

COUNTING PHYLOGENETIC NETWORKS OF LEVEL 1 AND 2

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ABSTRACT. Phylogenetic networks generalize phylogenetic trees, and have been introduced in order to describe evolution in the case of transfer of genetic material between coexisting species. There are many classes of phylogenetic networks, which can all be modeled as families of graphs with labeled leaves. In this paper, we focus on rooted and unrooted level- k networks and provide enumeration formulas (exact and asymptotic) for rooted and unrooted level-1 and level-2 phylogenetic networks with a given number of leaves. We also prove that the distribution of some parameters of these networks (like their number of cycles) are asymptotically normally distributed. These results are obtained by first providing a recursive description (also called combinatorial specification) of our networks, and by next applying classical methods of enumerative, symbolic and analytic combinatorics.

Keywords: phylogenetic networks, level, galled trees, counting, combinatorial specification, generating function, asymptotic normal distribution

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1. INTRODUCTION

Phylogenetic networks generalize phylogenetic trees introducing reticulation vertices, which have two parents, and represent ancestral species resulting from the transfer of genetic material between coexisting species, through biological processes such as lateral gene transfer, hybridization or recombination. More precisely, binary phylogenetic networks are usually defined as rooted directed acyclic graphs whose vertices have either

- in-degree 0 and out-degree 2 (the root),
- in-degree 1 and out-degree 2 (tree vertices),
- in-degree 2 and out-degree 1 (reticulation vertices),
- in-degree 1 and out-degree 0 (leaves), such vertices being bijectively labeled by a set of *taxa*, which correspond to currently living species.

An important parameter that allows to measure the complexity of a phylogenetic networks is its *level*. Phylogenetic trees are actually phylogenetic networks of level 0, and the level of a network N measures “how far from a tree” N is.

As for trees, phylogenetic networks can be rooted or unrooted. Ideally, phylogenetic networks should be rooted, the root representing the common ancestor of all taxa labeling the leaves. But several methods which reconstruct phylogenetic networks, such as distance-based or parsimony-based methods, do not produce inherently rooted networks.

The problem of enumerating (rooted or unrooted) trees is a very classical one in enumerative combinatorics. Solving this problem actually led to general methods for enumerating other tree-like structures, where *generating functions* play a key role. We will review some of these methods in Section 3. These methods have successfully been used by Semple and Steel [SS06] to enumerate two families of phylogenetic networks, namely unicyclic networks and unrooted level-1 networks (also called *galled trees*). Their results include an equation defining implicitly the generating function for unrooted level-1 networks (refined according to two parameters), which yields a closed formula for the number of unrooted level-1 networks with n (labeled) leaves, k cycles, and a total of m edges (also called arcs) across all the cycles. An upper bound on the number of unlabeled galled trees is also provided in [CHT18]. Other counting results have been more recently obtained on other families of phylogenetic networks, for example on so called “normal” and “tree-child networks” [MSW15, FGM19] and on “galled networks” [GRZ18].

In this paper, we extend the results of Semple and Steel in several ways. First, about unrooted level-1 networks, we provide an asymptotic estimate of the number of such networks with n (labeled) leaves. We also prove that the two parameters considered by Semple and Steel are asymptotically normally distributed. Second, we consider rooted level-1 networks, whose enumeration does not seem to have been considered so far in the literature. For these networks, we provide a closed formula counting them by number of leaves, together with an asymptotic estimate, and a closed formula for their enumeration refined by two parameters (the number of cycles and number of edges across all the cycles). Moreover, we show that these two parameters are asymptotically normally distributed. Finally, we consider both unrooted and rooted level-2 networks. Similarly, we provide in each case exact and asymptotic formulas for their enumeration, and prove asymptotic normality for some parameters of interest, namely: the number of bridgeless components of strictly positive level, and the number of edges across them. These parameters are a generalization for level- k ($k > 2$) of those considered by Semple and Steel for level-1, in the sense that they quantify how different from a tree these phylogenetic networks are.

