

Coalescent Histories for Lodgepole Species Trees

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ABSTRACT

Coalescent histories are combinatorial structures that describe for a given gene tree and species tree the possible lists of branches of the species tree on which the gene tree coalescences take place. Properties of the number of coalescent histories for gene trees and species trees affect a variety of probabilistic calculations in mathematical phylogenetics. Exact and asymptotic evaluations of the number of coalescent histories, however, are known only in a limited number of cases. Here we introduce a particular family of species trees, the *lodgepole* species trees $(\lambda_n)_{n \geq 0}$, in which tree λ_n has $m=2n+1$ taxa. We determine the number of coalescent histories for the lodgepole species trees, in the case that the gene tree matches the species tree, showing that this number grows with $m!$ in the number of taxa m . This computation demonstrates the existence of tree families in which the growth in the number of coalescent histories is faster than exponential. Further, it provides a substantial improvement on the lower bound for the ratio of the largest number of matching coalescent histories to the smallest number of matching coalescent histories for trees with m taxa, increasing a previous bound of $(\sqrt{\pi}/32)[(5m-12)/(4m-6)]m\sqrt{m}$ to $[\sqrt{m-1}/(4\sqrt{e})]^m$. We discuss the implications of our enumerative results for phylogenetic computations.

Key words: coalescence, genealogy, phylogeny.

1. INTRODUCTION

ADVANCES IN THE MATHEMATICAL INVESTIGATION OF GENE GENEALOGIES and the increasing availability of genetic data from diverse taxa have clarified that species trees, representing the branching histories of populations of organisms, need not be reflected in gene trees that represent the histories of individual genomic regions (Pamilo and Nei, 1988; Maddison, 1997; Nichols, 2001). New developments concerning the relationship between gene trees and species trees have now led to new methods for species tree inference, new approaches to inferences about evolutionary phenomena from gene tree discordance, and an improved understanding of the branching descent process (Degnan and Rosenberg, 2009; Liu et al., 2009; Knowles and Kubatko, 2010).

Investigations of the evolution of genomic regions along the branches of species trees have also generated new combinatorial structures that can assist in studying gene trees and species trees (Maddison, 1997; Degnan and Salter, 2005; Than and Nakhleh, 2009; Wu, 2012). Among these structures are coalescent histories, structures that for a given gene tree topology and species tree topology represent possible pairings of coalescences in the gene tree with branches of the species tree on which the coalescences take place (Degnan and Salter, 2005; Rosenberg, 2007).

Coalescent histories are important in a number of types of studies of the relationship between gene trees and species trees. They have appeared in empirical investigations of the gene tree topologies likely to be produced along the branches of a given species tree (Rosenberg and Tao, 2008). They are a component of mathematical proofs that concern properties of evolutionary models of gene trees conditional on species trees (Allman et al., 2011; Than and Rosenberg, 2011). Coalescent histories also arise in studying state spaces for models that consider transitions along the genome among the gene genealogies represented at specific sites (Hobolth et al., 2007, 2011; Duteil et al., 2009).

Many coalescent histories might be possible for a given gene tree and species tree, and the number of possible coalescent histories is a key quantity in the study of gene trees and species trees. In particular, because the probability of a gene tree topology conditional on a species tree can be written as a sum over coalescent histories (Degnan and Salter, 2005), the time required for computing gene tree probabilities is proportional to the number of coalescent histories compatible with a given gene tree and species tree. Thus, to study computational aspects of the use of coalescent histories, it has been of interest to evaluate the number of coalescent histories permissible for a given pair consisting of a gene tree and a species tree.

Degnan and Salter (2005), who initiated the study of coalescent histories, reported that if the labeled gene tree topology and species tree topology have the same matching ‘‘caterpillar’’ shape with m taxa, then the number of coalescent histories is the Catalan number,

$$c_{m-1} = \frac{1}{m} \binom{2m-2}{m-1}. \quad (1)$$

The Catalan sequence c_m is asymptotic to $4^m/(m^{3/2}\sqrt{\pi})$. Rosenberg (2007) and Than et al. (2007) provided recursive procedures that list all possible coalescent histories given a gene tree and species tree, and Rosenberg (2007) offered simple recursive formulas for counting them. Rosenberg (2007, 2013) and Rosenberg and Degnan (2010) then solved the recursion in a number of specific cases.

What is the asymptotic behavior of the number of coalescent histories as the number of taxa increases? In Figure 1, we show values taken from Rosenberg (2007) for the number of coalescent histories for matching gene trees, for all species trees with $m \leq 9$ taxa. On a logarithmic scale, a linear model fits the values quite well, suggesting that in general, the number of coalescent histories for matching gene trees and species trees might grow exponentially in the number of taxa. Existing enumerations of coalescent histories in particular cases, both for the caterpillar trees in Equation 1 and in related caterpillar-like families (Rosenberg, 2013),

