\right\} - \mathbb{E}\left\{P_n\right\}^2 \sim \mathbb{E}\left\{P_n^2\right\}$ follows by recalling that $\pi_n = o(1)$.

We will show that (8) implies (11). We first prove by induction that $d_{h-1} < 0.9^{2^{h-3}} c_h$ for all $h \geq 3$. This statement is readily verified for $h = 3$ and $h = 4$. Now assume that the inequality holds for some positive integer $h \geq 4$, and write $Q_h = 0.9^{-(2^{h-3})} > 1$, so that $c_h > Q_h d_{h-1}$. It follows from the recursions (6) and (7) that

$$\frac{d_h}{c_{h+1}} = \frac{d_{h-1}^2 - d_{h-1} + 4}{c_h^2 - c_h + 4} < \frac{d_{h-1}^2 - d_{h-1} + 4}{Q_h^2 d_{h-1}^2 - Q_h d_{h-1} + 4}$$

$$= \frac{1}{Q_h^2} - \frac{(Q_h - 1)(Q_h d_{h-1} - 4Q_h - 4)}{Q_h^2(Q_h^2 d_{h-1}^2 - Q_h d_{h-1} + 4)}.$$

The final fraction is positive since $Q_h > 1$ and $d_{h-1} \geq d_3 \geq 8$. Thus,

$$\frac{d_h}{c_{h+1}} < \frac{1}{Q_h^2} = 0.9^{2^{h-2}},$$

completing the induction.

It follows (for $n \geq 4$) that

$$\log \frac{d_{n-2}}{\pi_n c_{n-1}} \leq \log \left(\frac{1}{\pi_n} 0.9^{2^{n-4}} \right) = 2^{n-4} \log 0.9 - \log \pi_n = 2^{n-4} \log 0.9 + o(2^n)$$

by the assumption (8). Because this last expression goes to $-\infty$ as n increases without bound, we have verified (11). This completes the proof. □

The theorem finds that the asymptotic mean is simply the product of the CP rank of the caterpillar and the probability that a tree is a caterpillar. In all four types of random trees that we consider, we verify that π_n satisfies (8), so that the theorem applies. This verification amounts to demonstrating that caterpillars are sufficiently probable as n grows large; if π_n were to decrease too quickly, then the condition would not be satisfied.

The number of caterpillar cladograms is $n!/2$, so that for a random cladogram (and equivalently, for a random Catalan tree), (4) gives

$$\pi_n = \frac{n!}{2} \frac{1}{(2n-3)!!} = \frac{2^{n-2}}{\frac{1}{n}\binom{2n-2}{n-1}} \sim \frac{2^{n-2}}{\pi^{-1/2} n^{-3/2} 4^{n-1}} \sim \frac{n^{3/2}\sqrt{\pi}}{2^n}. \tag{12}$$

For a random Otter tree on n leaves, we have no simple explicit expression for π_n. However, we have the asymptotic probability from (2) that a random Otter tree is the unique caterpillar:

$$\pi_n = \frac{1}{u_n} \sim \kappa n^{3/2} \rho^n. \tag{13}$$

Finally, for a random binary search tree [28, p. 92],

$$\pi_n = \frac{n!}{2} \frac{1}{\frac{n!\,(n-1)!}{2^{n-1}}} = \frac{2^{n-2}}{(n-1)!} \sim \left(\frac{2e}{n}\right)^n \frac{\sqrt{n}}{4\sqrt{2\pi}}. \tag{14}$$

Verifying in (12), (13), and (14) that condition (8) is satisfied, we have shown the following theorem.