The results of this paper rely heavily on analytic combinatorics [FS08]. This framework can also be used to derive uniform random generators (for example with the recursive method [FZC94] or with a Boltzmann sampler [DFLS04]) directly from the specifications of the classes of phylogenetic networks given below. This could be useful for applications in bioinformatics, especially to generate simulated data in order to evaluate the speed or the quality of the output of algorithms dealing with phylogenetic networks.

Table 1 provides an overview of our results, and of where they can be found in the paper.

Type of network	Unrooted, level-1	Rooted, level-1	Unrooted, level-2	Rooted, level-2
Letter \mathcal{X} denoting the class	\mathcal{G} (galled)	\mathcal{R} (rooted)	\mathcal{U} (unrooted)	\mathcal{L} (last)
Eq. for the EGF $X(z)$	Thm. 4.1 (*)	Thm. 5.1	Thm. 6.1	Thm. 7.1
Exact formula for x_n	Prop. 4.2 (*)	Prop. 5.2	Prop. 6.2	Prop. 7.2
Asymptotic estimate of x_n	Prop. 4.3	Prop. 5.3	Prop. 6.3	Prop. 7.3
Eq. for the multivariate EGF	Eq. (\star_G) (*)	Eq. (\star_R)	Eq. (\star_U)	Eq. (\star_L)
Refined enumeration formula	[SS06, Thm. 4]	Prop. 5.4	-	-
Asymptotic normality	Prop. 4.4	Prop. 5.5	Prop. 6.4	Prop. 7.4

TABLE 1. Overview of our results. EGF means exponential generating function. The results marked with (*) also appear in the work of Semple and Steel [SS06]. We did not derive explicitly the results in the two cells marked -, although such refined formulas could be derived from Eq. (\star_U) and Eq. (\star_L) as in the level-1 case. (The computations would however be rather intricate, and the interest *a priori* of the formulas so obtained questionable, hence our choice not to do it.)

For the reader's convenience, we also include in this introduction the beginnings of the enumeration sequences of the four types of networks we consider, as well as their asymptotic behavior – see Table 2. We have added these sequences to the OEIS [OEI19], and we also include in Table 2 their OEIS reference.

The article is organized as follows. First, Section 2 recalls definitions and properties of phylogenetic networks that are important for our purpose. Next, Section 3 reviews some methods of enumerative and analytic combinatorics which we will apply to solve the enumeration of our networks in the following sections. Precisely, Sections 4 and 5 deal with level-1 networks, unrooted and rooted, while Sections 6 and 7 focus on level-2 networks.

2. SOME PROPERTIES OF PHYLOGENETIC NETWORKS

2.1. Rooted binary phylogenetic networks. In graph theory, a *cut arc* or *bridge* of a directed graph or multi-graph G is an arc whose deletion disconnects G . A *bridgeless component* of a graph or multi-graph G is a maximal induced subgraph of G without cut arcs.

n	g_{n-1}	r_n	u_{n-1}	ℓ_n
1	0	1	0	1
2	1	3	1	24
3	2	36	9	1 935
4	15	723	282	259 098
5	192	20 280	14 697	48 547 410
6	3 450	730 755	1 071 750	11 693 494 530
as $n \rightarrow \infty$	$c_1 \approx 0.20748$	$c_1 \approx 0.1339$	$c_1 \approx 0.0589$	$c_1 \approx 0.0238$
$x_n \sim c_1 c_2^n n^{n-1}$ with	$c_2 \approx 1.89004$	$c_2 \approx 2.943$	$c_2 \approx 7.662$	$c_2 \approx 19.685$
OEIS reference	A328121	A328122	A328123	A328126

TABLE 2. The numbers of rooted and unrooted level-1 or level-2 networks on n leaves.

