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Squaring within the Colless index yields a better balance index

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Abstract

The Colless index for bifurcating phylogenetic trees, introduced by Colless \cite{Colless1973}, is defined as the sum, over all internal nodes $v$ of the tree, of the absolute value of the difference of the sizes of the clades defined by the children of $v$. It is one of the most popular phylogenetic balance indices, because, in addition to measuring the balance of a tree in a very simple and intuitive way, it turns out to be one of the most powerful and discriminating phylogenetic shape indices. But it has some drawbacks. On the one hand, although its minimum value is reached at the so-called maximally balanced trees, it is almost always reached also at trees that are not maximally balanced. On the other hand, its definition as a sum of absolute values of differences makes it difficult to study analytically its distribution under probabilistic models of bifurcating phylogenetic trees. In this paper we show that if we replace in its definition the absolute values of the differences of clade sizes by the squares of these differences, all these drawbacks are overcome and the resulting index is still more powerful and discriminating than the original Colless index.

\textit{Keywords:} Phylogenetic tree, Balance index, Colless index, Yule model, uniform model

1. Introduction

Evolutionary biology is concerned, among other major things, about understanding what forces influence speciation and extinction processes, and how they affect macroevolution \cite{Gavrilets2004}. In order to do so, there has been a natural interest in the development of techniques and measures whose goal is to assess the imprint of these forces in what has become the standard representation of
joint evolutionary histories of groups of species: phylogenetic trees [37, 44, 61]. There are two aspects of a phylogenetic tree that can expose such an imprint: its branch lengths —determined by the timing of speciation events—, and its shape, or topology —which, in turn, is determined by the differences in the diversification rates among clades [22, Chap. 33]. But, as it turns out, the accurate reconstruction of branch lengths associating, to a given phylogenetic tree, a robust timeline is not straightforward [19] while, on the other hand, phylogenetic reconstruction methods over the same empirical data tend to agree on the topology of the reconstructed tree [9, 32, 49]. Therefore, the shape of phylogenetic trees has become the focus of most of the studies performed on this topic, be it via the definition of indices quantifying topological features —see, for instance, [26, 44, 58] and the references on balance indices given below— or the frequency distribution of small rooted subtrees [40, 55, 57, 65].

In his 1922 paper, Yule [64] first observed that taxonomic trees have a tendency towards asymmetry, with most clades being small and only a few of them large at every taxonomic level. Thus, balance, understood as the propensity of the children of any given node to have the same number of descendant leaves, has become the most popular topological measure used to describe the topology of a phylogenetic tree. Therefore, per negationem, the imbalance of a phylogenetic tree gives a measure of the tendency of diversification events to occur mostly along specific lineages [45, 56]. Several such measures have been proposed, in order to quantify the balance (or, in many cases, the imbalance) of a phylogenetic tree, and they are referred to in the literature as balance indices. For example, see [13, 16, 24, 26, 36, 40, 42, 43, 53, 56] and the section “Measures of overall asymmetry” in [22] (pp. 562–563).

For instance, these indices have then been thoroughly used in order to test the validity evolutionary models [3, 7, 20, 36, 44, 63]; to assess possible biases in the distribution of shapes that are obtained through different phylogenetic tree reconstruction methods [14, 21, 33, 58, 59]; to compare tree shapes [4, 28, 34]; as a tool to discriminate between input parameters in phylogenetic tree simulations [46, 54]; or simply to describe phylogenies existing in the literature [12, 18, 41, 48].

Introduced in [13], the Colless index has become one of the most popular balance indices in the literature. Given a bifurcating tree $T$, it is defined as the sum, overall internal nodes $v$ in $T$, of the absolute value of the difference between the numbers of descendant leaves of the pair of children of $v$ (even so, there exists a recent extension to multifurcating trees, see [43]). Its popularity springs from several sources. First of all, its antiquity: it is one of the first balance indices found in the literature, dating back to 1982. Secondly, the way it measures the “global imbalance” by adding the “local imbalances” of each internal node in $T$ is fairly intuitive. Finally, it has been classified as one of the most powerful tree shape statistics in goodness-of-fit tests of probabilistic models of phylogenetic trees [1, 36, 38], as well as one of the most shape-discriminant balance indices [29].

Due to this popularity, the statistical properties of the Colless index under several probabilistic models have been thoroughly studied [3, 10, 25, 31] as well
as its maximum $[43]$ and minimum $[15]$ values. The characterization of this last value, as well as that of the trees attaining it, apart from recent turns out to be rather complex and fails to shed light on the intuitive concept of balance. Indeed, other balance indices, such as the total cophenetic index $[42]$ and the rooted quartet index $rQI$ $[16]$ classify as “most balanced” trees only those that are maximally balanced, in the sense that the imbalance of each internal node is either 0 or 1. Even though these trees are effectively considered to be “most balanced” by the Colless index, they are seldom the only ones being so considered.

In this manuscript, we introduce a modification of the Colless index that offers some benefits over the original definition, consisting in squaring the difference of the number of descendant leaves to each child of an internal node instead of considering its absolute value. On the one hand, we have been able to compute both its expected value and its variance under the Yule and uniform probabilistic models for phylogenetic trees. In contrast, notice that the expected value of the Colless index under the uniform model is still unknown in the literature. On the other hand, its maximum and minimum values are attained exactly at the caterpillars and the maximally balanced trees, respectively, and the proofs of these results are rather easy —more so when compared to those concerning the Colless index. Furthermore, it proves to be less prone to have ties between different trees than any other balance index in the literature is, as well as more shape-discriminant than any of the balance indices tested in $[29]$ are.

Before leaving the Introduction, we want to note that, even though the Colless index, as well as other indices, was invented for its application to the description and analysis of phylogenetic trees, it is a shape index, i.e. one whose value does not depend on the specific labels associated to the leaves of the tree, but on its underlying topological features. Thus, in the rest of this manuscript we will restrict ourselves to unlabeled trees.

2. Preliminaries

2.1. Trees

In this paper, by a tree $T$ we always mean a bifurcating rooted tree, that is, a directed tree with one, and only one, node of in-degree 0 (called the root of the tree) and all its nodes of out-degree either 0 (the leaves, forming the set $L(T)$) or 2 (the internal nodes, forming the set $V_{int}(T)$). For every $n \geq 1$, we denote by $T_n^*$ the set of (isomorphism classes of) trees with $n$ leaves.

Let $T$ be a tree. If there exists an edge from a node $u$ to a node $v$ in $T$, we say that $v$ is a child of $u$ and that $u$ is the parent of $v$. Notice that, since $T$ is bifurcating, all internal nodes of $T$ have exactly two children. In addition, if there exists a path from a node $u$ to a node $v$ in $T$, we say that $v$ is a descendant of $u$. For every node $v$ of $T$, we denote by $\kappa_T(v)$ the number of its descendant leaves. If $n \geq 2$, the maximal pending subtrees of $T$ are the pair of subtrees rooted at the children of its root. We shall denote the fact that $T_1$ and $T_2$ are
the maximal pending subtrees of $T$ by writing $T = T_1 \ast T_2$. This notation is commutative, that is $T_1 \ast T_2 = T_2 \ast T_1$.

For every $n \geq 1$, the comb with $n$ leaves, $K_n$, is the unique tree in $T_n$ all whose internal nodes have different numbers of descendant leaves; cf. Figure 1(a).

\begin{figure}[h]
\centering
\includegraphics[width=0.6\textwidth]{figure1.png}
\caption{(a) The comb $K_7$ with 7 leaves; (b) The maximally balanced tree $B_7$ with 7 leaves.}
\end{figure}

2.2. The Colless index and the maximally balanced trees

Given a tree $T$ and an internal node $v \in V_{\text{int}}(T)$ with children $v_1$ and $v_2$, the balance value of $v$ is $\text{bal}_T(v) = |\kappa_T(v_1) - \kappa_T(v_2)|$. The Colless index [13] of a tree $T \in T_n$ is the sum of the balance values of its internal nodes:

$$C(T) = \sum_{v \in V_{\text{int}}(T)} \text{bal}_T(v).$$

An internal node $v$ is balanced when $\text{bal}_T(v) \leq 1$, i.e. when its two children have $\lceil \kappa_T(v)/2 \rceil$ and $\lfloor \kappa_T(v)/2 \rfloor$ descendant leaves, respectively. A tree is maximally balanced if all its internal nodes are balanced (cf. Figure 1(b)). Recursively, a bifurcating tree is maximally balanced if its root is balanced and its two maximal pending subtrees are maximally balanced. This easily implies that, for every $n \in \mathbb{N}$, there exists a unique maximally balanced tree with $n$ leaves, which we denote by $B_n$.