Theorem 11. *With π_n as in* (12), (13), *and* (14), *and with P_n corresponding to either C_n (the random Catalan tree), O_n (the random Otter tree), L_n (the random cladogram), or S_n (the random binary search tree), we have*

$$\mathbb{E}\left\{P_n\right\} \sim \pi_n c_{n-1},$$

$$\mathbb{V}\left\{P_n\right\} \sim \mathbb{E}\left\{P_n^2\right\} \sim \pi_n c_{n-1}^2.$$

7. Numerical computations

We informally examine the extent to which the asymptotic approximations for $\mathbb{E}\{\log_2 \log f(\tau_n)\}$, $\mathbb{E}\{f(\tau_n)\}$, and $\mathbb{V}\{f(\tau_n)\}$ agree with the exact values for small n. First, Tables 1 and 2 show the CP rank and the probabilities of all unlabeled unordered binary trees for $n = 1$ to 8 under each of three models: uniformly random unlabeled unordered trees, uniformly random leaf-labeled trees, and Yule–Harding leaf-labeled trees. The much larger CP rank for the caterpillar compared to the pseudocaterpillar (and all other trees) is already visible for $n = 8$.

Figure 2 plots the values of $\mathbb{E}\{\log_2 \log f(\tau_n)\}$, the mean height H_n, and the asymptotic approximation for $\mathbb{E}\{\log_2 \log f(\tau_n)\}$ under the three models. For each of the three models, we can observe similar shapes in plots for its three quantities. The values are greatest for the uniformly random leaf-labeled trees, with asymptotic approximation $2\sqrt{\pi n} \approx 3.54491\sqrt{n}$, followed by the uniformly random unlabeled unordered trees, with asymptotic approximation $3.13699\sqrt{n}$, and finally, the Yule–Harding leaf-labeled trees, with asymptotic approximation $4.31107 \log n$.

Figures 3 and 4 plot the exact mean and variance of $f(\tau_n)$ under the three models alongside the asymptotic approximation based on the contribution of the caterpillar tree, taking the $\log_2 \log$ of these quantities to produce a comparable scale to Figure 2. In the figure, we observe that even for quite small n, the exact mean and variance are closely approximated by the asymptotic $\pi_n c_{n-1}$. The mean and variance are greatest for the uniformly random leaf-labeled trees, for which $\pi_n \sim \sqrt{\pi}(n^{3/2})(0.5^n)$ (12), followed by the uniformly random unlabeled unordered trees, with asymptotic approximation $\pi_n \sim \kappa n^{3/2}\rho^n \approx 3.13699(n^{3/2})(0.40270^n)$ (13). For the Yule–Harding model, caterpillars are least probable (14).

8. Discussion

We have analyzed the Colijn–Plazzotta rank of rooted binary trees, showing that the rank of a tree is largely determined by its height. Indeed, the ranking proceeds through all trees of a given height h before moving on to trees of height $h+1$. We have also obtained asymptotic properties of the trees under three different models for selecting random trees, finding in particular the asymptotics of $\mathbb{E}\{\log_2 \log f(\tau_n)\}$ for random trees τ_n. The asymptotic mean and variance of the CP rank across trees with n leaves depend only on the probability and CP rank of the n-leaf caterpillar, as the product of the probability and the CP rank of the caterpillar grows faster than the next-highest rank. A summary of mathematical results appears in Table 3.

Numerical investigations clarify a pattern observable in the mathematical results, namely that the "uniform" model—uniformly random leaf-labeled trees—has CP ranks greater than the Yule–Harding model on leaf-labeled trees (Figures 2–4). This observation can be viewed as a consequence of the greater probability of the caterpillar shape in the uniform (12) than in the Yule–Harding model (14).

It has been suggested that CP rank can serve as a measure of tree balance and imbalance in empirical studies [14, 26]. We have found that as n grows, the CP rank of the caterpillar grows so fast that for both the uniform and Yule–Harding models on leaf-labeled trees, the mean CP rank across trees with n leaves is asymptotically determined by the contribution of the caterpillar. Hence, as a balance statistic beyond the smallest tree sizes, the use of CP rank $f(\tau)$ would amount primarily to distinguishing caterpillars from non-caterpillars. A potentially more suitable statistic is $\log_2 \log f(\tau)$, which places the CP ranks of different trees on a similar scale. Due to its extremely large values, the CP rank has been omitted from an empirical comparison of tree balance statistics [21]; we suggest that this problem could be resolved by including its double-logarithm in its place.