We define a *binary rooted phylogenetic network* N on a set X of leaf labels as a directed acyclic multi-graph having:

- (1) exactly one *root*, that is an in-degree-0 out-degree-2 vertex (or an in-degree-0 out-degree-0 vertex if N only has one leaf);
 - (2) *leaves*, that is in-degree-1 out-degree-0 vertices (or an in-degree-0 out-degree-0 vertex if N only has one leaf) which are bijectively labeled by elements of X ;
 - (3) *tree vertices*, that is in-degree-1 out-degree-2 vertices;
 - (4) *reticulation vertices*, that is in-degree-2 out-degree-1 vertices;
- and such that
- (5) for each bridgeless component B of N , there exist at least two cut arcs of N whose tail¹ belongs to B .

As illustrated in Fig. 1, a binary rooted phylogenetic network N is said to be *level- k* (or called a *level- k network* for short) if the number of reticulation vertices contained in any bridgeless component of N is less than or equal to k . In a level-1 network N , each bridgeless component B having strictly more than one vertex consists of the union of two directed paths, which start and end at the same vertices, called *source* and *sink* respectively. The source is actually either the root of N , or the head of a cut arc of N , and the sink is the unique reticulation vertex of B . Such bridgeless components are called *cycles*. (Note that a multiple edge is a particular case of such a cycle, where both directed paths consist of just one edge.)

Note that variations on the definition of rooted binary phylogenetic networks are around in the literature, and a few comments on our choice of definition are in order. Our definition of binary rooted phylogenetic networks allows multiple arcs, similarly to [GBP09], but contrary to several other articles about phylogenetic networks. Our goal is indeed to study the most general model of binary phylogenetic networks that could be counted if their number of leaves and level are fixed. Condition (5) is necessary to ensure that there are finitely many phylogenetic networks with a given number of leaves and level. Indeed, without it, such networks have unbounded number of vertices: this can be seen by replacing any cut arc of the network by a sequence of multiple arcs separated by cut arcs. (Note however that allowing multiple arcs inside bridgeless components does not create this problem from the counting point of view, because adding such multiple arcs increases the level.)

Similarly in some algorithmic-oriented papers about phylogenetic networks, bridgeless components with three vertices and two outgoing arcs are forbidden because the information needed to distinguish those components from simple tree vertices also connected with two outgoing arcs is not available in the input data. In the perspective of counting those objects we do not impose this restriction. But it could easily be added to our combinatorial descriptions and formulas below, to be taken into account if needed.

¹The *tail* of an arc is by definition its starting point. Its arrival point is called *head*.

2.2. Unrooted binary phylogenetic networks. Now, we extend the latter definition to unrooted phylogenetic networks. A *cut-edge* or *bridge* of a(n undirected) graph or multi-graph G is an edge whose removal disconnects the graph. A *bridgeless component* of a graph or multi-graph G is a maximal induced subgraph of G without cut-edges.

An *unrooted binary phylogenetic network* N on a set X of leaf labels is a loop-less (undirected) graph whose vertices have either degree 3 (*internal vertices*) or degree 1 (*leaves*), such that its set $L(N)$ of leaves is bijectively labeled by X and such that for each bridgeless component B of N having strictly more than one vertex, the set of cut-edges incident with some vertex of B has size at least 3. An unrooted binary phylogenetic tree is an unrooted binary phylogenetic network with no bridgeless component containing strictly more than one vertex. An unrooted binary phylogenetic network is said to be *level- k* (or called an *unrooted level- k network* for short) if an unrooted binary phylogenetic tree can be obtained by first removing at most k edges per bridgeless component, and then, for each degree-2 vertex, contracting the edge between this vertex and one of its neighbours. We denote by *cycles* the bridgeless components of unrooted level-1 networks having strictly more than one vertex. (Indeed, they are just cycles – of size at least 3 – in the graph-theoretical sense.)