The maximum Colless index in $T_n$ is reached exactly at the comb $K_n$. The fact that $C(K_n)$ is maximum was already hinted at by Colless in [13], but to our knowledge a formal proof that $C(K_n) > C(T)$ for every $T \in T_n \setminus \{K_n\}$ was not provided until [13] Lem. 1. As to the minimum Colless index in $T_n$, it is proved in [13] Thm. 1 that it is achieved at the maximally balanced tree $B_n$, although (unlike the situation with the maximum Colless index) for almost every $n \in \mathbb{N}_{\geq 1}$ there exist other trees in $T_n$ with minimum Colless index (see [15] Cor. 7). If we write $n = \sum_{j=1}^{\ell} 2^{m_j}$, with $\ell \geq 1$ and $m_1, \ldots, m_\ell \in \mathbb{N}$ such that $m_1 > \cdots > m_\ell$, then

$$C(B_n) = \sum_{j=2}^{\ell} 2^{m_j}(m_1 - m_j - 2(j - 2)). \quad (1)$$

For a proof, see Thm. 2 in [15].
2.3. Phylogenetic trees

A phylogenetic tree on a set $X$ is a (rooted and bifurcating) tree with its leaves bijectively labeled by the elements of $X$. We shall denote by $T_X$ the space of (isomorphism classes of) phylogenetic trees on $X$. When the specific set of labels $X$ is irrelevant and only its cardinality $|X| = n$ matters, we shall write $T_n$ instead of $T_X$, and we shall call the members of this set phylogenetic trees with $n$ leaves.

A probabilistic model of phylogenetic trees $P_n$, $n \geq 1$, is a family of probability mappings $P_n : T_n \to [0, 1]$, each one sending each phylogenetic tree in $T_n$ to its probability under this model.

The two most popular probabilistic models of phylogenetic trees are the Yule, or Equal-Rate Markov, model \cite{30, 64} and the uniform, or Proportional to Distinguishable Arrangements, model \cite{11, 51}. The Yule model produces bifurcating phylogenetic trees on $[n]$ through the following stochastic process: starting with a single node, at every step a leaf is chosen randomly and uniformly and it is replaced by a pair of sister leaves; when the desired number $n$ of leaves is reached, the labels are assigned randomly and uniformly to these leaves. The probability $P_{Y,n}(T)$ of each $T \in T_n$ under this model is the probability of being obtained through this process. As to the uniform model, it assigns the same probability to all trees $T \in T_n$, which is then $P_{U,n} = 1 / (2^n - 3)!!$. For more information on these two models, see \cite{60, §3.2}.

3. Main theoretical results

The Quadratic Colless index, $Q$-Colless index for short, of a bifurcating tree $T$ is the sum of the squared balance values of its internal nodes:

$$QC(T) = \sum_{v \in V_{int}(T)} bal_T(v)^2 = \sum_{v \in V_{int}(T)} (\kappa_T(v_1) - \kappa_T(v_2))^2,$$

where $v_1$ and $v_2$ denote the children of each $v \in V_{int}(T)$.

For instance, the trees depicted in Figure 1 have $Q$-Colless indices $QC(K_7) = 55$ and $QC(B_7) = 2$. As we shall see, these are the maximum and minimum values of $QC$ on $T_7$.

It is straightforward to check that the Q-Colless index satisfies the following recurrence; cf. \cite{50} for the corresponding recurrence for the “classical” Colless index.

**Lemma 1.** For every $T \in T_n$, with $n \geq 2$, if $T = T_k \ast T'_{n-k}$, with $T_k \in T_k$ and $T'_{n-k} \in T_{n-k}$, then

$$QC(T) = QC(T_k) + QC(T'_{n-k}) + (n - 2k)^2.$$

The Colless index and the Q-Colless index satisfy the following relation.

**Lemma 2.** For every $T \in T_n$, $QC(T) \geq C(T)$ and the equality holds if and only if $T$ is maximally balanced.
Proof. By definition,
\[ QC(T) = \sum_{u \in V_{\text{int}}(T)} \text{bal}_T(u)^2 \geq \sum_{u \in V_{\text{int}}(T)} \text{bal}_T(u) = C(T) \]
because \( \text{bal}_T(u) \in \mathbb{N} \) for all \( u \in V_{\text{int}}(T) \). This inequality is an equality if, and only if, each \( \text{bal}_T(u) \) is either 0 or 1, and, by definition, this only happens in the maximally balanced trees. 

3.1. Extremal values

In this subsection we prove that, according to the Q-Colless index, the most balanced trees are exactly the maximally balanced trees and the most unbalanced trees are exactly the combs.

Theorem 3. The minimum of the Q-Colless index on \( \mathcal{T}_n^* \) is always reached at the maximally balanced tree \( B_n^* \), and only at this tree. Moreover, \( QC(B_n^*) = C(B_n^*) \) and hence this minimum value is given by Eqn. (1).

Proof. Let \( T \in \mathcal{T}_n^* \). By [15, Thm. 1], we know that \( C(T) \geq C(B_n^*) \). Therefore, by Lemma 2,
\[ QC(T) \geq C(T) \geq C(B_n^*) = QC(B_n^*) \]
and therefore \( QC(B_n^*) \) is minimum on \( \mathcal{T}_n^* \). Furthermore, the first inequality is strict if \( T \neq B_n^* \), and therefore \( QC(T) > QC(B_n^*) \) if \( T \neq B_n^* \). 

Theorem 4. The maximum of the Q-Colless index on \( \mathcal{T}_n^* \) is always reached at the comb \( K_n^* \), and only at this tree, and it is equal to.
\[ QC(K_n^*) = \binom{n}{3} + \binom{n-1}{3} \]

Proof. The formula for \( QC(K_n^*) \) comes from the fact that the balance values of the internal nodes of \( K_n \) are \( \{0, 1, \ldots, n-2\} \) and therefore
\[ QC(K_n) = \sum_{i=1}^{n-2} i^2 = \frac{(n-1)(n-2)(2n-3)}{6} = \binom{n}{3} + \binom{n-1}{3} \]

We prove now the maximality assertion in the statement by induction on the number \( n \) of leaves. For \( n \in \{1, 2, 3\} \), the assertion is obviously true because in these cases \( \mathcal{T}_n^* \) consists of a single tree. Assume now that \( n \geq 4 \) and that, for every \( m < n \), \( QC(K_m^*) > QC(T_m^*) \) for every \( T_m^* \in \mathcal{T}_m^* \setminus \{K_m^*\} \). Let \( T \in \mathcal{T}_n^* \) and let \( T_{n_1} \) and \( T_{n-n_1} \) be its two maximal pending subtrees, with \( T_{n_1} \in \mathcal{T}_{n_1}^* \) and \( T_{n-n_1} \in \mathcal{T}_{n-n_1}^* \) and, say, \( n_1 \leq n/2 \). In this way, by Lemma 1
\[ QC(T) = QC(T_{n_1}^*) + QC(T_{n-n_1}^*) + (n-2n_1)^2. \]

We want to prove that \( QC(K_n^*) \geq QC(T) \) and that the equality holds only when \( T = K_n = K_1 \ast K_{n-1} \). Since, by induction, \( QC(K_{n_1}^*) \geq QC(T_{n_1}^*) \) and
\[ QC(K_n - n_1) \geq QC(T_n - n_1) \] and the corresponding equalities hold only when 
\( T_n = K_n \) and \( T_n - n_1 = K_{n - n_1} \), it is enough to prove that

\[ QC(K_n) \geq QC(K_{n_1}) + QC(K_{n - n_1}) + (n - 2n_1)^2, \]
i.e., that
\[
\frac{(n - 1)(n - 2)(2n - 3)}{6} \geq \frac{(n_1 - 1)(n_1 - 2)(2n_1 - 3)}{6} + \frac{(n - n_1 - 1)(n - n_1 - 2)(2n - 2n_1 - 3)}{6} + (n - 2n_1)^2,
\]
for every \( 1 \leq n_1 \leq n/2 \), and that the equality holds only when \( n_1 = 1 \).

Consider now the function \( \kappa : [1, n/2] \to \mathbb{R} \), defined as
\[
\kappa(x) = \frac{1}{6} (x - 1)(x - 2)(2x - 3) + (n - x - 1)(n - x - 2)(2n - 2x - 3) + 6(n - 2x)^2.
\]
The graph of this function is a convex parabola with vertex at \( x = n/2 \). Therefore, the maximum value of \( \kappa \) on the interval \( [1, n/2] \) is reached at \( x = 1 \), which is exactly what we wanted to prove.

By [15 Cor. 5],
\[ QC(B_n) = C(B_n) < \min\{n/2, 2^{\lceil \log_2(n) \rceil}/3\} \]
and therefore the range of values of \( QC \) on \( T_n \) goes from below this bound to \( \binom{n}{3} + \binom{n - 1}{3} \) and hence its width grows in \( n^3/3 \), one order of magnitude larger than the range of the Colless index.

### 3.2. Statistics under the uniform and the Yule model

Let \( QC_n \) be the random variable that chooses a phylogenetic tree \( T \in T_n \) and computes \( QC(T) \).

**Theorem 5.** For every \( n \geq 1 \):

(a) The expected value of \( QC_n \) under the uniform model is
\[
E_U(QC_n) = \binom{n + 1}{2} \cdot \frac{(2n - 2)!!}{(2n - 3)!!} - n(2n - 1).
\]

(b) The variance of \( QC_n \) under the uniform model is
\[
\sigma_U^2(QC_n) = \frac{2}{15} (2n - 1)(7n^2 + 9n - 1) \binom{n + 1}{2} - \frac{1}{8} (5n^2 + n + 2) \binom{n + 1}{2} \frac{(2n - 2)!!}{(2n - 3)!!} - \binom{n + 1}{2}^2 \frac{(2n - 2)!!}{(2n - 3)!!}^2.
\]
Regarding the Yule model, we have the following result. In it, $H_n$ and $H^{(2)}_n$ denote, respectively, the $n$-th harmonic number and second order harmonic number:

$$H_n = \sum_{i=1}^{n} \frac{1}{i}, \quad H^{(2)}_n = \sum_{i=1}^{n} \frac{1}{i^2}.$$ 

**Theorem 6.** For every $n \geq 1$:

(a) The expected value of $QC_n$ under the Yule model is

$$E_Y(QC_n) = n(n + 1) - 2nH_n.$$ 

(b) The variance of $QC_n$ under the Yule model is

$$\sigma_Y^2(QC_n) = \frac{1}{3} n(n^3 - 8n^2 + 50n - 1 - 30H_n - 12nH^{(2)}_n).$$ 

We prove these theorems in the Appendix at the end of the paper.

Using Stirling’s approximation for large factorials it is easy to prove that

$$\frac{(2n - 2)!!}{(2n - 3)!!} \sim \sqrt{\pi n}$$

(see, for instance, [17, Rem. 2]). Moreover, it is known (see, for instance, [35]) that

$$H_n \sim \ln(n), \quad H^{(2)}_n \sim \frac{\pi^2}{6}.$$ 

Then, from the last two theorems we obtain the following limit behaviours:

$$E_U(QC_n) \sim \frac{\sqrt{\pi}}{2} n^{5/2}, \quad \sigma_U(QC_n) \sim \sqrt{\frac{14}{15}} n^{5/2}$$

$$E_Y(QC_n) \sim n^2, \quad \sigma_Y(QC_n) \sim \frac{1}{\sqrt{3}} n^2.$$ 

So, both under the Yule and the uniform models, the Q-Colless index satisfies that the expected value and the standard deviation grow with $n$ in the same order. This is in contrast with the Colless index, for which it only happens under the uniform model (see [8] for details):

$$E_U(C_n) \sim \sqrt{\pi n^{3/2}}, \quad \sigma_U(C_n) \sim \sqrt{\frac{10 - 3\pi}{3}} n^{3/2}$$

$$E_Y(C_n) \sim n \log(n), \quad \sigma_Y(C_n) \sim \sqrt{\frac{18 - 6 \log(2) - \pi^2}{6}} n.$$
3.3. Limit distribution under the Yule distribution

Let us now consider the following Yule-normalized version of the random variable $QC_n$:

$$Y_n = QC_n - E_Y(QC_n) \frac{1}{n^2},$$

where notice that the denominator $n^2$ is the order of growth of $\sigma_Y(QC_n)$.

The limit distribution of this random variable under the Yule model satisfies the following theorem.

Theorem 7. As $n \to \infty$, the distribution under the Yule model of $Y_n$ tends to the distribution of a random variable $Y$ satisfying the following equality in distribution:

$$Y \overset{D}{=} \tau^2 Y' + (1 - \tau)^2 Y'' + (1 + 6\tau^2 - 6\tau),$$

where $\tau \sim \text{Unif}[0,1]$ and $Y', Y''$ are independent and distributed according to the same law as $Y$.

We also postpone the proof of this theorem to the Appendix at the end of the paper. It is interesting to compare the formula obtained in this theorem with the formula of the limit distribution of the corresponding normalization of the Colless index,

$$Z_n = C_n - E_Y(C_n) \frac{1}{n}.$$

Blum, François and Janson proved in [8] that as $n \to \infty$, the distribution under the Yule model of $Z_n$ tends to the distribution of a random variable $Z$ such that

$$Z \overset{D}{=} \tau Z' + (1 - \tau) Z'' + \tau \log(\tau) + (1 - \tau) \log(1 - \tau) + 1 - 2 \min(\tau, 1 - \tau), \quad (2)$$

where $\tau \sim \text{Unif}[0,1]$ and $Z', Z''$ are independent and distributed according to the same law as $Z$. So, the independent term of the recurrent equation for the limit distribution is much simpler for the Q-Colless index than for the Colles index.

We have not carried out here a similar study for the uniform model, because in this case the random variable $L_n$ that chooses a tree in $T_n$, and then chooses a maximal pending subtree of it and counts the number of leaves of the latter (cf. Appendix A.3) has a more complicated behaviour than in the Yule case (cf. the $\beta \leq -1$ case in [2, Lemma 3]). Similarly, the weak convergence results obtained in [9] cannot be carried over to this model (see Remark 4.2 in loc. cit.).

4. Numerical results

4.1. Discriminative power of $QC$

Since the range of values of the Q-Colless index on $T_n^*$ is wider than those of the Colless index $C$, the Sackin index $S$ \cite{Sackin1976} \cite{Sackin1976a} or the total cophenetic index $\Phi$ (see Table 1), our intuition told us that the probability of two trees with the same number of leaves having the same Q-Colless index would be smaller than...
Index | Minimum | Maximum
--- | --- | ---
\(C\) | \(\Theta(n)\) | \(\binom{n}{2}\)
\(S\) | \(\Theta(n \log(n))\) | \(\binom{n+1}{2} - 1\)
\(\Phi\) | \(\Theta(n^2)\) | \(\binom{n}{3}\)
\(QC\) | \(\Theta(n)\) | \(\binom{n}{3} + \binom{n-1}{3}\)

Table 1: Range of values of the Colless index \(C\), the Sackin index \(S\), the total cophenetic index \(\Phi\) and the Q-Colless index \(QC\); recall that a function \(f(n)\) is in \(\Theta(n^k)\) when there exist constants \(0 < c_1 \leq c_2\) such that, for large enough values of \(n\), \(c_1 \cdot n^k \leq f(n) \leq c_2 \cdot n^k\).

for these other balance indices. To simplify the language, when a balance index \(I\) takes the same value on two trees in the same space \(\mathcal{T}_n^*\), we call it a tie. Of course, since for \(n \geq 12\) the range of possible \(QC\) values is narrower than the number of trees in \(\mathcal{T}_n^*\) (see [22, Table 3.3] for the cardinality of \(\mathcal{T}_n^*\) for small values of \(n\)), the pigeonhole principle implies that the Q-Colless index cannot avoid ties for large numbers of leaves.

To check the discriminative power of \(QC\) with respect to \(C\), \(S\), and \(\Phi\), we have computed the probability of tie \(p_n(I)\) for these four balance indices \(I\) and for number of leaves of \(n\) between \(n = 4\) and \(n = 20\).

More concretely, first of all, for every balance index \(I = C, S, \Phi, QC\) and for \(n = 4, \ldots, 20\), we have considered all pairs of different trees \((T_1, T_2)\) in \(\mathcal{T}_n^* \times \mathcal{T}_n^*\) and we have calculated the number \(n_I\) of such pairs of trees such that \(I(T_1) = I(T_2)\). Finally, we have computed the probability \(p_n(I)\) as \(p_n(I) = \frac{n_I}{\left|\mathcal{T}_n^*\right|^2}\), where \(\left|\mathcal{T}_n^*\right|\) is the cardinal of the set \(\mathcal{T}_n^*\).

The results obtained are shown in figure 2. The Q-Colless balance index is the balance index with the least probability of a tie.

In relation with this last point, another way to assess the discriminating skill of an index is to evaluate its power to distinguish between dissimilar trees, and compare it with that of other shape indices. In their paper [29], the authors (whom we thank for their support with the software provided in the article) develop a new resolution function to evaluate the power of tree shape statistics when it comes to discriminate between dissimilar trees (based on the Laplacian matrix of the tree, which allows for less spatial and time complexity in the operations), and then test it together with the usual resolution function based on the NNI metric. Therefore, they are able to rank some balance indices according to their power in discriminating all possible phylogenetic trees on the same number of leaves.

We have performed the same experiment on the same data (which was provided along with [29]). It turns out that the \(QC\) performs better than all the other tested indices do, including the Sales index [29], a linear combination of the Sackin and Colless indices which was introduced in the same article and performed best when tested under the NNI metric — although not with the resolution function proposed in the article, under which it was the Colless index that performed better. We present here the two tables, the first of them comput-
4.2. Limit behaviour of QC

We can use Theorem 7 to simulate directly the behaviour of QC in the limit, using Algorithm 3 in [5]. We have simulated 10000 values of Y using this algorithm, with recursion depth 10. It has to be noted that the drawn number will come from the limiting distribution only when the recursion depth is infinite. We have also generated 10000 independent phylogenetic trees in \( T_{1000} \) under the Yule model, and calculated their Yule normalized Q–Colless indices

\[
Y(T) = \frac{QC(T) - E_Y(QC_n)}{n^2}.
\]

The corresponding histograms are shown in Fig. 3. As it can be seen, they are indistinguishable. Performing a t-test on the two simulated samples yields a p-value of 0.2315, and an F-test (R's `var.test()`), to compare the sample variances, yields a p-value of 0.199. We can also notice that both sample variances are close to 1/3, as they should be according to Theorem [6].

In Fig. 3, we also compare the (Yule-normalized) Q-Colles index limit distribution with the limit distribution of the (Yule-normalized) Colless index simulated by means of Eqn. (2). We can see that the Colless index is more symmetric and also has wider support than the Q-Colless index. This in turn implies that a statistical test based on the Q-Colless index should have better power at detecting deviations from the Yule model, in line with the conclusions concerning its discriminating abilities given in the previous subsection. Interestingly, the histogram of the limit of the normalized Q-Colless index exhibits a similar skewness.
Figure 2: Probability of tie using the Colless, Total cophenetic, Quadratic Colless, Rooted Quartet (rQI), and Sackin balance indices as function of the trees' number of leaves $n$, for $n = 4, \ldots, 20$. 
Table 3: Scaled resolution scores for shape indices on the resolution function presented in [29]. The value of the resolution is between 0 and 1. Lower values represent more discriminating power.

| n  | Colless | Sackin | Variance | $I_2$ | $B_1$ | $B_2$ | Q-Colless |
|----|---------|--------|----------|------|------|------|----------|
| 7  | 0.0984  | 0.0937 | 0.1082   | 0.1115 | 0.1178 | 0.0989 | 0.0948   |
| 8  | 0.0808  | 0.0955 | 0.111    | 0.0893 | 0.1164 | 0.0965 | 0.0941   |
| 9  | 0.0507  | 0.0566 | 0.0662   | 0.068  | 0.0797 | 0.0653 | 0.0558   |
| 10 | 0.0327  | 0.0379 | 0.0471   | 0.0535 | 0.0629 | 0.0451 | 0.0357   |
| 11 | 0.0222  | 0.0255 | 0.0326   | 0.0458 | 0.0511 | 0.0348 | 0.0236   |
| 12 | 0.0183  | 0.0217 | 0.0282   | 0.0429 | 0.0473 | 0.0304 | 0.0194   |
| 13 | 0.016   | 0.0185 | 0.0238   | 0.0413 | 0.0441 | 0.0283 | 0.0163   |
| 14 | 0.0147  | 0.0170 | 0.0217   | 0.04   | 0.0421 | 0.0265 | 0.0147   |
| 15 | 0.0137  | 0.0157 | 0.0197   | 0.039  | 0.0404 | 0.0256 | 0.0134   |
| 16 | 0.013   | 0.0148 | 0.0184   | 0.038  | 0.0389 | 0.0247 | 0.0126   |
| 17 | 0.0123  | 0.014  | 0.017    | 0.037  | 0.0375 | 0.0238 | 0.0118   |
| 18 | 0.0117  | 0.0132 | 0.016    | 0.0358 | 0.0361 | 0.0229 | 0.0111   |
| 19 | 0.0112  | 0.0127 | 0.015    | 0.0347 | 0.0349 | 0.0222 | 0.0105   |
| 20 | 0.0107  | 0.012  | 0.0141   | 0.0339 | 0.0338 | 0.0217 | 0.01   |
| 21 | 0.0102  | 0.0114 | 0.0133   | 0.0329 | 0.0327 | 0.0209 | 0.01    |

The Colless index [13] is one of the oldest and most popular balance indices appearing in the literature. Its number of cites more than doubles that of the second most cited balance index in Google Scholar, the Sackin index. Nevertheless, it presents some drawbacks related to the difficult characterisation of the trees that achieve its minimum value—which clashes with the intuition that only the maximally balanced trees should be considered the most balanced bifurcating trees—and the fact that its moments under one of the most widely used probabilistic models for bifurcating phylogenetic trees, the uniform model, are still unknown.

In this paper we have presented an alternative to the Colless index that captures both its intuitive definition and its statistical benefits. In the first part of this manuscript we have proved that its extremal values are attained exactly by the trees that are usually considered to be the “most” and “least” balanced family of bifurcating trees, respectively. This contrasts vividly with the Colless and Sackin indices, whose minimum value, although being always reached by the maximally balanced trees, is seldom attained only by it; although the Colless index was defined in 1982 [13], these characterizations have been only very recently found [15, 23]. We have thus shown that the range of values of
the Quadratic Colless index, $O(n^3)$, is bigger than that of the original Colless index, $O(n^2)$, on pair with that of the total cophenetic index.

Then, we have proceeded to the computation of both the expected value and the variance under the Yule and the Uniform models of the Q-Colless index. We want to remark to the reader that the expected value and the variance of the Colless index in its original definition are, under the uniform model, still unknown. So, in this regard the Quadratic Colless index presents an improvement over the original measure of balance. We have also obtained a recurrent equation for the limit distribution of the Q-Colless index under the Yule model.

Finally, we have empirically shown that it possesses more discriminatory power than the original Colless index does by, firstly, computing the probability of producing a tie between a pair of trees for numbers of leaves up to 20, and, secondly, testing it under the metrics provided in [29]. In both cases, it has systematically been one of the best performing measures, being often superior to the Colless and Sackin indices. All scripts and data used in these computations are available at the GitHub repository associated to this paper (https://github.com/biocom-uib/QColless).

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Appendices

A.1 Proof of Theorem 7

The following lemma summarizes Lemma 16 in [42] and Lemma 2 in [10].

**Lemma 8.** Let \( I : \bigcup_{n \geq 1} T_n \to \mathbb{R} \) be a mapping satisfying the following two conditions:

- It is invariant under phylogenetic tree isomorphisms and relabelings of leaves.
- There exists a symmetric mapping \( f_I : \mathbb{N}_{n \geq 1} \times \mathbb{N}_{n \geq 1} \to \mathbb{R} \) such that, for every pair of phylogenetic trees \( T, T' \) on disjoint sets of taxa \( X, X' \), respectively,

\[
I(T \star T') = I(T) + I(T') + f_I(|X|, |X'|).
\]

For every \( n \geq 1 \), let \( I_n \) and \( I^2_n \) be the random variables that choose a tree \( T \in T_n \) and compute \( I(T) \) and \( I(T)^2 \), respectively. Then, for every \( n \geq 2 \), their expected values under the Yule model are:

\[
E_Y(I_n) = \frac{1}{n-1} \sum_{k=1}^{n-1} (2E_Y(I_k) + f_I(k, n-k))
\]

\[
E_Y(I^2_n) = \frac{1}{n-1} \sum_{k=1}^{n-1} \left( 2E_Y(I_k^2) + 4f_I(k, n-k)E_Y(I_k) + 2E_Y(I_k)E_Y(I_{n-k}) + f_I(k, n-k)^2 \right).
\]

**Claim.** For every \( n \geq 1 \), the expected value of \( QC_n \) under the Yule model is

\[
E_Y(QC_n) = n(n+1) - 2nH_n.
\]
Proof. By Lemma 8.(a),
\[ E_Y(QC_n) = \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(QC_k) + \frac{1}{n-1} \sum_{k=1}^{n-1} (n-2k)^2 \]
\[ = \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(QC_k) + \frac{1}{3} n(n-2) \]
\[ = \frac{2}{n-1} E_Y(QC_{n-1}) + \frac{n-2}{n-1} \left( \frac{2}{n-2} \sum_{k=1}^{n-2} E_Y(QC_k) \right) + \frac{1}{3} n(n-2) \]
\[ = \frac{2}{n-1} E_Y(QC_{n-1}) + \frac{n-2}{n-1} \left( E_Y(QC_{n-1}) - \frac{1}{3} (n-1)(n-3) \right) \]
\[ + \frac{1}{3} n(n-2) \]
\[ = \frac{n}{n-1} E_Y(QC_{n-1}) + n - 2 \]
Dividing this equation by \( n \) and setting \( X_n = E_Y(QC_n)/n \), we obtain the equation
\[ X_n = X_{n-1} + 1 - \frac{2}{n} \]
whose solution with initial condition \( X_1 = E_Y(QC_1) = 0 \) is
\[ X_n = \sum_{k=2}^{n} \left( 1 - \frac{2}{k} \right) = n + 1 - 2H_n \]
and hence, finally,
\[ E_Y(QC_n) = nX_n = n(n + 1) - 2nH_n. \]

Claim. For every \( n \geq 1 \), the variance of \( QC_n \) under the Yule model is
\[ \sigma_Y^2(QC_n) = \frac{1}{3} n(n^3 - 8n^2 + 50n - 1 - 30H_n - 12nH_n^{(2)}) \]

Proof. We shall compute the variance \( \sigma_Y^2(QC_n) \) by means of the identity
\[ \sigma_Y^2(QC_n) = E_Y(QC_n^2) - E_Y(QC_n)^2 \]
where the value of \( E_Y(QC_n) \) is given by Theorem. What remains is to compute
$E_Y(QC_n^2)$. Now, by Lemma 8.(b),

$$E_Y(QC_n^2) = \frac{1}{n-1} \sum_{k=1}^{n-1} \left( 2E_Y(QC_k^2) + (n-2k)^4 ight)$$

$$+ 4(n-2k)^2E_Y(QC_k) + 2E_Y(QC_k)E_Y(QC_{n-k})$$

$$= \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(QC_k^2) + \frac{1}{n-1} \sum_{k=1}^{n-1} (n-2k)^4$$

$$+ \frac{4}{n-1} \sum_{k=1}^{n-1} (n-2k)^2k(k+1-2H_k)$$

$$+ \frac{2}{n-1} \sum_{k=1}^{n-1} k(n-k)(k+1-2H_k)(n-k+1-2H_{n-k})$$

Let us denote by $T_n$ the independent term in this equation, so that this equation can be written as

$$E_Y(QC_n^2) = \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(QC_k^2) + T_n$$

$$= \frac{2}{n-1} E_Y(QC_{n-1}^2) + \frac{n-2}{n-1} \frac{2}{n-2} \sum_{k=1}^{n-2} E_Y(QC_k^2) + T_n$$

$$= \frac{2}{n-1} E_Y(QC_{n-1}^2) + \frac{n-2}{n-1} \left( E_Y(QC_{n-1}^2) - T_{n-1} \right) + T_n$$

$$= \frac{n}{n-1} E_Y(QC_{n-1}^2) + T_n - \frac{n-2}{n-1} T_{n-1}$$

Dividing this equation by $n$ and setting $Y_n = E_Y(QC_n^2)/n$, we obtain the equation

$$Y_n = Y_{n-1} + \frac{1}{n} \left( T_n - \frac{n-2}{n-1} T_{n-1} \right). \quad (4)$$

We want to compute now the independent term in this equation as an explicit expression in $n$. To do that, we first compute the three sums that form $T_n$. On the one hand,

$$\frac{1}{n-1} \sum_{k=1}^{n-1} (n-2k)^4 = \frac{1}{15} n(n-2)(3n^2 - 6n - 4). \quad (5)$$
On the other hand,

\[
\frac{4}{n-1} \sum_{k=1}^{n-1} (n - 2k)^2 k (k + 1 - 2H_k)
\]

\[
= \frac{4}{n-1} \left( \sum_{k=1}^{n-1} (n - 2k)^2 k (k + 1) - 2(n - 2)^2 \sum_{k=1}^{n-1} k H_k 
\right.
\]

\[
+ 16(n - 3) \sum_{k=1}^{n-1} \binom{k}{2} H_k - 48 \sum_{k=1}^{n-1} \binom{k}{3} H_k 
\left.
\right)
\]

\[
= \frac{4}{n-1} \left( \frac{1}{15} (n-1)n(n+1)(2n^2 - 5n + 2) - 2(n - 2)^2 \binom{n}{2} \left( H_n - \frac{1}{2} \right) 
\right.
\]

\[
+ 16(n - 3) \left( \binom{n}{3} \left( H_n - \frac{1}{3} \right) - 48 \binom{n}{4} \left( H_n - \frac{1}{4} \right) \right) 
\left.
\right)
\]

\[
= \frac{2}{45} n(n - 2)(12n^2 + 16n + 9) - \frac{4}{3} n^2(n - 2)H_n 
\]

(6)

using, in the second last equality above, that

\[
\sum_{k=1}^{n-1} \binom{k}{m} H_k = \left( \frac{n}{m+1} \right) \left( H_n - \frac{1}{m+1} \right); 
\]

(7)

see Eqn. (6.70) in [35].
As to the third sum,
\[
\frac{2}{n-1} \sum_{k=1}^{n-1} k(n - k)(k + 1 - 2H_k)(n - k + 1 - 2H_{n-k})
\]
\[
= \frac{2}{n-1} \left[ \sum_{k=1}^{n-1} k(k + 1)(n - k)(n - k + 1) \\
- 2 \sum_{k=1}^{n-1} k(n - k)(n - k + 1)H_k - 2 \sum_{k=1}^{n-1} k(n - k)(k + 1)H_{n-k} \\
+ 4 \sum_{k=1}^{n-1} k(n - k)H_k H_{n-k} \right]
\]
\[
= \frac{2}{n-1} \left[ \sum_{k=1}^{n-1} k(k + 1)(n - k)(n - k + 1) - 4 \sum_{k=1}^{n-1} k(n - k)(n - k + 1)H_k \\
+ 4n \sum_{k=1}^{n-1} kH_k H_{n-k} - 4 \sum_{k=1}^{n-1} k^2 H_k H_{n-k} \right]
\]
\[
= \frac{2}{n-1} \left[ \sum_{k=1}^{n-1} k(k + 1)(n - k)(n - k + 1) \\
- 4 \sum_{k=1}^{n-1} \left( 6 \binom{k}{3} - 4(n - 1) \binom{k}{2} + n(n - 1)k \right) H_k \\
+ 4n \sum_{k=1}^{n-1} kH_k H_{n-k} - 4 \sum_{k=1}^{n-1} k^2 H_k H_{n-k} \right]
\]
\[
= \frac{2}{n-1} \left[ 4 \binom{n + 3}{5} - 24 \binom{n}{4} \left( H_n - \frac{1}{4} \right) \\
+ 16(n - 1) \binom{n}{3} \left( H_n - \frac{1}{3} \right) - 4n(n - 1) \binom{n}{2} \left( H_n - \frac{1}{2} \right) \\
+ 4n \binom{n + 1}{2} \left( H_{n+1}^2 - H_{n+1}^{(2)} - 2H_{n+1} + 2 \right) \\
- \frac{4}{3} \binom{n + 1}{2} \left( (2n + 1)(H_{n+1}^2 - H_{n+1}^{(2)}) - \frac{13n + 5}{3} H_{n+1} + \frac{71n + 37}{18} \right) \right]
\]
\[
= \frac{1}{270} n(18n^3 + 303n^2 + 1163n + 98) - \frac{2}{9} n(n + 1)(3n + 16) H_n \\
+ \frac{4}{3} n(n + 1)(H_{n+1}^2 - H_{n+1}^{(2)})
\]
using, in the second last equality above, Eqn. (7) and the identities

\[
\begin{align*}
\sum_{k=1}^{n-1} kH_k H_{n-k} &= \binom{n+1}{2} \left( H_{n+1}^2 - H_{n+1}^{(2)} - 2H_{n+1} + 2 \right) \\
\sum_{k=1}^{n-1} k^2 H_k H_{n-k} &= \frac{n(n+1)}{6} \left[ (2n+1)(H_{n+1}^2 - H_{n+1}^{(2)}) - \frac{13n+5}{3} H_{n+1} + \frac{71n+37}{18} \right]
\end{align*}
\]

proved in [62].

So,

\[
T_n = \frac{1}{15} n(n-2)(3n^2 - 6n - 4) \\
+ \frac{2}{45} n(n-2)(12n^2 + 16n + 9) - \frac{4}{3} n^2(n-2)H_n \\
+ \frac{1}{270} n(18n^3 + 303n^2 + 1163n + 98) - \frac{2}{9} n(n+1)(3n+16)H_n \\
+ \frac{4}{3} n(n+1)(H_{n+1}^2 - H_{n+1}^{(2)}) \\
= \frac{1}{270} n(216n^3 - 9n^2 + 1031n + 26) - \frac{2}{9} n(9n^2 + 7n + 16)H_n \\
+ \frac{4}{3} n(n+1)(H_{n+1}^2 - H_{n+1}^{(2)})
\]
and, hence, the independent term in Eqn. (4) is

\[
\frac{1}{n} \left( T_n - \frac{n-2}{n-1} T_{n-1} \right) = \frac{1}{n} \left[ \frac{1}{270} n(216n^3 - 9n^2 + 1031n + 26) - \frac{2}{9} n(9n^2 + 7n + 16) H_n \\
+ \frac{4}{3} n(n+1)(H_{n+1}^2 - H_{n+1}^{(2)}) \\
- \frac{n-2}{n-1} \left( \frac{1}{270} (n-1)(216(n-1)^3 - 9(n-1)^2 + 1031(n-1) + 26) \\
- \frac{2}{9} (n-1)(9(n-1)^2 + 7(n-1) + 16) H_{n-1} \\
+ \frac{4}{3} (n-1)(H_n^2 - H_{n-1}^{(2)}) \right) \right]
\]

\[
= \frac{1}{n} \left[ \frac{1}{270} n(216n^3 - 9n^2 + 1031n + 26) \\
- \frac{2}{9} n(9n^2 + 7n + 16) H_{n-1} - \frac{2}{9} (9n^2 + 7n + 16) \\
+ \frac{4}{3} n(n+1)(H_n^2 - H_{n}^{(2)}) + \frac{8}{3} n H_{n-1} + \frac{8}{3} \\
- \frac{1}{270} (n-2)(216n^3 - 657n^2 + 1697n - 1230) \\
+ \frac{2}{9} (n-2)(9n^2 - 11n + 18) H_{n-1} \\
- \frac{4}{3} (n-2)(H_n^2 - H_{n}^{(2)}) \right]
\]

\[
= \frac{1}{n} \left[ \frac{1}{3} (12n^3 - 28n^2 + 47n - 30) - 8(n^2 - n + 1) H_{n-1} \\
+ 4n(H_n^2 - H_{n}^{(2)}) \right]
\]

\[
= 4n^2 - \frac{28}{3} n + \frac{47}{3} - \frac{10}{n} - 8(n-1)H_{n-1} - \frac{8H_{n-1} - 4H_n}{n} + 4H_n^2 - 4H_{n}^{(2)}
\]
The solution of Eqn. (4) with initial condition $Y_1 = E_Y(QC_1^2) = 0$ is

$$Y_n = \sum_{k=2}^{n} \frac{1}{k} (T_k - \frac{k-2}{k-1} T_{k-1})$$

$$= \sum_{k=2}^{n} \left( 4k^2 - \frac{28}{3} k + \frac{47}{3} - \frac{10}{k} - 8(k-1)H_{k-1} - \frac{8H_{k-1}}{k} + 4H_k^2 - 4H_k^{(2)} \right)$$

$$= \sum_{k=1}^{n-1} \left( 4(k+1)^2 - \frac{28}{3} (k+1) + \frac{47}{3} - \frac{10}{k+1} - 8kH_k - \frac{8H_k}{k+1} + 4H_{k+1}^2 - 4H_{k+1}^{(2)} \right)$$

$$= \left( * \right) \frac{1}{3} (4n^3 - 8n^2 + 35n - 31) - 10(H_n - 1)

- 8 \left( \frac{n}{2} \right) (H_n - \frac{1}{2}) - 4(H_n^2 - H_n^{(2)})

+ 4((n+1)H_n^2 - (2n+1)H_n + 2n - 1)

- 4((n+1)H_n^{(2)} - H_n - 1)

$$= \frac{1}{3} (4n^3 - 2n^2 + 53n - 1) - 2(2n^2 + 2n + 5)H_n + 4n(H_n^2 - H_n^{(2)})$$

where, in the second last equality (marked with (*)) we have used Eqn. (7) and the identities

$$\sum_{k=1}^{n-1} \frac{H_k}{k+1} = \frac{1}{2} (H_n^2 - H_n^{(2)})$$

(cf. Eqn. (6.71) in [35]) and

$$\sum_{k=1}^{n-1} H_k^2 = nH_n^2 - (2n+1)H_n + 2n$$

$$\sum_{k=1}^{n-1} H_k^{(2)} = nH_n^{(2)} - H_n$$

(see [39], §1.2.7). Therefore, finally

$$E_Y(QC_n^2) = nY_n$$

$$= \frac{n}{3} (4n^3 - 2n^2 + 53n - 1) - 2n(2n^2 + 2n + 5)H_n + 4n^2(H_n^2 - H_n^{(2)})$$

and

$$\sigma_Y^2(QC_n) = E_Y(QC_n^2) - E_Y(QC_n)^2$$

$$= \frac{1}{3} n(n^3 - 8n^2 + 50n - 1 - 30H_n - 12nH_n^{(2)})$$

as we claimed.
A.2 Proof of Theorem 5

To simplify the notations, for every \( n \geq 2 \) and for every \( 1 \leq k \leq n - 1 \), set
\[
C_{k,n} := \frac{1}{2} \binom{n}{k} \frac{(2k-3)!!(2(n-k)-3)!!}{(2n-3)!!}.
\]

The proof of the following lemma is identical to the proof of Lemma 8 given in the references provided in the previous subsection, simply replacing the probabilities under the Yule model by probabilities under the uniform model. We leave the details to the reader.

**Lemma 9.** Let \( I : \bigcup_{n \geq 1} \mathcal{T}_n \to \mathbb{R} \) be a mapping satisfying the same conditions as in the statement of Lemma 8 and, for every \( n \geq 1 \), let \( I_n \) and \( I_n^2 \) be the random variables that choose a tree \( T \in \mathcal{T}_n \) and compute \( I(T) \) and \( I(T)^2 \), respectively. Then, for every \( n \geq 2 \), their expected values under the uniform model are:
\[
E_U(I_n) = \sum_{k=1}^{n-1} C_{k,n-k} \left( 2E_U(I_k) + f_I(k,n-k) \right)
\]
\[
E_U(I_n^2) = \sum_{k=1}^{n-1} C_{k,n-k} \left( 2E_U(I_k^2) + f_I(k,n-k)^2 + 4f_I(k,n-k)E_U(I_k) + 2E_U(I_k)E_U(I_{n-k}) \right).
\]

In the proofs provided in this subsection we shall use the following technical lemmas. They are proved in the Section SN-4 of the Supplementary Material of [17]; Lemma 12 is Proposition 6 in that paper.

**Lemma 10.** For every \( n \geq 2 \):

(a) \[ \sum_{k=1}^{n-1} C_{k,n-k} = 1 \]

(b) For every \( m \geq 1 \),
\[
\sum_{k=1}^{n-1} C_{k,n-k} \binom{k}{m} = \frac{1}{2} \binom{n}{m} \left( 1 - \frac{m-1}{n-1} \cdot \frac{(2m-3)!!}{(2m-2)!!} \cdot \frac{(2n-2)!!}{(2n-3)!!} \right).
\]

**Lemma 11.** For every \( n \geq 2 \),

(a) \[ \sum_{k=1}^{n-1} C_{k,n-k} \cdot \frac{(2k-2)!!}{(2k-3)!!} = \frac{1}{2} \frac{(2n-2)!!}{(2n-3)!!} + \frac{1}{4} (2H_{2n-2} - H_{n-1} - 2). \]

(b) For every \( m \geq 1 \),
\[
\sum_{k=1}^{n-1} C_{k,n-k} \binom{k}{m} \frac{(2k-2)!!}{(2k-3)!!} = \frac{1}{2} \binom{n}{m} \left( \frac{(2n-2)!!}{(2n-3)!!} - \frac{(2m-2)!!}{(2m-3)!!} \right).
\]
Lemma 12. The solution $X_n$ of the equation

$$X_n = 2 \sum_{k=1}^{n-1} C_{k,n-k} X_k + \sum_{l=1}^{r} a_l \binom{n}{l} + \frac{(2n-2)!!}{(2n-3)!!} \sum_{l=1}^{n} b_l \binom{n}{l}$$

with given initial condition $X_1$ is

$$X_n = \sum_{l=1}^{s+1} \hat{a}_l \binom{n}{l} + \frac{(2n-2)!!}{(2n-3)!!} \sum_{l=1}^{r} \hat{b}_l \binom{n}{l}$$

with

$$\hat{a}_1 = X_1 - a_1$$

$$\hat{a}_l = \frac{l \cdot (2l-2)!!}{(2l-3)!!} \left( \frac{b_l}{l-1} + \frac{b_{l-1}}{l} \right), \quad l = 2, \ldots, s$$

$$\hat{a}_{s+1} = \frac{(s+1) \cdot (2s)!!}{s \cdot (2s-1)!!} \cdot b_s$$

$$\hat{b}_l = \frac{(2l-3)!!}{(2l-2)!!} \cdot a_l, \quad l = 1, \ldots, r$$

Claim. For every $n \geq 1$, the expected value of $QC_n$ under the uniform model is

$$E_U(QC_n) = \left( n + 1 \right) \cdot \binom{n+1}{2} \cdot \frac{(2n-2)!!}{(2n-3)!!} - n(2n-1).$$

Proof. By Lemma 9(a),

$$E_U(QC_n) = 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k) + \sum_{k=1}^{n-1} C_{k,n-k} (n-k)^2$$

$$= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k) + n^2 \sum_{k=1}^{n-1} C_{k,n-k} - 4(n-1) \sum_{k=1}^{n-1} C_{k,n-k} k$$

$$+ 8 \sum_{k=1}^{n-1} C_{k,n-k} \binom{k}{2}$$

$$= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k) + n^2 - 2n(n-1)$$

$$+ 4 \binom{n}{2} \left( 1 - \frac{1}{2(n-1)} \cdot \frac{(2n-2)!!}{(2n-3)!!} \right)$$

$$= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k) + 2 \binom{n}{2} + n - n \cdot \frac{(2n-2)!!}{(2n-3)!!}$$

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where in the second last equality we have used Lemma 10. Therefore, by Lemma 12 and using that $E_U(QC_1) = 0$, we have that

$$E_U(QC_n) = \left(\binom{n}{2} + n\right) \frac{(2n - 2)!!}{(2n - 3)!!} - \left(\binom{n}{2} + n\right)$$

$$= \left(\binom{n+1}{2}\right) \frac{(2n - 2)!!}{(2n - 3)!!} - n(2n - 1)$$

as we claimed.

\[\square\]

**Claim.** *For every $n \geq 1$, the variance of $QC_n$ under the uniform model is*

$$\sigma^2_U(QC_n) = \frac{2}{15}(2n - 1)(7n^2 + 9n - 1)\left(\frac{n+1}{n+2}\right)$$

$$- \frac{1}{8}(5n^2 + n + 2)\left(\binom{n}{2}\right) \frac{(2n - 2)!!}{(2n - 3)!!} - \left(\binom{n+1}{2}\right)^2 \left(\frac{(2n - 2)!!}{(2n - 3)!!}\right)^2$$

**Proof.** To simplify the notations, we shall denote $(2n - 2)!!/(2n - 3)!!$ by $\alpha_n$. We shall compute the variance $\sigma^2_U(QC_n)$ by means of the identity

$$\sigma^2_U(QC_n) = E_U(QC_n^2) - E_U(QC_n)^2 \quad (9)$$

where the value of $E_U(QC_n)$ is given by Theorem. Now, we must compute
By Lemma 9(b),

\[
E_U(QC_n^2) = \sum_{k=1}^{n-1} C_{k,n-k} \left( 2E_U(QC_k^2) + (n - 2k)^4 + 4(n - 2k)^2 E_U(QC_k) + 2E_U(QC_k)E_U(QC_{n-k}) \right)
\]

\[
= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k^2)
\]

\[
+ \sum_{k=1}^{n-1} C_{k,n-k} \left[ (n - 2k)^4 + 4(n - 2k)^2 \left( \frac{k + 1}{2} \right) \alpha_k - k(2k - 1) \right]
\]

\[
+ 2 \left( \frac{k + 1}{2} \right) \alpha_k - k(2k - 1)
\]

\[
\cdot \left( \frac{n - k}{2} \right) \alpha_{n-k} - (n - k)(2(n - k) - 1) \right] \alpha_k
\]

\[
+ 2 \sum_{k=1}^{n-1} C_{k,n-k} \left( \frac{k + 1}{2} \right) \left( \frac{n - k}{2} \right) \alpha_k \alpha_{n-k}
\]

\[
= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k^2)
\]

\[
- \sum_{k=1}^{n-1} C_{k,n-k} \left( 8k^4 + 16(n - 1)k^3 - 2(12n^2 - 6n - 1)k^2 - (2n - 8n^3)k - n^4 \right)
\]

\[
+ \sum_{k=1}^{n-1} C_{k,n-k} \left[ 4(n - 2k)^2 \left( \frac{k + 1}{2} \right) - 4 \left( \frac{k + 1}{2} \right) (n - k)(2(n - k) - 1) \right] \alpha_k
\]

\[
+ 2 \sum_{k=1}^{n-1} C_{k,n-k} \left( \frac{k + 1}{2} \right) \left( \frac{n - k + 1}{2} \right) \alpha_k \alpha_{n-k}
\]
\begin{align*}
&= 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(Q C_k^2) \\
&\quad - \sum_{k=1}^{n-1} C_{k,n-k} \left[ 192 \binom{k}{4} + 96(n+2) \binom{k}{3} - 4(12n^2 - 30n - 5) \binom{k}{2} \\
&\quad \quad + (8n^3 - 24n^2 + 6n - 6)k - n^4 \right] \\
&\quad + \sum_{k=1}^{n-1} C_{k,n-k} \left[ 96 \binom{k}{4} + 156 \binom{k}{3} - 4(n^2 - n - 16) \binom{k}{2} \\
&\quad \quad - 4(n^2 - n - 1)k \right] \alpha_k \\
&\quad + 2 \sum_{k=1}^{n-1} C_{k,n-k} \binom{k+1}{2} \binom{n-k+1}{2} \alpha_k \alpha_{n-k}.
\end{align*}
\tag{10}

Let us compute the independent term in this equation. The first sum can be computed using Lemma [10].

\begin{align*}
&\sum_{k=1}^{n-1} C_{k,n-k} \left( 192 \binom{k}{4} + 96(n+2) \binom{k}{3} - 4(12n^2 - 30n - 5) \binom{k}{2} \\
&\quad + (8n^3 - 24n^2 + 6n - 6)k - n^4 \right) \\
&= 96 \binom{n}{4} \left( 1 - \frac{3}{n-1} \cdot \frac{5!!}{6!!} \cdot \alpha_n \right) \\
&\quad + 48(n+2) \binom{n}{3} \left( 1 - \frac{2}{n-1} \cdot \frac{3!!}{4!!} \cdot \alpha_n \right) \\
&\quad - 2(12n^2 - 30n - 5) \binom{n}{2} \left( 1 - \frac{1}{2(n-1)} \cdot \alpha_n \right) \\
&\quad + \frac{1}{2}(8n^3 - 24n^2 + 6n - 6)n - n^4 \\
&= (3n-2)n^3 - \frac{n(15n^2 - 15n + 4)}{4} \cdot \alpha_n.
\end{align*}
The second sum in this independent term can be computed using Lemma 11:

\[ \sum_{k=1}^{n-1} C_{k,n-k} \left[ 96 \binom{k}{4} + 156 \binom{k}{3} - 4(n^2 - n - 16) \binom{k}{2} - 4(n^2 - n - 1)k \right] \alpha_k \]

\[ = 48 \binom{n}{4} (\alpha_n - \frac{6!!}{5!!}) + 78 \binom{n}{3} (\alpha_n - \frac{4!!}{3!!}) \]

\[ - 2(n^2 - n - 16) \binom{n}{2} (\alpha_n - 2) - 2(n^2 - n - 1)n(\alpha_n - 1) \]

\[ = n^3(n + 1)\alpha_n - \frac{2n(33n^3 - 13n^2 - 12n + 7)}{15}. \]