The results have been obtained by connecting studies of CP rank as a quantity of mathematical phylogenetics to the extensive literature on tree height in studies grounded in theoretical computer science. As has been demonstrated here, such applications of theoretical computer science results on tree properties have the potential to provide solutions to unsolved problems in mathematical phylogenetics.

Although we have obtained the asymptotics of the mean and variance of the CP rank under the uniform and Yule–Harding models—the two models for which the mean and variance were noted by [14] as open problems—we have not commented on the *exact* mean and variance. For practical applications of CP rank, an understanding of the asymptotics likely suffices, but we note that the precise determination of the mean and variance of the CP rank remains an open problem.

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DATA AVAILABILITY STATEMENT. The study has no associated data.

CONFLICT OF INTEREST STATEMENT. The authors declare that they have no conflict of interest.

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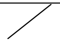
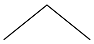
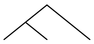
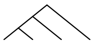
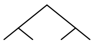
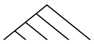
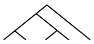
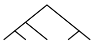
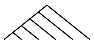
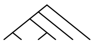
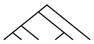
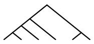
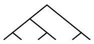
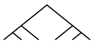
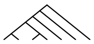
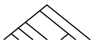
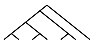
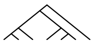
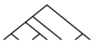
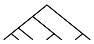
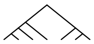
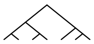
n	t_n	$f(t_n)$	Height	Model		
				Unlabeled uniform unordered	Leaf-labeled uniform	Leaf-labeled Yule–Harding
1		1	0	1	1	1
2		2	1	1	1	1
3		3	2	1	1	1
4		5	3	1/2	4/5	2/3
4		4	2	1/2	1/5	1/3
5		12	4	1/3	4/7	1/3
5		8	3	1/3	1/7	1/6
5		6	3	1/3	2/7	1/2
6		68	5	1/6	8/21	2/15
6		30	4	1/6	2/21	1/15
6		17	4	1/6	4/21	1/5
6		13	4	1/6	4/21	4/15
6		9	3	1/6	1/21	2/15
6		7	3	1/6	2/21	1/5
7		2280	6	1/11	8/33	2/45
7		437	5	1/11	2/33	1/45
7		138	5	1/11	4/33	1/15
7		80	5	1/11	4/33	4/45
7		38	4	1/11	1/33	2/45
7		23	4	1/11	2/33	1/15
7		69	5	1/11	4/33	1/9
7		31	4	1/11	1/33	1/18
7		18	4	1/11	2/33	1/6
7		14	4	1/11	4/33	2/9
7		10	3	1/11	1/33	1/9

TABLE 1. CP rank $f(t_n)$ and probability under three models for all unlabeled unordered binary trees t_n with n leaves, $1 \leq n \leq 7$. For unlabeled uniform unordered trees, the probability is the reciprocal of the number of such trees, the Wedderburn–Etherington number defined by (1). For leaf-labeled uniform trees, it is the ratio of $n!/2^{s(t_n)}$ (the number of ways of labeling shape t_n, where the number of symmetric nodes $s(t_n)$ is the number of internal nodes whose two descendant subtrees have the same unlabeled shape) and $(2n-3)!!$, the number of leaf-labeled trees with n leaves (4). For leaf-labeled Yule–Harding trees, it is the ratio of $[n!/2^{s(t_n)}][(n-1)!/\prod_{r=2}^{n}(r-1)^{d_r(t_n)}]$ and $n!(n-1)!/2^{n-1}$, where $d_r(t_n)$ is the number of internal nodes of t_n with r descendant leaves, $(n-1)!/\prod_{r=2}^{n}(r-1)^{d_r(t_n)}$ gives the number of *labeled histories* of a leaf-labeled tree (the number of sequences in which the tree can be produced by a sequence of bifurcations), and $n!(n-1)!/2^{n-1}$ is the total number of labeled histories for n labeled leaves.