Note that given a rooted level- k network N on n leaves, we can obtain an unrooted binary phylogenetic network N' on $n + 1$ leaves with the following *unrooting procedure*: add a vertex adjacent to the root of N , labeled with an extra leaf label (usually denoted $\#$), and ignore all arc directions. Theorem 1 of [GBP12] implies in addition that the network N' so obtained is an unrooted level- k network. This unrooting procedure which consists of building an unrooted level- k network from a rooted level- k network, illustrated in Fig. 1, can be reversed (see Lemma 4.13 of [JJE⁺09]), although not in a unique fashion. Indeed, given an unrooted level- k network N' on $n + 1$ leaves, it is possible to choose any leaf and delete it, making its neighbour become the root ρ of a rooted level- k network N obtained by:

- (1) placing the bridgeless component B containing ρ at the top;
- (2) orienting downwards all the cut edges incident with vertices of B ;
- (3) choosing the tail t of one of these cut arcs as the sink of B ;
- (4) computing an ρ - t numbering [LEC67] on the vertices of B if there are more than one, that is labeling vertices of B with integers from 1 to the number n_B of vertices of B , such that the labels of ρ and t are respectively 1 and n_B and such that any vertex of B except ρ and t is adjacent both to a vertex with a lower label and a vertex with a higher label;
- (5) orienting each edge of B by choosing its vertex with the lower label as the tail;
- and
- (6) moving downwards into the network, recursively applying this procedure on all other bridgeless components.

This correspondence is not one-to-one because of the choices of the leaf which is deleted, and most importantly because of the choices of sinks in step 3 above.

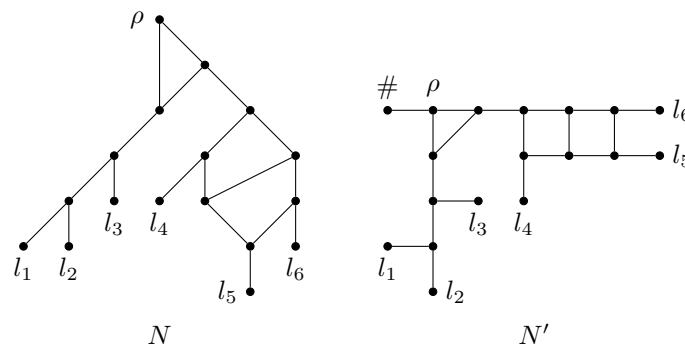


FIGURE 1. A rooted level-2 network N (where all arcs are directed downwards) and the unrooted level-2 network N' obtained by applying the unrooting procedure on N .

2.3. Decomposition of rooted and unrooted level- k networks. For any bridgeless component B with $k_B \leq k$ reticulation vertices of a rooted level- k network N , the directed multi-graph obtained by removing all outgoing arcs, and then contracting each arc from an in-degree-1 out-degree-1 vertex to its child, is called a *level- k_B generator* [vIKK⁺09, GBP09]. For each $k > 0$, there exists a finite list of *level- k generators* which can be built from level- $(k - 1)$ generators [GBP09]. Therefore, depending on the level k_ρ of the bridgeless component B_ρ of N containing its root ρ , N can be decomposed in the following way. It is either:

- a single leaf if $k_\rho = 0$ and ρ has out-degree 0;
- a root ρ being the parent of the root ρ_1 of a rooted level- k network N_1 and of the root ρ_2 of a rooted level- k network N_2 with disjoint sets of leaf labels, if $k_\rho = 0$ and ρ has out-degree 2;
- a level- k_ρ generator G_ρ containing the root, with $0 < k_\rho \leq k$, whose arcs are subdivided to create new in-degree-1 out-degree-1 vertices, to which we add a set of cut arcs, whose tails are the out-degree-0 vertices of G_ρ and the newly created in-degree-1 out-degree-1 vertices, and whose heads are roots of rooted level- k networks with disjoint sets of leaf labels.

Similarly, for any bridgeless component B of an unrooted level- k network N , the multi-graph obtained by first removing all outgoing arcs, then, for each degree-2 vertex, contracting the edge between this vertex and one of its neighbours, is called an *unrooted level- k_B generator* [GBP12, HMW16]. An unrooted level- k_B generator can also be defined as a single vertex for $k_B = 0$, as two vertices linked by a multiple edge for $k_B = 1$, and as a 3-regular bridgeless multi-graph with $2k_B - 2$ vertices for $k_B > 1$ (Lemma 6 of [HMW16]). Therefore, by considering a leaf $l_\#$ of any unrooted level- k network N and the bridgeless component B containing the vertex adjacent to this leaf, depending on the level k_B of B , N can be decomposed in the following way.