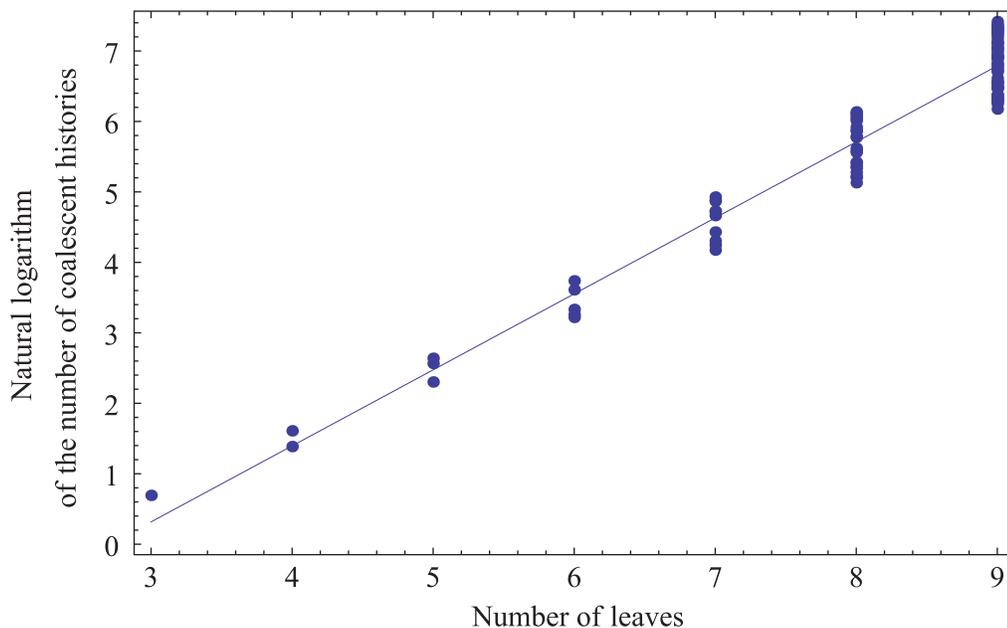


FIG. 1. Natural logarithm of the number of coalescent histories for all matching gene trees and species trees with at most nine taxa. The values plotted are taken from Tables 1–4 of Rosenberg (2007). Each dot corresponds to a tree of the specified size. The line represents a linear regression $y = a + bx$, with $a \approx -2.91891$ and $b \approx 1.07865$.

support this prediction. We might therefore expect that for a generic family of species trees of increasing size, the number of coalescent histories for the matching gene tree increases exponentially.

Here, we show that this prediction does not always hold. Indeed, we exhibit a family of species trees $(\lambda_n)_n$ —that we term the *lodgpole* family—whose number of coalescent histories grows with the double factorials, and thus increases at a rate that is faster than exponential in the number of taxa. We use the lodgpole family to further understand the variability at a given m of the number of coalescent histories for cases with matching gene trees and species trees. Rosenberg (2007) obtained a lower bound on the ratio of the largest number of coalescent histories to the smallest number of coalescent histories at m taxa, showing that this ratio was greater than a constant multiple of $(\sqrt{\pi}/32)[(5m-12)/(4m-6)]m\sqrt{m}$. Here we improve substantially upon this lower bound, demonstrating that it exceeds the much larger $[\sqrt{m-1}/(4\sqrt{e})]^m$.

2. PRELIMINARIES

2.1. Species trees and coalescent histories

A *species tree* is a binary rooted tree equipped with a labeling for the leaves. As in other studies of coalescent histories, a single labeling can without loss of generality be taken as representative of an unlabeled species tree topology. When the labeling is not needed, we abbreviate the arbitrarily labeled species tree by its unlabeled shape and consider the labeled and unlabeled topologies interchangeably. We consider matching gene trees and species trees with the same labeled topology t .

We term a coalescent history for the case when the gene tree and species tree have the same labeled topology a *matching coalescent history*. Given a species tree t , a mapping h from the internal nodes of t to the branches of t is a matching coalescent history of t when it satisfies both of the following two conditions: (a) for all leaves x in t , if x descends from internal node k in t , then x descends from branch $h(k)$ in t ; (b) for all internal nodes k_1 and k_2 in t , if k_2 is a descendant of k_1 in t , then branch $h(k_2)$ is descended from or coincides with branch $h(k_1)$ in t . Figure 2A shows an example of a matching coalescent history. The examples in Figure 2B and 2C are not matching coalescent histories; in Figure 2B, condition (a) is violated, and in Figure 2C, condition (b) is violated.

2.2. The lodgpole family of species trees

We focus here on the number of matching coalescent histories (*histories* or *coalescent histories* for short) for a particular family of species trees, $(\lambda_n)_{n \geq 0}$, that we call the *lodgpole* family. We define λ_0 as the 1-taxon tree. For $n \geq 0$, we inductively define λ_{n+1} by appending λ_n and a tree with two leaves (a *cherry*) to a common root (Fig. 3). Note that the tree λ_n has $m=2n+1$ rather than n taxa; we use n to denote the n th tree λ_n of the lodgpole family and perform our enumerations according to this parameter, later returning to m , the number of taxa. We view λ_n as unlabeled, or as having an arbitrary labeling.

The lodgpole family $(\lambda_n)_{n \geq 0}$ can be seen as a modification of the caterpillar family of species trees, in which a family of trees is generated by sequentially appending the previous tree in the family and a single taxon—instead of a cherry, as in the lodgpole family—to a common root.