Finally, the third sum in the independent term of this equation can be computed as follows:

\[ 2 \sum_{k=1}^{n-1} C_{k,n-k} \left( \begin{array}{c} k + 1 \\ 2 \end{array} \right) \left( \begin{array}{c} n - k + 1 \\ 2 \end{array} \right) \frac{(2k - 2)!! (2n - 2k - 2)!!}{(2k - 3)!! (2n - 2k - 3)!!} \]

\[ = \frac{n!}{(2n - 3)!!} \sum_{k=1}^{n-1} (k + 1)(n - k + 1) \frac{2^{n-k-4} (n-k)!}{(2n-3)!!} \]

\[ = \frac{n!2^{n-4}}{(2n-3)!!} \frac{12n^3(n-1)(n+1)(n+6)}{6} = \frac{n+6}{8} \binom{n+1}{3} \cdot \alpha_n. \]

So, the independent term of Eqn. (10) is

\[ \frac{n(15n^2 - 15n + 4)}{4} \cdot \alpha_n - (3n - 2)n^3 \]

\[ + n^3(n + 1)\alpha_n - \frac{2n(33n^3 - 13n^2 - 12n + 7)}{15} + \frac{n+6}{8} \binom{n+1}{3} \cdot \alpha_n \]

\[ = \frac{n(49n^3 + 234n^2 - 181n + 42)}{48} \cdot \alpha_n - \frac{n(111n^3 - 56n^2 - 24n + 14)}{15} \]

\[ = \left( 3n + 36 \binom{n}{2} + 66 \binom{n}{3} + \frac{49}{2} \binom{n}{4} \right) \alpha_n - 3n - 78 \binom{n}{2} - 244 \binom{n}{3} - \frac{888}{5} \binom{n}{4} \]

and, hence, Eqn. (10) simplifies to

\[ E_U(QC_n^2) = 2 \sum_{k=1}^{n-1} C_{k,n-k} E_U(QC_k^2) - 3n - 78 \binom{n}{2} - 244 \binom{n}{3} - \frac{888}{5} \binom{n}{4} \]

\[ + \left( 3n + 36 \binom{n}{2} + 66 \binom{n}{3} + \frac{49}{2} \binom{n}{4} \right) \alpha_n. \]
This equation can be solved using Lemma 12 and the fact that $E_U(QC^2_n) = 0$. Its solution is

$$E_U(QC^2_n) = 3n + 84\binom{n}{2} + 320\binom{n}{3} + 360\binom{n}{4} + 112\binom{n}{5} - \left(3n + 39\binom{n}{2} + \frac{183}{2}\binom{n}{3} + \frac{111}{2}\binom{n}{4}\right)\alpha_n$$

$$= \frac{n}{15}(14n^4 + 85n^3 - 60n^2 + 5n + 1) - \frac{n}{16}(37n^3 + 22n^2 - 13n + 2)\alpha_n.$$

Finally,

$$\sigma^2_Y(QC_n) = E_U(QC^2_n) - E_U(QC_n)^2$$

$$= \frac{2}{15}(2n - 1)(7n^2 + 9n - 1)\binom{n + 1}{2} - \frac{1}{8}(5n^2 + n + 2)\binom{n + 1}{2} \left(\frac{(2n - 2)!!}{(2n - 3)!!}\right)^2 - \frac{(2n - 2)!!}{(2n - 3)!!}^2$$

as we claimed. □

A3 Proof of Theorem 7

Recall from Lemma 1 that the Q-Colless index has the following recursive representation for a tree $T_n = T_k \ast T'_{n-k} \in T_n$:

$$QC(T_n) = QC(T_k) + QC(T'_{n-k}) + (n - 2k)^2.$$ 

Recall moreover from Theorem 5 that, under the Yule model, 

$$E_Y(QC_n) = n(n + 1) - 2nH_n$$ 

and

$$\sigma^2_Y(QC_n) = \frac{1}{3}n\left(n^3 - 8n^2 + 50n - 1 - 30H_n - 12nH^{(2)}_n\right) \sim n^4.$$ 

Let us now consider the following normalized version of the Q-Colless index on $T_n$:

$$Y(T) = \frac{QC(T) - E_Y(QC_n)}{n^2} = \frac{QC(T) - (n(n + 1) - 2nH_n)}{n^2}.$$
Then, if $T = T_k * T_{n-k}$,

$$Y(T) = n^{-2} \left( QC(T_k) + QC(T'_{n-k}) + (n - 2k)^2 - (n(n+1) - 2nH_n) \right)$$

$$= n^{-2} \left[ k^2 \left( \frac{QC(T_k) - (k(k + 1) - 2kH_k) + k(k + 1) - 2kH_k}{k^2} \right) \right.$$

$$+ (n - k)^2 \left( \frac{QC(T'_{n-k}) - ((n - k)(n - k + 1) - 2(n - k)H_{n-k})}{(n - k)^2} \right)$$

$$+ (n - k)(n - k + 1) - 2(n - k)H_{n-k}) \right]$$

$$= n^{-2}(k^2 Y(T_k) + (n - k)^2 Y(T'_{n-k}) + n^2 - 2nH_n - 2kH_k)$$

$$+ (n - k)(n - k + 1) - 2(n - k)H_{n-k})$$

$$= n^{-2}(k^2 Y(T_k) + (n - k)^2 Y(T'_{n-k}) + n^2 - 6nk + 2nH_n - 2kH_k - 2(n - k)H_{n-k})$$

$$= n^{-2}(k^2 Y(T_k) + (n - k)^2 Y(T'_{n-k}) + A_n(k)) \quad (11)$$

where

$$A_n(k) = n^2 + 6k^2 - 6nk + 2nH_n - 2kH_k - 2(n - k)H_{n-k}.$$ 

Let us denote now by $Y_n$ the random variable that chooses a tree $T \in \mathcal{T}_n$ and computes $Y(T)$. Moreover, and as it is usual in this context (see, e.g., [3]) let $L_n$ denote the random variable that chooses a tree $T \in \mathcal{T}_n$ and one of its maximal pending subtrees of $T$ and counts its number of leaves. Recall that, under the Yule model, $L_n$ is uniformly distributed on $\{1, \ldots, n-1\}$. When we translate Eqn. (11) in terms of these random variables, we obtain

$$Y_n = n^{-2}(L_n^2 Y_{L_n} + (n - L_n)^2 Y_{n-L_n} + A_n(L_n)).$$

We will now look at the limit in distribution of $Y_n$ under the Yule model as $n \to \infty$. If one simplifies the proof of Thm. 3.1 in [3] to the Yule case (which corresponds to Aldous’s $\beta$-model with $\beta = 0$ [2]), or, alternatively, follows the logic behind the proof Thm. 3.1 in [3] (which is a minor modification of the proof of Thm. 2.1 in [2]), using the function $A_n$ that gives the independent term in Eqn. (11), and noticing that $E_Y(Y_n^2)$ is uniformly bounded and that

$$E_Y(A_n(L_n)) = E_Y(n^2 + 6L_n(L_n - n) + 2nH_n - 2L_nH_{L_n} - 2(n - L_n)H_{n-L_n})$$

$$= n^2 + 6 \sum_{k=1}^{n-1} k(k - n) + 2nH_n - 2 \sum_{k=1}^{n-1} kH_k - 2 \sum_{k=1}^{n-1} kH_k$$

$$= n^2 - n(n+1) + 2nH_n - n(2H_n - 1) = 0$$

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(for the value of $\sum_{k=1}^{n-1} kH_k$, see Eqn. (6.68) in [35]), one obtains that $Y_n \xrightarrow{D} Y$, for a random variable $Y$ satisfying the equality in distribution

$$Y \overset{D}{=} \tau^2 Y' + (1 - \tau)^2 Y'' + (1 + 6\tau^2 - 6\tau),$$

where $\tau \sim \text{Unif}[0, 1]$ and $Y', Y''$ are independent, distributed according to the same law as $Y$. 

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