- If $k_B = 0$ and B consists of a single vertex of degree 1 in N , then N is just the leaf $l_\#$ adjacent to another leaf.
- If $k_B = 0$ and B is not a single vertex of degree 1 in N , then the leaf $l_\#$ is adjacent to a vertex v of degree 3 in N , such that the other two edges incident to v are cut edges. N is described by the edge between $l_\#$ and v , plus the two other edges incident with v , which are in turn identified with edges of two unrooted level- k networks N_1 and N_2 with disjoint sets of leaf labels (not containing $\#$) in such a way that v is identified with a leaf $l_{\#1}$ (resp. $l_{\#2}$) of N_1 (resp. N_2), removing the leaf labels of $l_{\#1}$ and $l_{\#2}$ during this identification.
- Otherwise $0 < k_B \leq k$. In this case, N is described by taking a level- k_B generator whose edges are subdivided to insert vertices, and then performing identification of these inserted vertices (in a same flavor as in the previous case). Specifically, one of these inserted vertices is identified with the neighbour of $l_\#$ in N , and all others are identified with leaves of unrooted level- k networks with disjoint sets of leaf labels (not containing $\#$). Again, each leaf that is identified with another vertex loses its label during this identification.

These decompositions of rooted and unrooted level- k networks will be the key to our counting results below.

3. GENERATING FUNCTIONS: SOME BASICS TOOLS AND TECHNIQUES

This section summarizes some of the basics on combinatorial classes and their generating functions that we will use in our work. Our presentation follows closely [FS08] (although with much less details), and the reader interested to know more on the topic is referred to [FS08, mainly Chapters I.5, II.1, II.5, VI.3, VII.3, VII.4].

3.1. (Univariate) generating functions and counting. Generally speaking, a *combinatorial class* \mathcal{C} is a set of discrete objects, equipped with a notion of size, such that for every integer n there is a finite number of objects of size n in \mathcal{C} . We denote by \mathcal{C}_n the set of objects of size n in \mathcal{C} , and by c_n the cardinality of \mathcal{C}_n . Specifically in this paper, each combinatorial class we consider is a family of level- k phylogenetic networks, and the size of such a network is its number of leaves.

Objects of size n in \mathcal{C} can be seen as an arrangement (following some rules to be made precise) of n atoms, which are objects of size 1. In our context, these atoms are the leaves of the networks, representing the current species, or *taxa*. In general, combinatorial objects may or may not be labeled, depending whether the atoms constituting an object are distinguishable from one another (*labeled case*) or not (*unlabeled case*). Because leaves of level- k networks correspond to taxa, our networks will be labeled combinatorial objects. Without loss of generality (*i.e.*, up to relabeling), atoms in a labeled object of size n are simply labeled by integers from 1 to n , and we will take this convention in our work.

To a combinatorial class \mathcal{C} , we can associate its *exponential* (resp. *ordinary*) *generating function* $C(z) = \sum_{n \geq 0} c_n \frac{z^n}{n!}$ (resp. $C_{ord}(z) = \sum_{n \geq 0} c_n z^n$), which is a formal power series in z encapsulating the entire enumeration of \mathcal{C} . Exponential (resp. ordinary) generating functions are particularly adapted to the study of labeled (resp. unlabeled) objects, so that we will only consider exponential generating functions in what follows.

A *specification* for a combinatorial class is an unambiguous description of the objects in the class using simpler classes and possibly the class itself. For instance, consider labeled rooted ordered binary trees, and define their size to be the number of their leaves. Such a tree is unambiguously described as being either a leaf or composed of a root to which a left and a right subtree are attached, which are themselves labeled rooted ordered binary trees, with a *consistent relabeling* of their atoms. By this, we mean the following: considering two trees whose atoms are labeled by $\{1, \dots, k\}$ and $\{1, \dots, k'\}$, we can build a tree using the first (resp. second) as left (resp. right) subtree; the atoms of this tree are labeled by $\{1, \dots, k+k'\}$, and need to be such that the relative order between the labels in the left (resp. right) subtree is preserved (and they may be in any such way). This specification for labeled rooted ordered binary trees can be formally written as follows: $\mathcal{B} = \bullet \uplus \begin{array}{c} \circ \\ \swarrow \quad \searrow \\ \mathcal{B} \quad \mathcal{B} \end{array}$, where \bullet represents a leaf (contributing 1 to the size of the object) and \circ

represents an internal node (which contributes 0 to the size).