2.3. Dyck paths

To enumerate histories for lodgpole species trees, we make use of results that involve certain lattice paths, the *Dyck paths* (Stanley, 1999). A Dyck path of size n is a lattice path that starts from $(0, 0)$ and ends

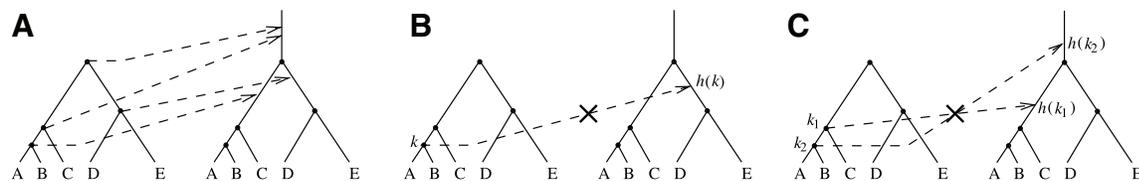


FIG. 2. Coalescent histories with matching gene trees and species trees. **(A)** A matching coalescent history. **(B)** Condition (a) for matching coalescent histories is violated because leaf B descends from node k but not from branch $h(k)$. **(C)** Condition (b) for matching coalescent histories is violated, as node k_2 descends from node k_1 , but the branch $h(k_2)$ remains strictly above the branch $h(k_1)$.

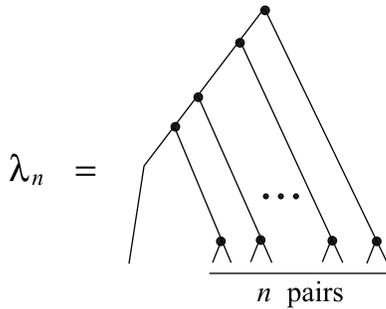


FIG. 3. The lodgepole family of species trees λ_n . Starting from the tree with one taxon (λ_0), by adding $n \geq 0$ cherries, we obtain the tree λ_n . The term *lodgepole* is after the lodgepole pine tree, *Pinus contorta*, one of a number of pine species in which needles extend from the main twig in bundles of two.

at $(2n, 0)$ in the quarter plane, that has n unit steps up (each labeled U) and n unit steps down (labeled D), and that never passes below the x -axis (Fig. 4A). It is useful to distinguish the *indecomposable* Dyck paths from the *decomposable* ones. A Dyck path of size n is said to be indecomposable when it touches the x -axis only at the extreme points $(0, 0)$ and $(2n, 0)$. A Dyck path is decomposable if it is not indecomposable. In Figure 4B, the two Dyck paths at the top are indecomposable, and the remaining three are decomposable.

3. THE NUMBER OF MATCHING COALESCENT HISTORIES FOR LODGEPOLE SPECIES TREES

3.1. Overview

We are now ready to compute the number h_n of matching coalescent histories for the lodgepole tree λ_n . We start in section 3.2 by obtaining a combinatorial formula that computes h_n as a sum over a certain set of vectors V_n . In section 3.3, we show that by a bijection of coalescent histories for λ_n with a certain set of labeled Dyck paths D_n —a set that is, in turn, related to structures known as indecomposable *histoires d’Hermite*—we can apply existing enumerative results to obtain a recursion for h_n . Finally, in section 3.4, we study the asymptotic behavior of h_n .

3.2. A first combinatorial formula for h_n

For $n \geq 1$, we define a set V_n of integer vectors $\bar{a} = (a_1, a_2, \dots, a_n)$ as

$$V_n = \{\bar{a} : a_1 = 2 \text{ and } 2 \leq a_i \leq a_{i-1} + 1 \text{ for } 2 \leq i \leq n\}.$$

Setting, for instance, $n = 3$, we obtain $V_3 = \{(2, 2, 2), (2, 2, 3), (2, 3, 2), (2, 3, 3), (2, 3, 4)\}$.

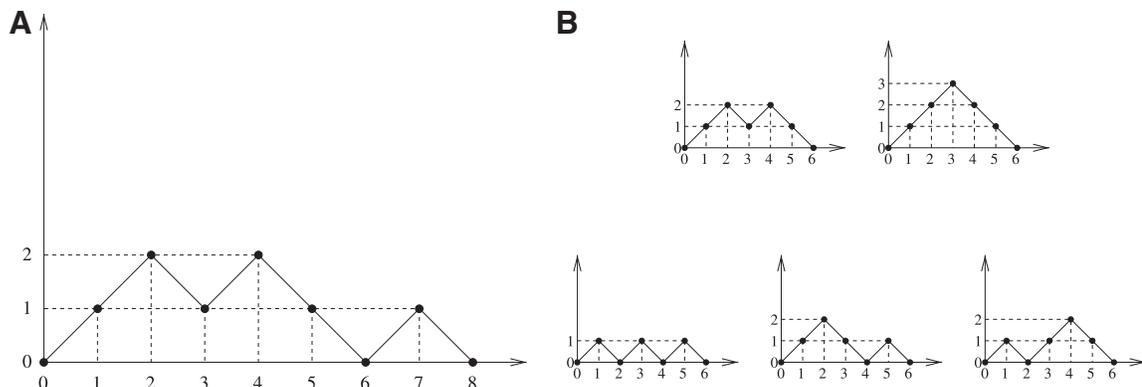


FIG. 4. Dyck paths: **(A)** The Dyck path of size 4 whose sequence of steps is $UUDUDDUD$. It contains four unit up-steps U and four unit down-steps D that never pass strictly below the x -axis. **(B)** The five possible Dyck paths of size 3. The two at the top are indecomposable because they touch the x -axis only at the endpoints $(0, 0)$ and $(6, 0)$.