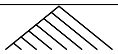
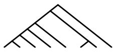
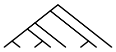
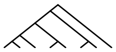
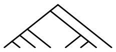
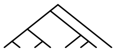
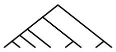
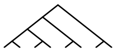
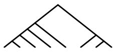
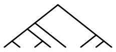
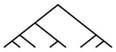
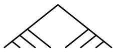
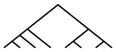
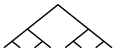
n	t_n	$f(t_n)$	Height	Model		
				Unlabeled uniform unordered	Leaf-labeled uniform	Leaf-labeled Yule–Harding
8		2598062	7	1/23	64/429	4/315
8		95268	6	1/23	16/429	2/315
8		9455	6	1/23	32/429	2/105
8		3162	6	1/23	32/429	8/315
8		705	5	1/23	8/429	4/315
8		255	5	1/23	16/429	2/105
8		2348	6	1/23	32/429	2/63
8		467	5	1/23	8/429	1/63
8		155	5	1/23	16/429	1/21
8		93	5	1/23	32/429	4/63
8		47	4	1/23	8/429	2/63
8		2281	6	1/23	32/429	4/105
8		438	5	1/23	8/429	2/105
8		139	5	1/23	16/429	2/35
8		81	5	1/23	16/429	8/105
8		39	4	1/23	4/429	4/105
8		24	4	1/23	8/429	2/35
8		70	5	1/23	32/429	2/21
8		32	4	1/23	8/429	1/21
8		19	4	1/23	16/429	1/7
8		16	4	1/23	16/429	4/63
8		15	4	1/23	8/429	4/63
8		11	3	1/23	1/429	1/63

TABLE 2. CP rank $f(t_n)$ and probability under three models for all unlabeled unordered binary trees t_n with n leaves, $n = 8$. The table design follows Table 1.

Property	Model		
	Unlabeled uniform unordered	Leaf-labeled uniform	Leaf-labeled Yule–Harding
$\mathbb{E}\{\log\log f(\tau_n)\}$	Theorem 5	Theorem 6	Theorem 7
$\log f(\tau_n)$	-	-	Theorem 8
$\mathbb{E}\{f(\tau_n)\}$	Theorem 10	Theorem 10	Theorem 10
$\mathbb{V}\{f(\tau_n)\}$	Theorem 10	Theorem 10	Theorem 10

TABLE 3. Summary of the main asymptotic results under three models. τ_n refers to a random tree with n leaves under the model, and $f(\tau_n)$ is the associated random CP rank. Properties of random trees are the same for uniformly random leaf-labeled unordered trees and for uniformly random unlabeled ordered trees.

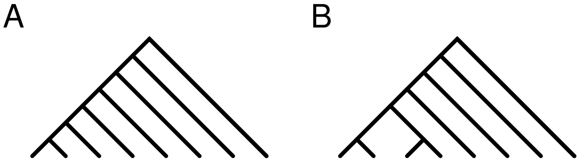


FIGURE 1. Caterpillar and pseudocaterpillar trees. (A) Caterpillar tree with $n = 8$ leaves. The height of the tree is $n - 1 = 7$. (B) Pseudocaterpillar tree with $n = 8$ leaves. The height of the tree is $n - 2 = 6$.

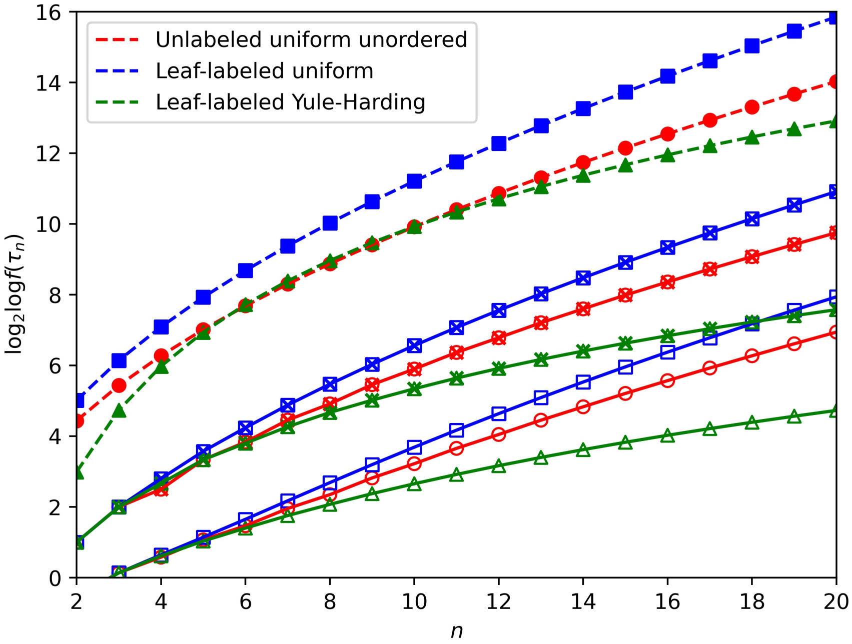


FIGURE 2. Expected value of the double logarithm of CP rank, $\mathbb{E}\{\log_2 \log f(\tau_n)\}$, under three models, for $n = 2$ to 20: uniformly random unlabeled unordered binary trees, uniformly random leaf-labeled binary trees, and Yule–Harding leaf-labeled binary trees. Exact values of $\mathbb{E}\{\log_2 \log f(\tau_n)\}$ (open symbols) appear alongside exact values of the expected tree height $\mathbb{E}\{H_n\}$ (open symbols superimposed with crosses) under the three models and the asymptotic expressions (closed symbols, dashed lines): $\kappa\sqrt{n}$ for unlabeled uniform unordered (Theorem 5ii), $2\sqrt{\pi n}$ for leaf-labeled uniform (Theorem 6), and $\alpha \log n$ for leaf-labeled Yule–Harding (Theorem 7). $\kappa \approx 3.13699$, $\alpha \approx 4.31107$.

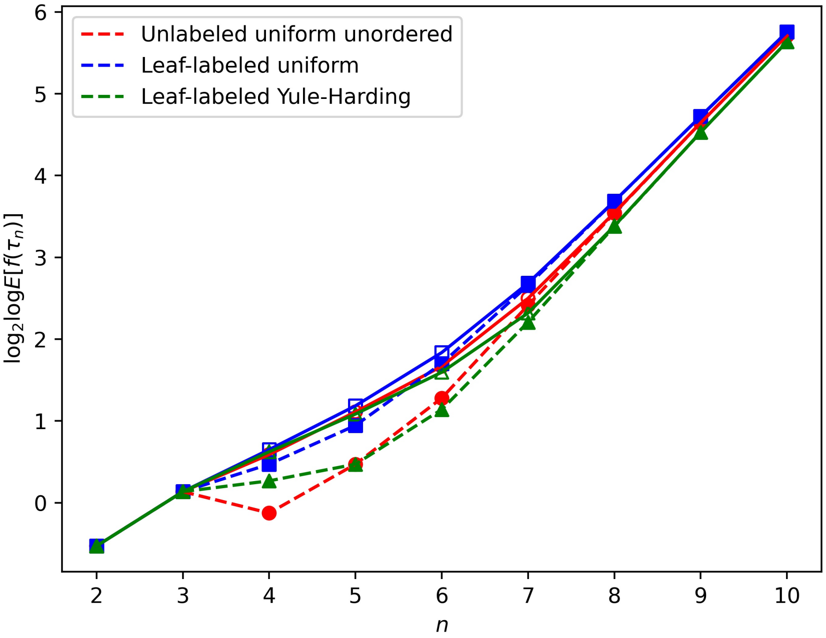


FIGURE 3. Expected value of the CP rank, $\mathbb{E}\{f(\tau_n)\}$, under three models, for $n = 2$ to 10: uniformly random unlabeled unordered binary trees, uniformly random leaf-labeled binary trees, and Yule–Harding leaf-labeled binary trees. Exact values of $\log_2 \log \mathbb{E}\{f(\tau_n)\}$ (open symbols) appear alongside asymptotic expressions $\log_2 \log(\pi_n c_{n-1})$ from Theorem 10 (closed symbols, dashed lines), where π_n follows (12) for leaf-labeled uniform and (14) for leaf-labeled Yule–Harding and c_{n-1} is the CP rank of the caterpillar with $n-1$ internal nodes and n leaves (6). For unlabeled uniform unordered, π_n is computed as the exact $1/u_n$, where u_n is the Wedderburn–Etherington number defined by (1).

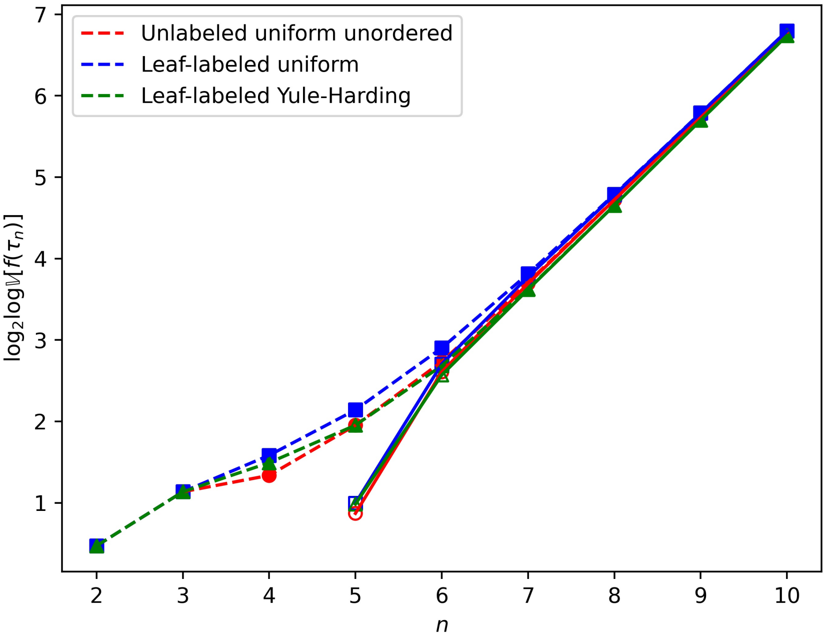


FIGURE 4. Variance of the CP rank, $\mathbb{E}\{f(\tau_n)\}$, under three models, for $n = 2$ to 10: uniformly random unlabeled unordered binary trees, uniformly random leaf-labeled binary trees, and Yule–Harding leaf-labeled binary trees. Exact values of $\log_2 \log \mathbb{V}\{f(\tau_n)\}$ (open symbols) appear alongside asymptotic expressions $\log_2 \log(\pi_n c_{n-1}^2)$ from Theorem 10 (closed symbols, dashed lines), where π_n follows (12) for leaf-labeled uniform and (14) for leaf-labeled Yule–Harding and c_{n-1} is the CP rank of the caterpillar with $n-1$ internal nodes and n leaves (6). For unlabeled uniform unordered, π_n is computed as the exact $1/u_n$, where u_n is the Wedderburn–Etherington number defined by (1).