Specifications describing combinatorial classes can be translated into *equations* satisfied by the corresponding generating functions. For instance, disjoint unions correspond to sums of series, Cartesian products (with consistent relabellings in the case of labeled objects) correspond to products of series, and sequences (*i.e.*, m -tuples of objects of a class \mathcal{C} , for any $m \geq 0$) to the quasi-inverse $\frac{1}{1-C(z)}$. This holds for both exponential generating functions of labeled objects, and for ordinary generating functions of unlabeled objects. For labeled classes, the precise statement that we refer to is [FS08, Theorem II.1]. On the previous example of binary trees, we get that the corresponding generating function satisfies $B(z) = z + B(z)^2$.

The next step is to have access to the enumeration sequence (c_n) of a class \mathcal{C} from an equation satisfied by the generating function $C(z)$ of \mathcal{C} . A possible way, especially in the case of tree-like objects, is to appeal to the *Lagrange inversion formula* ([FS08, Theorem A.2]). To state it, we introduce the notation $[z^n]C(z)$ to denote the n -th coefficient of the series $C(z)$; that is to say, writing $C(z) = \sum_{n \geq 0} \gamma_n z^n$, we have $[z^n]C(z) = \gamma_n$. In particular, when C is the ordinary (resp. exponential) generating function of a combinatorial class whose counting sequence is $(c_n)_{n \geq 0}$, we have that $[z^n]C(z)$ is c_n (resp. $\frac{c_n}{n!}$).

The Lagrange inversion formula is as follows. If the generating function C satisfies an equation of the form $C(z) = z\phi(C(z))$ for $\phi(z) = \sum_{n \geq 0} \phi_n z^n$ a formal power series such that $\phi_0 \neq 0$, then we have:

$$[z^n]C(z) = \frac{1}{n} [z^{n-1}] \phi(z)^n.$$

Even though defined as formal power series, it is often useful to consider that generating functions are *analytic functions* of the complex variable z , in a small disk of convergence around the origin of the complex plane. This sometimes allows to find a closed form for the generating function in its disk of convergence, but not always. Even in this least favorable case, it enables to inherit fundamental results from complex analysis, that can be used for the purpose of enumerating combinatorial objects. In particular, we have in this tool box the *Singular Inversion Theorem* (Theorem VI.6 of [FS08]), which allows to derive asymptotic estimates of the coefficients of generating functions.

Theorem 3.1 (Singular Inversion Theorem). *Let $C(z)$ be a generating function such that $C(0) = 0$, that satisfies the equation $C(z) = z\phi(C(z))$ for $\phi(z) = \sum_{n \geq 0} \phi_n z^n$ a power series such that $\phi_0 \neq 0$. Denote by R the radius of convergence of ϕ at 0. Assuming that ϕ is analytic at 0, that for all n , $\phi_n \in [0, +\infty)$, that $\phi(z) \neq \phi_0 + \phi_1 z$, and that the characteristic equation $\phi(z) - z\phi'(z) = 0$ has a solution $\tau \in (0, R)$ (that is necessarily unique), the followings hold:*

- $\rho = \frac{\tau}{\phi(\tau)}$ is the radius of convergence of C at 0;
- near ρ , $C(z) \sim \tau - \sqrt{\frac{2\phi(\tau)}{\phi''(\tau)}} \sqrt{1 - \frac{z}{\rho}}$;
- when n grows, $[z^n]C(z) \sim \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)}} \frac{\rho^{-n}}{\sqrt{\pi n^3}}$.

3.2. