DISTRIBUTION OF PHYLOGENETIC DIVERSITY UNDER RANDOM EXTINCTION

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ABSTRACT. Phylogenetic diversity is a measure for describing how much of an evolutionary tree is spanned by a subset of species. If one applies this to the (unknown) subset of current species that will still be present at some future time, then this ‘future phylogenetic diversity’ provides a measure of the impact of various extinction scenarios in biodiversity conservation. In this paper we study the distribution of future phylogenetic diversity under a simple model of extinction (a generalized ‘field of bullets’ model). We show that the distribution of future phylogenetic diversity converges to a normal distribution as the number of species grows (under mild conditions, which are necessary). We also describe an algorithm to compute the distribution efficiently, provided the edge lengths are integral, and briefly outline the significance of our findings for biodiversity conservation.

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1. Introduction

The current rapid rate of extinction of many diverse species has focused attention on predicting the loss of future biodiversity. There are numerous ways to measure the ‘biodiversity’ of a group of species, and one which recognises the evolutionary linkages between taxa (for example, species) is phylogenetic diversity ([3], [4], [8]). Briefly, given a subset of taxa, the PD (phylogenetic diversity) score of that subset is the sum of the lengths of the edges of the evolutionary tree that connects this subset (formal definitions are given shortly). Here the ‘length’ of an edge may refer to the amount of genetic change on that edge, its temporal duration or perhaps other features (such as morphological diversity).

Under the simplest models of speciation, each taxon has the same probability of surviving until some future time, and the survival of taxa are treated as independent events; this is a simple type of ‘field of bullets’ model ([9], [12], [14]). This model is quite restrictive ([11]) and a more realistic extension allows each species to have its own survival probability – this is the model we study in this paper. Under this model, we would like to be able to predict the PD score of the set of taxa that survive. This ‘future PD’ is a random variable with a well-defined distribution, but to date, most attention has focused on just its mean (that is, the expected PD score of the species that survive). For example, the ‘Noah’s Ark problem’ ([6] [13] [10]) attempts to maximize expected future PD by allocating resources that increase the survival probabilities in a constrained way. Clearly, one could consider other properties of the distribution of future PD – for example the probability (let us call it the $PL_0$ value) that future PD is less than some critical lower limit ($L_0$). Given different conservation strategies, we may wish to maximize expected PD or minimize the $PL_0$ value. A natural question is how are these two quantities related?

To address these sorts of questions, we need to know the full distribution of future PD. In this paper, we show that for large trees, future PD is (asymptotically) normally distributed. Given the increasing trend in biology of constructing and analysing phylogenetic trees that contain large numbers of species ($10^2 - 10^3$), we see this result as timely. Our work was also motivated by the suggestive form of distributions obtained by simulating future PD by sampling 12-leaf subtrees randomly from 64-leaf trees from Nee and May ([9], see also [14]). To formally prove the normal limit law requires some care, as future PD is not a sum of independent random variables (even though the survival events for the taxa at the leaves are treated independently); consequently, the usual central limit theory does not immediately apply.

This limit law has some useful consequences for applications. For example, it means that for a large tree, the $PL_0$ value can be estimated by the area under a normal curve to the left of $\frac{L_0 - \mathbb{E}(PD)}{\sqrt{\text{Var}(PD)}}$. In particular, we see that the relation between the $PL_0$ value and expected future PD ($\mathbb{E}(PD)$) involves scaling by the standard deviation of future PD (so strategies that aim to maximize expected future PD may not necessarily minimize the $PL_0$ value).
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Our normal distribution result is asymptotic - that is, it holds for large trees. However, it is also useful to have techniques for calculating the exact PD distribution on any given tree. In Section 3, we show how this may be achieved by a polynomial time algorithm under the mild assumption that each edge length is an integer multiple of some fixed length. In Section 4, we show how our results can be easily modified to handle an ‘unrooted’ form of PD that has also been considered in the literature.

1.1. Definitions and preliminaries. Throughout this paper $X$ will denote a set of taxa (for example, different species, different genera or populations of the same species) and $X'$ will denote a subset of $X$. A rooted phylogenetic $X$–tree is a rooted tree in which (i) all edges are oriented away from the root, (ii) $X$ is the set of leaves (vertices of the tree with no outgoing edges) and (iii) every vertex except the leaves (and also possibly the root) has at least two out-going edges (allowing the root to have just one outgoing arc will be useful later). In systematic biology, these trees are used to represent evolutionary development of the set $X$ of taxa from their common ancestor (the root of the tree), and the orientation of the edges corresponds to temporal ordering. Given a rooted phylogenetic $X$–tree $T$, we let $E(T)$ denote the set of edges, and $E_P(T)$ denote the set of pendant edges (edges that are incident with a leaf).

Suppose we have a rooted phylogenetic $X$–tree $T$ and a map $\lambda$ that assigns a non-negative real-valued length $\lambda_e$ to each edge $e$ of $T$. Given the pair $(T, \lambda)$ and a subset $X'$ of $X$, the phylogenetic diversity of $X'$, denoted $PD(T, \lambda)(X')$ – or, more briefly, $PD(X')$ – is the sum of the $\lambda_e$ values of all edges that lie on at least one path between an element of $X'$ and the root of $T$. In the (generalized) field of bullets model (g-FOB), we have a triple $(T, \lambda, p)$ where $T$ is a rooted phylogenetic $X$–tree, $\lambda$ is an edge length assignment map, and $p$ is a map that assigns to each leaf $i \in X$ a probability $p_i$. Construct a random set $X'$ by assigning each element $i$ of $X$ to $X'$ independently with probability $p_i$. In biodiversity conservation we regard $X'$ as the set of taxa that will still exist (that is, not be extinct) at some time $t$ in the future; accordingly, we call $p_i$ the survival probability of $i$.

Considering the random variable $\varphi = \varphi_T = PD(T, \lambda)(X')$, which is the phylogenetic diversity of the random subset $X'$ of $X$ (consisting of those taxa that ‘survive’)

![Figure 1](image-url)
according to the process just described, we call $\varphi$ future phylogenetic diversity. An example of this process is shown in Fig. 1.

Note that in the g-FOB model, we can write

$$\varphi = \sum_e \lambda_e Y_e,$$

where $Y_e$ is the binary random variable which takes the value 1 if $e$ lies on at least one path between an element of $X'$ and the root of $T$, and which is 0 otherwise.