We have the following combinatorial formula to compute, for $n \geq 1$, the number of matching coalescent histories h_n for the lodgpole species tree λ_n :

$$h_n = \sum_{\bar{a} \in V_n} \prod_{i=1}^n a_i. \tag{2}$$

Equation 2 can be justified by formulating the procedure of Rosenberg (2007) for tabulating coalescent histories specifically in the lodgpole case, observing that a history of λ_n can be constructed in two steps. In the tree λ_n , it is convenient to distinguish a main branch, that is, the one from which the n cherry nodes in λ_n descend (Fig. 5A). The main branch of λ_n thus contains n internal nodes that we treat as ordered from the root (the first node) toward the single leaf at the end of the branch. In step (a), we fix a history for the nodes of the main branch, ignoring the attached cherries. In Figure 5A, a possible history for the main branch is represented by the solid arcs: each arc maps a node of the main branch onto a permissible branch. In step (b), we choose a mapping for the cherry nodes (dashed arcs in the figure). The choice for the mapping of the cherry nodes must be compatible with the mapping in step (a) for the nodes of the main branch of λ_n . As required by the definition of coalescent histories in section 2.1, the image of a cherry node k cannot be placed on a branch above the one chosen in step (a) as the image of the node of the main branch to which node k is appended.

The two-step procedure translates into Equation 2. In fact, each possible history of the main branch of λ_n can be bijectively encoded by a vector of integers $(a_1, \dots, a_n) \in V_n$ by noting that the i th node of the main branch is mapped exactly $a_i - 2$ nodes above it, associating each node with its immediate ancestral branch (Fig. 5A). Once the vector has been fixed, the cherry node appended to the i th node of the main branch can be mapped in exactly a_i compatible ways. Therefore, with the sum in Equation 2, we are considering all the possible histories of the main branch—those constructed in step (a)—and for each of these histories, the product counts the number of compatible mappings of the cherry nodes as considered in step (b).

By applying Equation 2, setting $h_0 = 1$ for convenience, we computed the first terms of the sequence h_n (Table 1). The values for $n = 1, 2, 3, 4$ accord with the values computed in the enumerations of coalescent histories reported for small trees in Tables 1 and 4 of Rosenberg (2007).

3.3. Correspondence with the histoires d’Hermite and a recursion for h_n

We now show that a bijective correspondence exists between histories of the lodgpole family $(\lambda_n)_{n \geq 0}$ and certain labeled paths in the plane. Indeed, note that as in the example in Figure 5B, each vector $\bar{a} \in V_n$

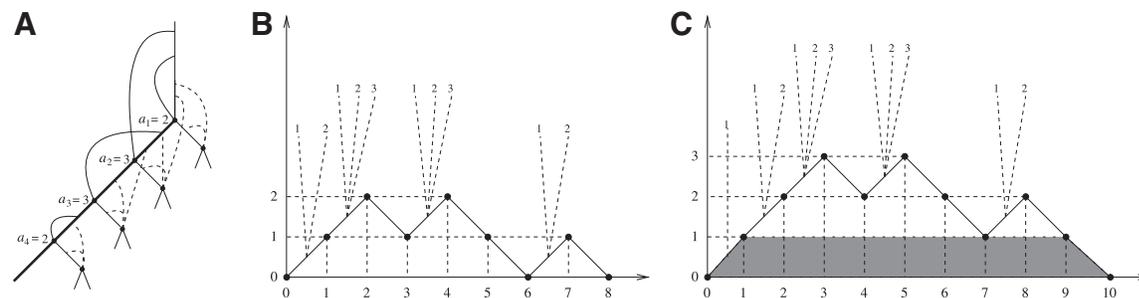


FIG. 5. Combinatorial structures for computation of h_n : coalescent histories, labeled Dyck paths, and histoires d’Hermite. **(A)** Coalescent histories of λ_4 . Arcs represent the mapping of the nodes of λ_4 to its branches. Each history of λ_n can be constructed in two steps. First, a mapping of the nodes of the main branch to branches of the tree is fixed. Next, a compatible mapping of the cherry nodes is constructed. For the nodes of the main branch, the mapping in the figure is encoded by the vector $\bar{a} = (a_1, a_2, a_3, a_4) = (2, 3, 3, 2) \in V_4$: for $i = 1, 2, 3, 4$, the i th node of the main branch is mapped onto the branch $a_i - 2$ nodes above it (solid arcs). Dashed arcs represent possible mappings of the cherry nodes that are compatible with the mapping for the main branch determined by the vector \bar{a} . The i th cherry node can be mapped in exactly a_i compatible ways. **(B)** A labeled Dyck path of size 4, encoding the vector $(a_1, a_2, a_3, a_4) = (2, 3, 3, 2) \in V_4$ from **(A)**. The ordinate y_i of the endpoint of the i th up-step U_i satisfies $y_i = a_i - 1$. By labeling each up-step U_i of the path with an integer $\ell(U_i) \in [1, y_i + 1]$, we obtain a path in D_4 . The number of ways that the underlying Dyck path can be labeled is thus given by the product $\prod_{i=1}^4 a_i = 36$. **(C)** The indecomposable histoire d’Hermite of size 5 associated with the Dyck path of size 4 in **(B)**. The histoire is obtained by adding an up-step labeled 1 at the beginning of the path in **(B)** and a down-step at the end and keeping the labels of the remaining up-steps as in **(B)**. In this way, the i th up-step U_i of the histoire in **(C)** has an integer label $\ell^*(U_i) \in [1, y_i]$, where, as in **(B)**, y_i is the ordinate of the endpoint of the i th up-step.

TABLE 1. THE NUMBER OF MATCHING COALESCENT HISTORIES

Number of taxa m ($m=2n+1$)	Number of matching coalescent histories			
	Predicted by the linear regression model	Exact value of $h_{(m-1)/2}$ for the lodgepole tree	Upper bound for h_m^- based on “bicaterpillars”	Lower bound for h_m^+ based on lodgepole trees
3	1	2	2	2
5	12	10	10	14
7	103	74	65	138
9	888	706	481	1,663
11	7,679	8,162	5,544	6,237
13	66,406	110,410	56,628	90,090
15	574,261	1,708,394	613,470	1,447,875
17	4,966,073	29,752,066	6,952,660	25,844,568
19	42,945,396	576,037,442	81,662,152	509,233,725

Given m , we exponentiate the value from the regression model in Figure 1 and round to the nearest integer. The exact $h_{(m-1)/2} = h_n$ is computed from Equation 2 or 6. For $m \leq 9$, the upper bound for h_m^- and the lower bound for h_m^+ are computed exactly from Tables 1–4 of Rosenberg (2007). For $m \geq 11$, the upper bound for h_m^- is computed as $c_n c_{n+1}$, with c_n as in Equation 1. Applying Proposition 1 and noting that $(n-2)/n = (m-5)/(m-1)$, the lower bound for h_m^+ is computed as $m!(m-5)/(m-1)$, rounding down where necessary.

bijectionally encodes a Dyck path of size $n \geq 1$. More precisely, starting from the vector \bar{a} , a Dyck path with n up-steps is uniquely determined by fixing for each i the ordinate y_i of the endpoint of the i th up-step according to

$$a_i = y_i + 1. \tag{3}$$

For instance, in Figure 5B, we depict the Dyck path $UUDUDDUD$ associated with the vector $\bar{a} = (2, 3, 3, 2) \in V_4$: in fact, as in Equation 3, we have $y_1 = 1 = a_1 - 1$, $y_2 = 2 = a_2 - 1$, $y_3 = 2 = a_3 - 1$, and $y_4 = 1 = a_4 - 1$.

Defining D_n as the set of Dyck paths of size n that for each i have the i th up-step U_i labeled by an integer

$$\ell(U_i) \in [1, y_i + 1], \tag{4}$$

we can also interpret Equation 2 as the formula that computes the cardinality $|D_n|$, so that

$$h_n = |D_n|. \tag{5}$$

Equation 5 holds for $n \geq 0$ including the case $n=0$, as we set $h_0 = 1$, and by counting the empty path, $D_0 = 1$. In interpreting Equation 2 as an enumeration of labeled Dyck paths in D_n , the sum in Equation 2 traverses all possible Dyck paths of size n as encoded by vectors in V_n . For each of these Dyck paths, the product $\prod_{i=1}^n a_i$ computes the number of ways that the path can be labeled. By Equations 3 and 4, each label $\ell(U_i)$ has a_i possible values.

This result, similar to a bijection with monotonic paths used by Degnan (2005) to count coalescent histories in the caterpillar case, allows us to switch from counting the histories of λ_n to counting labeled paths in D_n . The correspondence in Equation 5 can be used to obtain a recursion for h_n . Starting with $h_0 = 1$, we have for $n \geq 1$,

$$h_n = (2n+1)!! - \sum_{k=0}^{n-1} (2k+1)!! h_{n-1-k}. \tag{6}$$

To prove Equation 6, we make use of the relationship between the labeled Dyck paths in D_n and the so-called *histoires d’Hermite* of size $n+1$ (*histoires* for short, Fig. 5C).

An *histoire* of size $n \geq 1$ is a labeled Dyck path of size n , but with a labeling scheme $\ell^*(U_i)$ for its up-steps that slightly differs from the scheme $\ell(U_i)$ considered in Equation 4 for the paths of D_n . Indeed, in an *histoire*, for each i , the i th up-step U_i carries an integer label

$$\ell^*(U_i) \in [1, y_i], \tag{7}$$

where y_i is, as before, the ordinate of the endpoint of step U_i . Note that for histoires of size n , we have y_i possible values for each label $\ell^*(U_i)$, whereas for Dyck paths in D_n , we had $y_i + 1$ possibilities for label $\ell(U_i)$.

Denote by H_n the set of histoires of size n . Section 1.2 of Roblet and Viennot (1996) reported that for $n \geq 1$,

$$|H_n| = (2n - 1)!! = (2n - 1) \times (2n - 3) \times \dots \times 3 \times 1. \tag{8}$$

We say that an histoire of size n is *indecomposable* if its underlying Dyck path is indecomposable (Fig. 5C). It can be observed that, denoting by H'_n the set of indecomposable histoires of size n , we have for $n \geq 0$

$$|D_n| = |H'_{n+1}|. \tag{9}$$

Indeed, as depicted in Figure 5B and C, each labeled Dyck path $P \in D_n$ can be bijectively mapped onto a labeled path $P' \in H'_{n+1}$ that is obtained by adding an up-step U labeled with the integer 1 and a down-step D respectively at the beginning and at the end of P and keeping unchanged the labels of the remaining up-steps of P . In symbols, we have for $n \geq 0$ the bijective correspondence

$$P \in D_n \Leftrightarrow UPD = P' \in H'_{n+1}. \tag{10}$$

Note in fact that according to the labeling scheme ℓ^* for histoires (Eq. 7), in P' only the label $\ell^*(U_1) = 1$ is possible for the new first up-step U_1 . The up-step U_1 has ordinate 1. Furthermore, for all i with $1 \leq i \leq n$, the ordinate y'_{i+1} of the $(i + 1)$ th up-step in P' satisfies

$$y'_{i+1} = y_i + 1,$$

where y_i is the ordinate of the i th up-step in P . Therefore, keeping the labels of the up-steps of P unchanged, the labeling scheme ℓ^* for the histoires is satisfied by P' , as can be seen by comparing Equations 4 and 7. Finally, by construction, the path P' touches the x -axis only in the extreme points and is by definition indecomposable. By the bijection in Equation 10, we thus have Equation 9.

Combining Equations 5 and 9, we obtain for $n \geq 0$

$$h_n = |H'_{n+1}|. \tag{11}$$

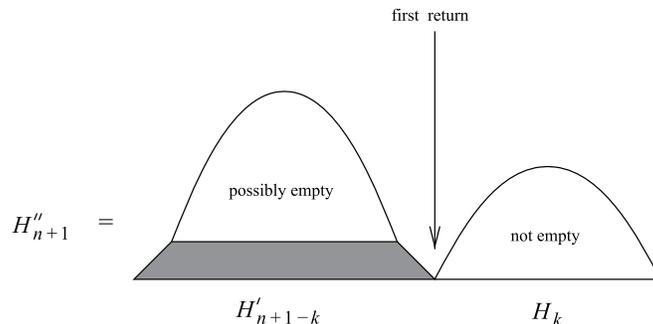
We denote by H''_n the set of *decomposable* (not indecomposable) histoires of size $n \geq 1$. An histoire in H''_{n+1} can be decomposed uniquely as a concatenation of an indecomposable histoire in H'_{n+1-k} for some k , $1 \leq k \leq n$, and a second histoire that is either decomposable or indecomposable and hence lies in H_k (Fig. 6). The endpoint of the indecomposable histoire in H'_{n+1-k} provides the first return of the decomposable histoire in H''_{n+1} to the x -axis, after which the histoire in H_k might or might not touch the x -axis at a point in its interior.

Applying the decomposition, we have for $n \geq 1$

$$|H''_{n+1}| = \sum_{k=1}^n |H'_{n+1-k}| |H_k|.$$

Because the number of histoires in H_n is known from Equation 8, and because each histoire is either decomposable or indecomposable, we obtain a recursion for the number of indecomposable histoires of size $n + 1$:

FIG. 6. A decomposition of a decomposable histoire d’Hermite. Any decomposable histoire in H''_{n+1} for $n \geq 1$ is uniquely obtained by concatenating an indecomposable histoire in H'_{n+1-k} with $1 \leq n + 1 - k \leq n$ (Fig. 5C) and an histoire in H_k with $1 \leq k \leq n$. The point at which they touch corresponds to the first return to the x -axis of the entire path. The shading indicates that the indecomposable histoire on the left begins with an up-step, ends with a down-step, and does not reach the x -axis within the shaded trapezoid.



$$\begin{aligned} |H'_{n+1}| &= |H_{n+1}| - |H''_{n+1}| \\ &= (2n+1)!! - \sum_{k=1}^n |H'_{n+1-k}| |H_k| \\ &= (2n+1)!! - \sum_{k=1}^n |H'_{n+1-k}| (2k-1)!! \end{aligned}$$

By Equation 11, we have demonstrated Equation 6.

The fact that h_n can be computed as in Equation 6 shows that the matching coalescent histories of λ_n are equinumerous with other combinatorial structures. In particular, in addition to being the number of coalescent histories for lodgepole trees and the number of indecomposable histories d’Hermite of size $n+1$, h_n appears in enumerating topologically distinct Feynman diagrams of order n (Jacobs, 1981; Battaglia and George, 1988), as well as in counting for an alphabet of size $n+1$ a class of “irreducible” words in which each letter appears exactly twice, and in which the first appearances of the letters are in a canonical order (Burns and Muche, 2011).

3.4. Asymptotic behavior of h_n and its consequences

We now turn to using our recursion in Equation 6 to determine asymptotic properties of the number h_n of matching coalescent histories for lodgepole species trees. From Equation 6, it immediately follows for $n \geq 0$ that

$$h_n \leq (2n+1)!! \tag{12}$$

Therefore, dividing both sides of Equation 6 by $(2n+1)!!$, for $n \geq 1$, we can write

$$1 \geq \frac{h_n}{(2n+1)!!} = 1 - \sum_{k=0}^{n-1} \frac{(2k+1)!!}{(2n+1)!!} h_{n-1-k} \geq 1 - \sum_{k=0}^{n-1} \frac{(2k+1)!! [2(n-1-k)+1]!!}{(2n+1)!!} \tag{13}$$

The final step in Equation 13 follows by replacing h_{n-1-k} with the upper bound $[2(n-1-k)+1]!!$ from inequality 12.

Using the fact that

$$(2n+1)!! = \frac{(2n+1)!}{2^n n!}, \tag{14}$$

the sum in Equation 13 can be simplified as

$$s_n = \sum_{k=0}^{n-1} \frac{(2k+1)!! [2(n-1-k)+1]!!}{(2n+1)!!} = \sum_{k=0}^{n-1} \frac{\binom{n+1}{k+1}}{\binom{2n+2}{2k+2}} \tag{15}$$

For $n=1$, we have $s_1 = \frac{1}{3}$. In the Appendix, we show that for $n \geq 1$, the sequence $(s_n)_{n \geq 1}$ satisfies the recursion

$$(2n+3)s_{n+1} = (n+2)s_n + 1. \tag{16}$$

For $n \geq 1$, the upper bound

$$s_n \leq \frac{2}{n} \tag{17}$$

can be verified by induction. Because $s_1 = \frac{1}{3}$, $s_2 = \frac{2}{5}$, and $s_3 = \frac{13}{35}$, inequality 17 holds for $n=1, 2, 3$. By Equation 16, the inductive hypothesis yields $(2n+3)s_{n+1} \leq 2(n+2)/n + 1 = (3n+4)/n$, so that

$$s_{n+1} \leq \frac{3n+4}{n(2n+3)} \leq \frac{2}{n+1},$$

where the latter inequality holds for $n \geq 3$.

Therefore, from inequalities 13 and 17, we have for $n \geq 1$

$$1 - \frac{2}{n} \leq 1 - s_n \leq \frac{h_n}{(2n+1)!!} \leq 1,$$

which finally gives the bounds

$$(2n+1)!! \left(\frac{n-2}{n} \right) \leq h_n \leq (2n+1)!!,$$

and the asymptotic relationship $h_n \sim (2n+1)!!$. We summarize our results in a proposition.

Proposition 1 *The number h_n of matching coalescent histories for the lodgpole family $(\lambda_n)_{n \geq 0}$ is*

$$h_n = (2n+1)!! - \sum_{k=0}^{n-1} (2k+1)!! h_{n-1-k}, \quad (18)$$

where we set $h_0 = 1$. The following bounds hold for $n \geq 1$:

$$(2n+1)!! \left(\frac{n-2}{n} \right) \leq h_n \leq (2n+1)!! \quad (19)$$

and asymptotically, we have

$$h_n \sim (2n+1)!! \sim \sqrt{2} \left[\frac{2(n+1)}{e} \right]^{n+1}. \quad (20)$$

The asymptotic approximation in eq. 20 follows from Stirling's approximation $n! \sim \sqrt{2\pi n} (n/e)^n$ and from an equivalent form of Equation 14, $(2n+1)!! = (2n+2)! / [2^{n+1} (n+1)!]$. By Proposition 1, using an odd number $m = 2n+1$ describing the number of taxa in the lodgpole species tree λ_n , we have the following corollary.

Corollary 1 *There exists a family of species trees whose number of matching coalescent histories grows faster than exponentially in the number of taxa m . In particular, when m is odd, the number of matching coalescent histories for the lodgpole species tree $\lambda_{(m-1)/2}$ with $m \geq 1$ leaves is asymptotically*

$$h_{(m-1)/2} \sim m!! \sim \sqrt{2} \left(\sqrt{\frac{m+1}{e}} \right)^{m+1}. \quad (21)$$

Rosenberg (2007) studied the variability across all species trees for a fixed number of taxa m of the number of matching coalescent histories by examining a ratio

$$R(m) = \frac{h_m^+}{h_m^-},$$

where h_m^+ denotes the number of coalescent histories for the m -taxon species tree with the greatest number of matching coalescent histories and h_m^- denotes the corresponding value for the smallest number of histories (h_m^-). In Theorem 3.18, Rosenberg (2007) reported a lower bound on $R(m)$ for $m \geq 2$:

$$R(m) \geq \left(\frac{\sqrt{\pi}}{32} \right) \left(\frac{5m-12}{4m-6} \right) m \sqrt{m}. \quad (22)$$

Our computations with lodgpole species trees substantially increase the lower bound for h_m^+ . By using inequality 19, we can improve on the lower bound on $R(m)$ for the case of m odd.

Corollary 2 *Let $R(m) = h_m^+ / h_m^-$ denote the ratio of the numbers of matching coalescent histories for the m -taxon species trees with the greatest and smallest numbers of coalescent histories. Then, for odd $m \geq 7$,*

$$R(m) \geq \left(\frac{\sqrt{m-1}}{4\sqrt{e}} \right)^m. \quad (23)$$

Proof. Because m is odd, we fix $m=2n+1$ and switch between indexing by m and by n . First, for h_m^- , Rosenberg (2007) considered a “bicaterpillar” tree from whose root descended two caterpillar subtrees, with $\lfloor m/2 \rfloor = n$ and $\lceil m/2 \rceil = n+1$ taxa. This tree has $c_n c_{n+1}$ histories (Rosenberg, 2007, Theorem 3.10), where c_n is the Catalan number as in Equation 1, so that $h_m^- \leq c_n c_{n+1}$.

Now, for h_m^+ , we use the lodgepole species tree λ_n with $m=2n+1$ leaves to provide a lower bound on the number of matching coalescent histories for the tree with the largest number of matching coalescent histories, so that $h_m^+ \geq h_n$. By inequality 19,

$$h_m^+ \geq h_n \geq (2n+1)!! \left(\frac{n-2}{n} \right).$$

Therefore, with c_n as in Equation 1,

$$R(m) = \frac{h_m^+}{h_m^-} \geq \frac{(2n+1)!! \left(\frac{n-2}{n} \right)}{c_n c_{n+1}} = \frac{(2n+1)(n-2)(n+1)(n+2)}{2^n n} \frac{n!}{\binom{2n+2}{n+1}},$$

where we have again used Equation 14. Using the Stirling bound $n! \geq \sqrt{2\pi n} (n/e)^n$ and noting that $\binom{2n}{n} \leq 4^n$, we have

$$\begin{aligned} R(m) &\geq \frac{(2n+1)(n-2)(n+1)(n+2)}{2^n n} \frac{\sqrt{2\pi n} (n/e)^n}{4^{n+1}} \\ &= \frac{(2n+1)(n-2)(n+1)(n+2)\sqrt{2\pi n}}{4n} \left(\frac{n}{8e} \right)^n. \end{aligned} \quad (24)$$

Substituting $n=(m-1)/2$ in inequality 24 to consider the number of taxa $m=2n+1$ yields

$$R(m) \geq \frac{\sqrt{e\pi m}(m-5)(m+1)(m+3)}{4(m-1)} \left(\frac{\sqrt{m-1}}{4\sqrt{e}} \right)^m, \quad (25)$$

which gives, if $m \geq 7$, inequality 23 (and is in fact stronger than the simpler Equation 23). ■

4. DISCUSSION

We have defined the lodgepole family of species trees $(\lambda_n)_n$ and studied the growth of the number h_n of matching coalescent histories for λ_n as a function of n , showing that asymptotically, $h_n \sim (2n+1)!!$. For m odd, the number $h_{(m-1)/2}$ of matching coalescent histories for the lodgepole species tree with m taxa grows with $m!!$. Previous enumerative results for other species tree families have found that the number of coalescent histories increases only exponentially; we have demonstrated the existence of a family of species trees for which the number of matching coalescent histories grows more quickly than exponentially in the number of taxa (Corollary 1).

Our results for lodgepole species trees indicate that the exponential increase in the number of matching coalescent histories observed in Figure 1 is misleading, at least in regard to the largest numbers of matching coalescent histories at a fixed number of taxa. We can consider the linear regression model obtained in Figure 1—representing exponential growth—alongside an upper bound for h_m^- , the smallest number of matching coalescent histories at m taxa, and our new lower bound for h_m^+ , the largest number of matching coalescent histories at m taxa (Table 1). This comparison illustrates that whereas the linear model is reasonable at the small values of m depicted in Figure 1, it becomes increasingly unreasonable in predicting h_m^+ . Indeed, a consequence of the enumeration for lodgepole families is a substantially larger lower bound for the variability of the number of matching coalescent histories for species trees of fixed size (Corollary 2).

The lodgepole trees differ from the caterpillars in that pairs of leaves rather than single leaves are descended from the internal nodes along the main branch. That the lodgepole species trees have such faster growth in their number of matching coalescent histories compared to the caterpillar species trees indicates that this apparently minor change in the branching structure of species trees leads to qualitatively different results in the number of histories. By contrast, it has been found that certain other changes to the caterpillars, replacing a caterpillar subtree by a non-caterpillar subtree, change the asymptotic growth in the

number of matching coalescent histories only by a change to the constant multiple of the Catalan numbers, and do not change the overall growth rate (Rosenberg, 2007, 2013).

The results have the implication that although the numbers of coalescent histories for relatively small species trees remain small enough for reasonable computation times involving enumerations of coalescent histories, the most challenging cases can grow more rapidly in the number of taxa than has been suggested in the cases that have been previously examined. It will be important to determine whether the challenging lodgpole scenario arises in practical settings, as well as the possibility that even more challenging families exist, for which the growth rate is even faster than in the lodgpole case.

The links in our analysis to Dyck paths and the histories d'Hermite, and the appearance for the number of matching coalescent histories of lodgpole species trees of a sequence arising in other counting problems, identify known combinatorial structures to which coalescent histories can be related. These connections are promising for additional future computations about coalescent histories.

5. APPENDIX

This appendix proves Equation 16 from Equation 15. We define for $n \geq 1$ and $0 \leq k \leq n$, $F(k, n) = \binom{n+1}{k+1} / \binom{2n+2}{2k+2}$ and $R(k, n) = 2n - 2k + 1$. We use $F(k, n)$ and $R(k, n)$ to apply the summation methods of Petkovšek et al. (1996). It can be verified algebraically that

$$2(n+2)F(k, n) - 2(2n+3)F(k, n+1) = F(k+1, n)R(k+1, n) - F(k, n)R(k, n). \quad (26)$$

Indeed, the identity follows by dividing both sides of Equation 26 by the nonzero $F(k, n)$ and applying the ratios $F(k, n+1)/F(k, n) = (2n-2k+1)/(2n+3)$ and $F(k+1, n)/F(k, n) = (2k+3)/(2n-2k-1)$. Summing both sides of Equation 26 for k from 0 to $n-1$, the right-hand side telescopes, giving a final contribution of $F(n, n)R(n, n) - F(0, n)R(0, n)$. Therefore, we obtain

$$2(n+2) \left(\sum_{k=0}^{n-1} F(k, n) \right) - 2(2n+3) \left[\left(\sum_{k=0}^n F(k, n+1) \right) - F(n, n+1) \right] = F(n, n)R(n, n) - F(0, n)R(0, n).$$

Taking $s_n = \sum_{k=0}^{n-1} F(k, n)$ as in Equation 15 yields

$$2(n+2)s_n - 2(2n+3) \left(s_{n+1} - \frac{1}{2n+3} \right) = 0,$$

from which Equation 16 immediately follows.

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AUTHOR DISCLOSURE STATEMENT

The authors declare that no competing financial interests exist.

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