Moreover,

$$P[Y_e = 1] = 1 - \prod_{i \in C(e)} (1 - p_i),$$

where $C(e)$ is the set of elements of $X$ that are separated from the root of $T$ by $e$. Consequently, if we let

$$P_e := P[Y_e = 1] = 1 - \prod_{i \in C(e)} (1 - p_i),$$

then

$$\mathbb{E}[\varphi] = \sum_e \lambda_e P_e.$$

Equation (1) suggests that for large trees, $\varphi$ might be normally distributed, as it will be sum of many random variables (a normal distribution is also suggested by simulations described in [9, 14]). However, the random variables ($\lambda_e Y_e$) are not identically distributed and, more importantly, they are not independent. Therefore a straightforward application of the (usual) central limit theorem seems problematic. We show that under two mild restrictions, a normal law can be established for large trees. Moreover, neither of these two mild restrictions can be lifted (we exhibit a counter-example to a normal law in both cases).

Since a normal distribution is determined once we know both its mean and variance, it is useful to have equations for calculating both these quantities. Equation (3) provides a simple expression for the mean, and we now present an expression for the variance that is also easy to compute. Given two distinct edges of $T$, we write $e <_T f$ if the path from the root of $T$ to $f$ includes edge $e$ (or, equivalently, $C(f) \subseteq C(e)$).

**Lemma 1.1.**

$$\text{Var}[\varphi] = \sum_e \lambda_e^2 P_e (1 - P_e) + 2 \sum_{(e, f): e <_T f} \lambda_e \lambda_f P_f (1 - P_e).$$

**Proof.** From Equation (1) we have:

$$\text{Var}[\varphi] = \text{Cov}[\varphi, \varphi] = \sum_{e, f} \lambda_e \lambda_f \text{Cov}[Y_e, Y_f].$$

The covariance of $Y_e$ and $Y_f$ is

$$\text{Cov}[Y_e, Y_f] = \mathbb{E}[Y_e Y_f] - \mathbb{E}[Y_e] \mathbb{E}[Y_f] = P[Y_e = 1, Y_f = 1] - P[Y_e = 1] P[Y_f = 1].$$

Now, we have the following cases:
(1) $e \neq f$ and neither $e <_T f$ nor $f <_T e$. In this case, the subtree of $T$ with root edge $e$ and the subtree of $T$ with root edge $f$ do not have any leaves in common, and so $Y_e$ and $Y_f$ are independent. Thus, $\text{Cov}[Y_e, Y_f] = 0$.

(2) $e <_T f$. In this case, $C(f) \subset C(e)$ and so the survival of any taxon in $C(f)$ implies the survival of a taxon in $C(e)$; that is, $Y_f = 1$ implies $Y_e = 1$ and we have $\text{Cov}[Y_e, Y_f] = P[Y_f = 1] - P[Y_e = 1]P[Y_f = 1] = P_f(1 - P_e)$.

(3) $f <_T e$. This is analogous to case (2) (and, together with case (1), explains the factor of 2 in the expression on the right-hand side of our formula for $\text{Var}[\varphi]$).

(4) $e = f$. This case gives $\text{Cov}[Y_e, Y_f] = P[Y_e = 1](1 - P[Y_e = 1]) = P_e(1 - P_e)$ (and corresponds to the first term on the right hand-side of our formula for $\text{Var}[\varphi]$).

By considering these cases for $\text{Cov}[Y_e, Y_f]$, we obtain the result claimed. \hfill \Box

A consequence of this lemma is the following lower bound on the variance of future PD which will be useful later.

**Corollary 1.2.** Consider the $g$-FOB model on $(T, \lambda, p)$. Then,

$$\text{Var}[\varphi] \geq \sum_{e \in E_P(T)} \lambda_e^2 P_e(1 - P_e).$$

**Proof.** Notice that all the terms in the summation expression for $\text{Var}[\varphi]$ in Lemma 1.1 are non-negative, and so a lower bound on $\text{Var}[\varphi]$ is obtained by summing over those pairs $(e, f)$ for which $e = f$ is a pendant edge of $T$. This gives the claimed bound. \hfill \Box

2. **ASYMPTOTIC NORMALITY OF FUTURE PHYLOGENETIC DIVERSITY UNDER THE G-FOB MODEL**

Consider a sequence of such rooted phylogenetic trees:

$$T_1, T_2, \ldots, T_n \ldots$$

where $T_n$ has a leaf label set $X = \{1, \ldots, n\}$. Furthermore, suppose that for each tree we have an associated edge length function $\lambda = \lambda^{(n)}$ and a survival probability function $p = p^{(n)}$. For the sequence of $g$-FOB models $(T_n, \lambda^{(n)}, p^{(n)})$, we impose the following conditions (where $E_P(T_n)$ is the set of pendant edges of $T_n$):

**(C1)** For some $\epsilon > 0$ and for each $n$, we have:

$$\epsilon \leq p_i^{(n)} \leq 1 - \epsilon,$$

for all $i \in \{1, \ldots, n\}$ except for at most $A n^{\alpha}$ values of $i$, where $A, \alpha \geq 0$ are constants, with $\alpha < \frac{1}{2}$. 
(C2) Let $L(n) = \max\{\lambda_e^{(n)} : e \in E(T_n)\}$. Then, for each $n$, we have:

$$\sum_{e \in E_p(T_n)} \left(\lambda_e^{(n)}\right)^2 \geq B n^\beta L(n)^2,$$

for some constants $B > 0, \beta > 2\alpha$.

**Remarks concerning conditions (C1), (C2).**

Condition (C1) simply says that the survival of most taxa is neither (arbitrarily close to) certain nor impossible. The term $A n^\alpha$ provides the flexibility to allow for some of the taxa to have a survival probability that is very close to, or even equal to, 0 or 1.

Condition (C2) says, roughly speaking, that the pendant edges are, on average, not too short in relation to the longest edge in the tree. This is relevant for evolutionary biology, as it follows that for trees generated by a constant speciation rate ‘pure birth’ model (see, for example, [2]) condition (C2) holds in expectation (for any $\alpha \in (0, \frac{1}{2})$). A more formal statement of this claim, and its proof, is given in the Appendix.

Note that if condition (C2) holds for a value $\beta > 0$ then, $\beta$ is at most 1, since the terms in the summation expression in (C2) are all at most 1 and there are $O(n)$ of them.

Next, we state our main theorem, which describes the asymptotic normality of future phylogenetic diversity $\varphi_n = \varphi_{T_n}$. Since phylogenetic trees often contain a large number of taxa, the result allows one to approximate the distribution of future phylogenetic diversity with a normal distribution.

**Theorem 2.1.** Under conditions (C1) and (C2), $(\varphi_n - \mathbb{E}[\varphi_n]) / \sqrt{\text{Var}[\varphi_n]}$ converges in distribution to $N(0, 1)$ as $n \to \infty$, where $N(0, 1)$ denotes a standard normally distributed random variable.

We pause to note that one cannot drop either condition (C1) or (C2) in Theorem 2.1. It is clear that dropping (C1) is problematic (for example, set $p_i^{(n)} \in \{0, 1\}$ for all $i$ which leads to a degenerate distribution); as for (C2) the following example shows that we require $\beta$ to be strictly positive.

**Example: Condition (C2) cannot be removed**

Consider a tree $T_n$ with $n$ leaves. Leaves $1, \ldots, n - 1$ have incident edges that each have length $\frac{1}{\sqrt{n-1}}$ and all these edges are incident with a vertex that is adjacent to the root by an edge of length 1. Leaf $n$ has edge length 1 (see Fig. 2). Consider a sequence of $g$-FOB models with $p_i^{(n)} = s$ for all $i, n$, where $s$ is any number strictly between 0 and 1. Then $\varphi_n = A_n + B_n + C_n$ where $A_n$ is the contribution to $\varphi_n$ of the $n-1$ edges that are incident with leaves $1, \ldots, n-1$; $B_n$ is the contribution to $\varphi_n$ of the edge that connects these $n-1$ edges to the root of $T_n$.
and $C_n$ is the contribution to $\varphi_n$ of the edge incident with leaf $n$. Notice that $A_n$ is a sum of $n - 1$ i.i.d. binary $(0, 1)$ random variables, each of which takes the value 1 with probability $s$, and $C_n$ is a binary random variable which takes the value 1 with probability $s$. Consequently, $A_n$ is $n - 1$ i.i.d. binary $(0, 1)$ random variables, each of which takes the value 1 with probability $s$, and $C_n$ is a binary random variable which takes the value 1 with probability $s$. Furthermore, by the standard central limit theorem, $\frac{A_n - E[A_n]}{\sqrt{V\text{ar}[A_n]}}$ converges in distribution to $N(0, \frac{1}{2})$ (a normal random variable with mean 0 and variance $\frac{1}{2}$). Thus, $(\varphi_n - E[\varphi_n]) / \sqrt{\text{Var}[\varphi_n]}$ converges to the random variable $N(0, \frac{1}{2}) + W$ where $W$ is independent of $N(0, \frac{1}{2})$ and takes the value $s$ with probability $\frac{1-s}{\sqrt{2s(1-s)}}$ with probability $1 - s$. In particular, $(\varphi_n - E[\varphi_n]) / \sqrt{\text{Var}[\varphi_n]}$ does not converge in distribution to $N(0, 1)$. Notice that in this example, (C1) is satisfied, but (C2) fails since $\sum_{e \in E(T_n)} (\lambda_e^{(n)})^2 = 2L(n)^2$.

**Figure 2.** A tree for which future phylogenetic diversity does not become normally distributed as $n$ grows.

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We now provide a brief, informal outline of the approach we use to prove Theorem 2.1. The main idea is to decompose $T_n$ into a ‘central core’ and a large number of ‘moderately small’ pendant subtrees. Each edge in the central core separates the root from enough leaves so that we can be very sure that at least one of these leaves survives – consequently the combined PD-contribution of this central core converges in probability to a fixed (non-random) function of $n$. Regarding the pendant subtrees, their contributions to the PD score are independent and although they are not identically distributed random variables, their combined variance grows sufficiently quickly that we can establish a normal law for their sum by a standard central limit theorem.

**Proof of Theorem 2.1** We first note that it is sufficient to establish Theorem 2.1 under (C1) and the seemingly stronger condition:

$$(C2^*) \quad L(n) = 1, \quad \sum_{e \in E_p(T_n)} (\lambda_e^{(n)})^2 \geq Bn^\beta \text{ for constants } B > 0, \beta > 2\alpha.$$  

To see why, suppose we have established Theorem 2.1 under (C1), (C2*). For a sequence $T_n$ (with associated maps $\lambda^{(n)}$, $p^{(n)}$) satisfying (C1), (C2), let $\mu_e^{(n)} = L(n)^{-1}\lambda_e^{(n)}$ for each edge $e$ of $T_n$ and each $n$. Note that, by Equation (1), the
normalized $\varphi$ score (namely $(\varphi_n - E[\varphi_n]) / \sqrt{\text{Var}[\varphi_n]}$) for $(T_n, \mu(n), p(n))$ equals the normalized $\varphi$ score for $(T_n, \lambda(n), p(n))$ and that $(T_n, \mu(n), p(n))$ satisfies (C2*). Thus we will henceforth assume conditions (C1) and (C2*).

Next, we make a notational simplification: for the remainder of the proof, we will write $\lambda(n)_e$ as $\lambda_e$ and $p(n)_i$ as $p_i$ (but respecting in the proof that these quantities depend on $n$). Also, for a sequence of random variables $(Y_n)$, we write $Y_n \xrightarrow{P} a$ to denote that $Y_n$ converges in probability to a constant $a$, and $Y_n \xrightarrow{D} Y$ to denote that $Y_n$ converges in distribution to a random variable $Y$.

Since $\beta > 2\alpha$, we may select a value $\gamma$ with $\alpha < \gamma < \beta/2$, and set $f(n) := n^\gamma$. We partition the edges of $T_n$ into two classes $E_{1}^n$ and $E_{2}^n$ and we define a third class $E_{12}^n \subseteq E_{1}^n$ as follows: Let $n_e$ denote the number of leaves of $T_n$ that are separated from the root by $e$. Then set:

- $E_{1}^n$: edges $e$ of $T_n$ with $n_e \leq f(n)$;
- $E_{2}^n$: edges $e$ of $T_n$ with $n_e > f(n)$;
- $E_{12}^n$: edges $e \in E_{1}^n$ such that $e$ is adjacent to an edge $f \in E_{2}^n$.

For an edge $e \in E_{12}^n$ of $T_n$, we make the following definitions:

- $t_e$ denotes the subtree of $T_n$ consisting of edge $e$ and all other edges of $T_n$ that are separated from the root by $e$.
- $\varphi_e^n$ denotes the future phylogenetic diversity of $t_e$, under the probabilistic model described above.

See Fig. 3 for a schematic summary of these concepts.

**Figure 3.** A representation of the decomposition of $T_n$ in the proof of Theorem 2.1.

For $\varphi_n$, Equation 1 gives

\[
\varphi_n = \sum_{e \in E_{1}^n} \lambda_e Y_e + \sum_{e \in E_{2}^n} \lambda_e Y_e = \sum_{e \in E_{12}^n} \varphi_e^n + \sum_{e \in E_{2}^n} \lambda_e Y_e.
\]
Let
\[ \lambda_n = \sum_{e \in E_2^n} \lambda_e, \quad Z_n = \sum_{e \in E_{12}^n} \varphi_e^n, \quad \text{and} \quad R_n = \sum_{e \in E_2^n} \lambda_e (1 - Y_e). \]

With this notation, we can re-write (4) as
\[ \varphi_n = \lambda_n + Z_n - R_n. \]

**Lemma 2.2.** \( R_n \xrightarrow{P} 0. \)

**Proof.** Since \( \text{Var}[R_n] = \mathbb{E}[R_n^2] - \mathbb{E}[R_n]^2 \) and \( \mathbb{E}[R_n^2] \geq \mathbb{E}[R_n]^2 \), it is sufficient to show that \( \mathbb{E}[R_n^2] \xrightarrow{P} 0 \) (the claim that \( R_n \xrightarrow{P} 0 \) then follows by Chebyshev’s inequality).

We have
\[ \lambda_n = \sum_{e \in E_2^n} \lambda_e \lambda_f (1 - Y_e)(1 - Y_f) \leq |E_2^n| \sum_{e \in E_2^n} (1 - Y_e), \]

since \( \lambda_e, \lambda_f \leq 1 \) by \( (C2^*) \), and \( (1 - Y_f) \leq 1 \) for all \( f \in E_2^n \). Thus,
\[ \mathbb{E}[R_n^2] \leq |E_2^n| \cdot \max \{ P[Y_e = 0] : e \in E_2^n \}. \]

Now, for any edge \( e \in E_2^n \) there are at least \( n^\gamma - An^\alpha \) elements \( i \) of \( C(e) \) for which \( p_i \geq \epsilon \) (by \( (C1) \)) and thus
\[ P[Y_e = 0] \leq (1 - \epsilon)^{n^\gamma - An^\alpha}. \]

Since \( |E_2^n| < 2n \), Equation (6) and the inequality \( \alpha < \gamma \) gives
\[ \mathbb{E}[R_n^2] \leq 4n^2 \cdot (1 - \epsilon)^{n^\gamma - An^\alpha} \xrightarrow{n \to \infty} 0, \]
as required. \( \square \)

**Lemma 2.3.** Under conditions \( (C1) \) and \( (C2^*) \), we have
\[ \sum_{e \in E_P(T_n)} (\lambda_e^{(n)})^2 P_e (1 - P_e) \geq B \epsilon^2 (1 + o(1)) n^\beta, \]
where \( o(1) \) denotes a term that tends to 0 as \( n \to \infty \).

**Proof.** Let \( U_n \) be the set of those pendant edges \( e \) of \( T_n \) for which the leaf incident with \( e \) has its survival probability in the interval \( [\epsilon, 1 - \epsilon] \), and let \( V_n \) denote the set of the remaining pendant edges of \( T_n \). Clearly,
\[ \sum_{e \in E_P(T_n)} (\lambda_e^{(n)})^2 P_e (1 - P_e) \geq \epsilon^2 \sum_{e \in U_n} (\lambda_e^{(n)})^2, \]
and by \( (C2^*) \) we have
\[ Bn^\beta \leq \sum_{e \in E_P(T_n)} (\lambda_e^{(n)})^2 \leq \sum_{e \in U_n} (\lambda_e^{(n)})^2 + |V_n| \]
where the last term ($|V_n|$) is an upper bound on $\sum_{e \in V_n} (\lambda^{(n)}_e)^2$ by virtue of the bound $|\lambda^{(n)}_e| \leq 1$ (by (C2*)). Since $|V_n| \leq An^\alpha$, Equations (11) and (12) give

$$\sum_{e \in E_P(T_n)} (\lambda^{(n)}_e)^2 P_e (1 - P_e) \geq \epsilon^2 (Bn^\beta - An^\alpha) = B\epsilon^2 (1 + o(1)) n^\beta.$$  

Lemma 2.4. The random variable $\psi_n = (Z_n - \mathbb{E}[Z_n]) / \sqrt{\text{Var}(Z_n)} \xrightarrow{D} N(0, 1)$.

Proof. We can apply a version of the central limit theorem for double arrays of random variables. The required theorem can be found in [13] and states the following. For each $n$, let $X_{n1}, \ldots, X_{nr}$ be $r = r(n)$ independent random variables with finite $p$th moments for some $p > 2$. Let

$$A_n = \sum_j \mathbb{E}[X_{nj}], \quad B_n = \sum_j \text{Var}[X_{nj}].$$

If

$$B_n^{-p/2} \sum_j \mathbb{E}[[X_{nj} - \mathbb{E}[X_{nj}]]^p] \to 0 \text{ as } n \to \infty,$$

then $W_n = (\sum_j X_{nj} - A_n) / \sqrt{B_n} \xrightarrow{D} N(0, 1)$. We apply this theorem by taking $X_{n1}, \ldots, X_{nr} = \{\phi^n_e : e \in E_{12}^n\}$, since the random variables $\{\phi^n_e : e \in E_{12}^n\}$ are clearly independent. With our notation $Z_n = \sum_{e \in E_{12}^n} \phi^n_e$, we have $A_n = \mathbb{E}[Z_n]$, $B_n = \text{Var}[Z_n]$ and $W_n = \psi_n$. Thus, we only need to verify condition (9) in order to establish Lemma 2.4.

By Corollary 1.2 we have:

$$\text{Var}[\phi^n_e] \geq \sum_{f \in E_P(t_e)} \lambda^2_f P_f (1 - P_f).$$

This lower bound and the independence of $\{\phi^n_e : e \in E_{12}^n\}$, implies:

$$B_n = \text{Var}[Z_n] = \sum_{e \in E_{12}^n} \text{Var}[\phi^n_e] \geq \sum_{e \in E_{12}^n} \sum_{f \in E_P(t_e)} \lambda^2_f P_f (1 - P_f)$$

Consequently, by Lemma 1.3, and the fact that every pendant edge occurs in $E_P(t_e)$ for some $e \in E_{12}^n$, we obtain

$$B_n \geq B\epsilon^2 (1 + o(1)) n^\beta.$$  

Consider now the absolute central moments in (9). We have

$$\mathbb{E}[[X_{nj} - \mathbb{E}[X_{nj}]]^p] = \mathbb{E}[[\phi^n_e - \mathbb{E}[\phi^n_e]]^p] \leq L^p_e,$$

where $L_e$ is the sum of the lengths of the edges of $t_e$. Since $t_e$ has less than $2n_e$ edges, and the edge lengths are bounded from above by 1 (under (C2*)) and $e \in E_{12}^n$ implies $n_e \leq f(n)$, we obtain $L_e \leq 2n_e \leq 2f(n)$. Now we have

$$\mathbb{E}[[\phi^n_e - \mathbb{E}[\phi^n_e]]^p] \leq 2^p f(n)^p.$$

□
Combining the bounds (10) and (11), and noting that \(|E_{12}^n| \leq 2n\) and \(f(n) = n^\gamma\) we obtain:

\[
B_n^{-p/2} \sum_{e \in E_{12}^n} \mathbb{E}[|\varphi_e^n - \mathbb{E}[\varphi_e^n]|^p] \leq \frac{|E_{12}^n| 2^p f(n)^p}{(Be^2(1 + o(1)))^{p/2}n^{\beta p/2}} \leq C(p)n^{1 + p(\gamma - \beta/2)},
\]

for some constant \(C(p) > 0\) independent of \(n\). Now, since \(\gamma < \beta/2\), the exponent of \(n\) in the obtained upper bound is negative for any \(p > (\beta/2 - \gamma)^{-1}\). Since there are some \(p > 2\) satisfying this inequality and consequently satisfying condition (9), the proof of Lemma 2.4 is complete. \(\square\)

We return to the proof of Theorem 2.1. Using Equation (5) and the notation of Lemma 2.4, we get

\[
\varphi_n - \mathbb{E}[\varphi_n] = \frac{\lambda_n + Z_n - R_n - (\lambda_n + \mathbb{E}[Z_n] - \mathbb{E}[R_n])}{\sqrt{\text{Var}[\varphi_n]}} = C_n \psi_n + D_n
\]

where

\[
C_n = \frac{\sqrt{\text{Var}[Z_n]}}{\sqrt{\text{Var}[\varphi_n]}}, \quad D_n = -\frac{R_n - \mathbb{E}[R_n]}{\sqrt{\text{Var}[\varphi_n]}}.
\]

By Lemma 2.2 and the fact that \(\text{Var}[\varphi_n]\) does not converge to 0 (by Corollary 1.2 Lemma 2.3 and condition (C2*)), we have:

(12) \(D_n \overset{p}{\rightarrow} 0\).

Moreover, by (5), \(\text{Var}[\varphi_n] = \text{Var}[Z_n] + \text{Var}[R_n] - 2 \text{Cov}[Z_n, R_n]\), so that

\[
C_n^{-2} - 1 = \frac{\text{Var}[R_n]}{\text{Var}[Z_n]} - 2\rho \frac{\sqrt{\text{Var}[R_n]}}{\sqrt{\text{Var}[Z_n]}},
\]

where \(\rho\) is the correlation coefficient of \(R_n\) and \(Z_n\). Now, by Lemma 2.2 we have \(\lim_{n \rightarrow \infty} \text{Var}[R_n] = 0\). Thus, since \(\text{Var}[Z_n]\) is bounded away from 0 (by (10)), and \(\rho \in [-1, 1]\) we have:

(13) \(\lim_{n \rightarrow \infty} C_n = 1\).

To complete the proof of Theorem 2.1 we apply Slutsky’s Theorem [11] which states that if \(X_n, Y_n, W_n\) are sequences of random variables, and \(X_n \overset{p}{\rightarrow} a, Y_n \overset{p}{\rightarrow} b\), (where \(a, b\) are constants) and \(W_n \overset{D}{\rightarrow} W\) (for some random variable \(W\)) then \(X_nW_n + Y_n \overset{D}{\rightarrow} aW + b\). In our setting, we will take \(X_n = C_n, Y_n = D_n, W_n = \psi_n,\) and \(W = N(0, 1)\) (the standard normal random variable). The condition that \(\psi_n \overset{D}{\rightarrow} N(0, 1)\) was established in Lemma 2.4 and the conditions \(C_n \overset{p}{\rightarrow} 1, D_n \overset{p}{\rightarrow} 0\) were established in (13) and (12) (note that the convergence of a sequence of real numbers in (13) is just a special case of convergence in probability). Thus,

\[
(\varphi_n - \mathbb{E}[\varphi_n]) / \sqrt{\text{Var}[\varphi_n]} = C_n \psi_n + D_n \overset{D}{\rightarrow} N(0, 1),
\]
which completes the proof of Theorem 2.1.

3. Computing the PD distribution

In this section we describe an algorithm to calculate the distribution of \( \varphi_T \) efficiently under the g-FOB model. An approximate distribution could also be obtained by simulation, but the approach we present here allows us to derive the exact distribution of \( \varphi_T \). Note that we do not require conditions (C1) or (C2) in this section. We make the simplifying assumption that the edge lengths are non-negative integer-valued, which implies that \( \varphi_T \) can only have values in the set \( \{0, 1, \ldots, L\} \), where \( L = PD(X) = \sum \lambda_e \). This assumption is not problematic in practice, as we can rescale all the edge lengths so that they are (arbitrarily close to) integer multiples of some small value.

We also assume that the input tree is such that the root has one outgoing edge and all other non-leaf vertices have exactly two outgoing edges. This assumption does not affect the generality of our method, as any tree can be modified to satisfy it, without changing the distribution for \( \varphi_T \): one can resolve multifurcations arbitrarily and possibly insert an edge below the root, always assigning length 0 to the newly introduced edges.

Consistent with the notation used before, \( \varphi_e \) denotes the contribution to \( \varphi_T \) that comes from \( e \) and the edges separated from the root by \( e \). Then, for any edge \( e \) and integer \( x \), define

\[
 f_e(x) := \mathbb{P}[\varphi_e = x, Y_e = 1].
\]

Also recall that \( P_e = \mathbb{P}[Y_e = 1] \).

Clearly, if \( e \) is the only edge attached to the root of \( T \), then \( f_e \) and \( P_e \) are all that is needed to derive the distribution of \( \varphi_T \): simply observe that

\[
 \mathbb{P}[\varphi_T = x] = \mathbb{P}[\varphi_e = x, Y_e = 1] + \mathbb{P}[\varphi_e = x, Y_e = 0] = f_e(x) + (1 - P_e) \cdot I_{x=0},
\]

where \( I_p \) equals 0 or 1 depending on proposition \( p \) being false or true, respectively.

The algorithm then consists in doing a depth-first (bottom-up) traversal of all the edges, so that each time an edge \( e \) is visited, the values of \( P_e \) and \( f_e(x) \), for all \( x \in \{\lambda_e, \lambda_e + 1, \ldots, L\} \), are calculated using the following recursions. We may then use the \( P_e \) and \( f_e(x) \) values of the root edge to calculate the distribution of \( \varphi_T \).

**Recursion for** \( f_e(x) \).

- If \( e \) leads into leaf \( i \), then

\[
 f_e(x) = \mathbb{P}[\varphi_e = \lambda_e, Y_e = 1] \cdot I_{x=\lambda_e} = p_i \cdot I_{x=\lambda_e}.
\]
is 0 and that therefore there is no need to calculate and store \( f_x \) with \( x > \lambda_c \).

Equation (14) is easily proved; we have

\[
\begin{align*}
\phi_c \cdot \phi_d &= \sum_{i=0}^{x-\lambda_c} \phi_c \cdot \phi_d(x-\lambda_c-i) + (1-P_d) \cdot \phi_c(x-\lambda_c) + (1-P_c) \cdot \phi_d(x-\lambda_c).
\end{align*}
\]

where the second equality is obtained by restating event \( \phi_c = x \) in terms of \( \phi_c \) and \( \phi_d \), which is possible since we make assumptions on \( Y_c \) and \( Y_d \). Thus,

\[
\phi_c = \sum_{i=0}^{x-\lambda_c} \phi_c \cdot \phi_d(x-\lambda_c-i) + (1-P_d) \cdot \phi_c(x-\lambda_c) + (1-P_c) \cdot \phi_d(x-\lambda_c).
\]

where the first equality is obtained by using the independence between the survival events in \( C(c) \) and \( C(d) \). Note that in the first expression in the second equality, the range of the sum has been reduced, as \( \phi_c(i) = 0 \) for \( i < \lambda_c \) and \( \phi_d(x-\lambda_c-i) = 0 \) for \( x - \lambda_c - i < \lambda_d \).

Recursion for \( P_c \).

- If \( c \) leads into leaf \( i \), then \( P_c = p_i \).
- If \( c \) leads into the tail of edges \( c \) and \( d \), then \( P_c = P_c + P_d - P_c P_d \).

**Computational complexity.** For any given \( c \), the calculation of \( P_c \) is done in \( O(1) \) time, whereas that of each of the \( f_c(x) \) values requires \( O(x) = O(L) \) time (see recursion (14)), giving a total of \( O(L^2) \). Calling \( n \) the number of leaves in \( T \), there are \( 2n - 1 \) edges in \( T \) and the entire procedure takes \( O(nL^2) \) time.

A more efficient version of the algorithm can be obtained by restricting the calculation of \( f_c(x) \) to the values of \( x \in \{\lambda_c, \lambda_c + 1, \ldots, L_c \} \), where \( L_c \) is the maximum value that \( \phi_c \) can attain (namely the sum of the lengths of all the edges separated from the root by \( c \), including \( c \) itself). Note that the sum in (14) can then be further restricted to the values of \( i \) such that \( i \leq L_c \) and \( x - \lambda_c - i \leq L_d \). Using this more efficient algorithm, it is easy to see that the calculation of all the \( f_c(x) \) values for a given internal edge \( c \) takes \( O(L_c L_d + L_c) \) time, where \( c \) and \( d \) are the edges that \( c \) leads into. Noting that the sum of all the \( L_c L_d \) terms, for all
sister edges \(c\) and \(d\), is bounded above by \(L^2\), this shows that the running time of the entire procedure is \(O(L^2 + nL)\). Since typically every pair of taxa in the tree is separated by at least one edge of positive length, we have that \(n = O(L)\) and therefore the running time above is equivalent to \(O(L^2)\).

Regarding memory requirements, note that each time we calculate the information relative to \(e\) (namely \(P_e\) and \(f_e(x)\)), the information relative to the edges it leads to (if any) can be deleted, as it will never be used again. So, at any given moment the information of at most \(n\) ‘active’ edges needs to be stored. If we use the range restriction just described, the sizes of the \(f_e(x)\) vectors for all the active edges sum to a number bounded above by \(n + L\), and therefore the algorithm requires \(O(n + L)\) space, equivalent to \(O(L)\) if \(n = O(L)\).

4. Extension to unrooted PD

There is a simple modification of the definition of phylogenetic diversity that is also relevant in biology ([5], [10]). Given a subset \(X'\) of \(X\), we can evaluate the sum of the lengths of the edges in the minimum subtree connecting (only) the leaves in \(X'\). This score – which we will denote by \(uPD(X')\) and refer to as the ‘unrooted PD’ score of \(X'\) – is equivalent to \(PD(X')\) if the path connecting two leaves in \(X'\) traverses the root of \(T\). However, in general, \(uPD(X') \leq PD(X')\) (Fig. 4 shows an example where \(uPD(X') < PD(X')\)). This alternative concept of phylogenetic diversity has the advantage that it can be defined on either rooted or unrooted phylogenetic trees. Of course, the g-FOB model is also defined naturally on unrooted trees, and so it makes sense to consider the distribution of \(uPD\) under the g-FOB model in this more general setting. A natural question is whether Theorem 2.1 is still valid, (that is, is the future \(uPD\) of (rooted or unrooted) trees also asymptotically normal under conditions (C1) and (C2)?)? We now answer this question (affirmatively) and also show how to extend the computation of the exact future PD distribution to unrooted trees.

Let the random variable \(\phi' = \varphi'_f\) denote the \(uPD\) score of the random subset \(X'\) of \(X\) (consisting of those taxa that will still exist at some time \(t\) in the future).
where $\lambda(18)$ and $\phi$ denote the subtree with root edge $T$ and $E\phi$ contribution to phylogenetic diversity of $E\phi$ functions. It can be shown that Theorem 2.1 is still valid for uPD; that is, under

$$\text{Var}(\lambda) = \sum_{e \in E_1} \lambda_e Y'_e,$$

where $X_1(e)$ and $X_2(e)$ are the bipartition of the two subsets of $X$ that are separated by edge $e$. Thus if we let $P_1(e)$ denote the probability that at least one taxon in $X_1(e)$ survives (for $i \in \{1, 2\}$), then the expected value of $\phi'$ (analogous to (3)) is

$$\mathbb{E}[\phi'] = \sum_{e \in E} \lambda_e P_1(e)P_2(e).$$

Regarding $\text{Var}[\phi']$ there is an analogous formula to that given in Lemma 1.1.

Consider now a sequence $T_1, T_2, \ldots, T_n$ of (rooted or unrooted) phylogenetic trees where $T_n$ has $n$ leaves, and assume that this sequence satisfies conditions (C1) and (C2) when each $T_n$ has associated edge length and leaf survival probability functions. It can be shown that Theorem 2.1 still is valid for uPD; that is, under the same conditions, $(\phi'_n - \mathbb{E}[\phi'_n])/\sqrt{\text{Var}[\phi'_n]}$ converges in distribution to $N(0, 1)$ as $n \to \infty$.

To establish this asymptotic normality of $\phi'_n$ under conditions (C1) and (C2*) (and thereby (C1) and (C2)) requires slight modifications to the proof of Theorem 2.1 and we now provide an outline of the argument. The main difference is that now each edge $e$ induces a bipartition $X = X_1(e) \cup X_2(e)$ of the taxon set and so we decompose $T_n$ in a slightly different way. For simplicity, assume that $|X_1(e)| \leq |X_2(e)|$ and consider the following edge sets (the definition of the function $f(n)$ is as in the rooted case):

$E_1^n$: edges $e$ of $T_n$ with $|X_1(e)| \leq f(n)$.

$E_2^n$: edges $e$ of $T_n$ with $|X_1(e)| > f(n)$.

$E_{12}^n$: edges $e \in E_1^n$ such that $e$ is adjacent to an edge $f \in E_2^n$.

For $\phi'_n$ we obtain the following equation:

$$\phi'_n = \sum_{e \in E_1^n} \lambda_e Y'_e + \sum_{e \in E_2^n} \lambda_e Y'_e = \sum_{e \in E_1^n} \lambda_e Y'_e + \lambda_n - R'_n,$$

where $\lambda_n = \sum_{e \in E_2^n} \lambda_e$ and $R'_n = \sum_{e \in E_2^n} \lambda_e (1 - Y'_e)$. For an edge $e \in E_1^n$, let $t_e$ denote the subtree with root edge $e$ and with leaf set $X_1(e)$. Let $(\phi'_e)n'$ denote the contribution to $\phi'_n$ by the edges in $t_e$. Furthermore, let $\phi_e^n$ be the rooted future phylogenetic diversity of $t_e$, $Z_n = \sum_{e \in E_{12}^n} \phi_e^n$ as in the rooted case, $W_e = \phi_e^n - (\phi'_e)n'$
and $V_n = \sum_{e \in E_{12}} W_e$. With this notation, we get

$$
(19) \quad \varphi'_n = \sum_{e \in E_{12}^u} \varphi_n^u + \lambda_n - R'_n = \sum_{e \in E_{12}^u} \varphi_n^u - \sum_{e \in E_{12}^u} W_e + \lambda_n - R'_n = Z_n - V_n + \lambda_n - R'_n.
$$

Now we can apply Lemma 2.4 and Slutsky’s Theorem to complete the proof.

### 4.1. Computing the uPD distribution

Finally we show how the algorithm described in Section 3 for computing the PD distribution can be modified to calculate the distribution of unrooted PD. As before, we assume the edge lengths are non-negative integers and we preprocess $T$ (possibly rooting it in an arbitrary vertex) so that the number of outgoing edges is 1 for the root and 2 for all the other non-leaf vertices. Since $T$ is now rooted, $C(e)$ and the random variables $Y_e$ are well defined. We also define $\varphi'_e$ as the uPD of the surviving taxa in $C(e)$. Then, for any integer $x$, define

$$
\varphi'_e(x) := \Pr[\varphi'_e = x, Y_e = 1].
$$

As before, if $e$ is the root edge of $T$, then $\varphi'_e$ and $P_e$ are sufficient to derive the distribution of $\varphi'_T$:

$$
\Pr[\varphi'_T = x] = \varphi'_e(x) + (1 - P_e) \cdot I_{x=0}.
$$

An algorithm to calculate the distribution of $\varphi'_T$ can be obtained with a simple modification of the algorithm for $\varphi_T$: for each edge $e$, in addition to calculating $P_e$ and $f_e(x)$, also calculate $\varphi'_e(x)$, for all $x \in \{0, 1, \ldots, L\}$. For this purpose, the following recursion is used (note that the $\varphi'_e$ values may depend on $f_e$ and $f_d$ as well as on $\varphi'_e$ and $\varphi'_d$), which is why we retain the calculation of the $\varphi'_e$ values even though they are not directly implicated in determining $\Pr[\varphi'_T = x]$).

### Recursion for $\varphi'_e(x)$.

- If $e$ leads into leaf $i$, then
  
  $$
  \varphi'_e(x) = p_i \cdot I_{x=0}.
  $$

- If $e$ leads into the tail of edges $c$ and $d$, then

$$
(20) \quad \varphi'_e(x) = \sum_{i=\lambda_e}^{x-\lambda_e} f_c(i) \cdot f_d(x - i) + (1 - P_d) \cdot \varphi'_c(x) + (1 - P_e) \cdot \varphi'_d(x),
$$

which is proved in a way similar to (14):

$$
\varphi'_e(x) = \Pr[\varphi'_e = x, Y_e = 1, Y_d = 1] + \Pr[\varphi'_e = x, Y_e = 1, Y_d = 0] + \Pr[\varphi'_e = x, Y_e = 0, Y_d = 1] \\
= \Pr[\varphi_c + \varphi_d = x, Y_e = 1, Y_d = 1] + \Pr[\varphi_c = x, Y_e = 1, Y_d = 0] + \Pr[\varphi_d = x, Y_e = 0, Y_d = 1] \\
= \sum_{i=\lambda_e}^{x-\lambda_e} f_c(i) \cdot f_d(x - i) + (1 - P_d) \cdot \varphi'_c(x) + (1 - P_e) \cdot \varphi'_d(x).
$$
5. Concluding remarks

The main result of this paper (Theorem 2.1) has been to establish a limiting normal distribution for future PD on large phylogenetic trees. This theorem assumes an underlying generalized ‘field of bullets’ model, and imposes two further mild conditions (conditions (C1) and (C2)). In this setting Theorem 2.1 reduces the problem of computing the distribution of future PD to that of determining just two parameters – its mean and variance – and these can be readily computed by Equation (3) and Lemma 1.1. Using the resulting normal distribution one can easily compute the probability under the model that future PD will fall below any given critical value. This may also be helpful in designing strategies to minimize this probability (analogous to the ‘Noah’s Ark problem’ which tries to maximize expected future PD).

In practice, the use of a normal distribution based on Theorem 2.1 requires that the number of taxa is moderate (> 50), that the survival probabilities are not too extreme (condition (C1)), and that the length of the pendant edges on average are not too small in relation to the largest edge length in the tree (condition (C2)). If these conditions are violated, it would be prudent to use the exact algorithm we have described in the paper, as this requires neither a large number of taxa nor condition (C1) or (C2). To apply this algorithm may involve some small adjustment to the edge lengths to make them integral multiples of some common value.

Regarding the ‘mild conditions’ for Theorem 2.1 (namely (C1) and (C2)), we showed that neither can be dropped completely from the statement of the theorem. However it is likely that both conditions could be weakened somewhat, though at the risk of complicating the description of the conditions and the proof of Theorem 2.1.

It would be interesting to explore other extinction models that weaken the strong assumption in the g-FOB model that taxon extinction events are independent. One such model would regard extinction as a continuous-time Markov process in which the extinction rate of a taxon \( i \) at any given time \( t \) is the product of an intrinsic extinction rate \( r_i \), with a factor that depends on the set of species in the tree that are extant at time \( t \). In general, such processes could be very complex, so a first step would be to identify a simple model that nevertheless captures more biological realism than the g-FOB model.

6. Appendix

Condition (C2) is satisfied in expectation for trees generated under a continuous-time pure-birth model.

Consider a model where each lineages persist for a random period of time before speciating, and that these persistence times are i.i.d. random variables with exponential distribution with mean \( s > 0 \) (This model is sometimes called the ‘Yule
model' in phylogenetics). Now suppose we sample the process at some time during which the tree has \( n \) leaves. Let \( T_n \) denote this tree (with its associated edge lengths) and let \( \mu_P(n) \) denote the average length of the pendant edges of \( T_n \).

**Proposition 6.1.** Under a constant birth model with speciation rate \( s \) and \( \beta \in (0,1) \) there is a constant \( B > 0 \) for which the expected value of

\[
\sum_{e \in E_P(T_n)} (\lambda_e(n))^2 - Bn^\beta L(n)^2
\]

is strictly positive for all \( n \geq 3 \).

**Proof.** By using the inequality \( \sum_{i=1}^{n} x_i^2 \geq \frac{1}{n} (\sum_{i=1}^{n} x_i)^2 \) we have

\[
E \left[ \sum_{e \in E_P(T_n)} (\lambda_e(n))^2 - Bn^\beta L(n)^2 \right] \geq nE[\mu_P(n)]^2 - Bn^\beta E[L(n)^2]
\]

and the proposition follows (by choice of a sufficiently small value of \( B > 0 \)) once we establish the following two results.

(i) \( E[\mu_P(n)] \geq s/6 \) for all \( n \geq 3 \).

(ii) \( n^{-\eta}E[L(n)^2] \to 0 \) as \( n \to \infty \), for any \( \eta > 0 \).

To establish result (i), let \( S_n \) denote the sum of the lengths of the pendant edges of \( T_n \) up till the point when the number of species first changes from \( n - 1 \) to \( n \), and excluding the (length of the) pendant edge on which this speciation event occurs. Thus \( S_n \) is a sum of lengths of \( n - 2 \) pendant edges. [For example, \( S_3 \) has an exponential distribution with mean \( s/2 \), as it is the length of the edge that does not first speciate, up until the time when one of the two edges in the tree first speciates]. Since we are observing the tree \( T_n \) at some later time (but while it still has \( n \) leaves) then we clearly have:

\[(21) \quad \mu_P(n) \geq \frac{1}{n} S_n.\]

We will derive a recursion for the sequence \( E[S_n], n = 3, 4, \ldots \). Let \( \theta_n \) be an exponentially-distributed random variable with mean \( s/n \). Now, the random variable \( S_{n+1} \) takes the value \( S_n + (n - 1)\theta_n \), with probability \( 2/n \) (this is the case where the next speciation event occurs on one of the two edges that develop from the last speciation event). Otherwise (and so with probability \( 1 - 2/n \), \( S_{n+1} \) takes the value \( S_n + (n - 1)\theta_n - \lambda_e \), where \( \lambda_e \) is the length of one of the \( n - 2 \) pendant edges that contribute to \( S_n \) (selected uniformly at random from this set of edges).

Consequently,

\[
E[S_{n+1}] = \frac{2}{n}E[S_n] + (n - 1)\frac{s}{n} + (1 - \frac{2}{n})(E[S_n](1 - \frac{1}{n-2}) + (n - 1)\frac{s}{n})
\]

\[= \frac{n - 1}{n}(E[S_n] + s).\]

By using the initial condition \( E[S_3] = s/2 \), and this recursion, we have that \( E[S_n] = ns/2 - s \) for all \( n \geq 3 \). Taking expectations on both sides of inequality \( (21) \) gives

\[
E[\mu_P(n)] \geq \frac{1}{n}(ns/2 - s) = \frac{s}{2} - \frac{s}{n} \geq \frac{s}{6}.
\]
for all $n \geq 3$, thus proving (i).

To establish result (ii), observe that length of the longest edge in $T_n$ (namely $L(n)$) is bounded above by the length of the longest edge in the tree obtained from $T_n$ by allowing each leaf to evolve until it next speciates. Now, the lengths of the edges in this resulting trees is a set of $|E(T_n)|$ independent random variables each having an exponential distribution with mean $s$ (here $|E(T_n)|$ is the number of edges of $T_n$, which is at most $2n - 1$). Thus, if we let $Y_n$ be the maximum of $2n - 1$ i.i.d exponentially-distributed random variables, each with mean $s$, then $L(n) \leq Y_n$. Moreover, for any $x > 0$ we have:

\[
E[Y_n^2] = \int_0^\infty P[Y_n^2 > y] dy \leq x^2 + \int_{x^2}^\infty P[Y_n^2 > y] dy,
\]

where the first equality in (22) is a standard identity in probability theory for any non-negative random variable $Y_n^2$. Now, by Boole’s inequality,

\[
P[Y_n^2 > y] = P[Y_n > \sqrt{y}] \leq (2n - 1) \exp(-\sqrt{y}/s).
\]

Making the substitution $y = x^2 + t^2$, and applying the inequality $\sqrt{x^2 + t^2} \geq x + t \sqrt{2}$ we obtain

\[
\int_{x^2}^\infty P[Y_n^2 > y] dy \leq 2(2n - 1) \exp(-x^{2}/s\sqrt{2}) \int_{t=0}^\infty t \exp\left(-\frac{t}{s\sqrt{2}}\right) dt.
\]

Thus, taking $x = cs \log(n)$, for any $c > \sqrt{2}$, in (22) we obtain

\[
E[L(n)^2] \leq E[Y_n^2] \leq c^2 s^2 (\log(n))^2 + o(1),
\]

(where $o(1)$ is a term that tends to 0 as $n \to \infty$) and result (ii) now follows. □

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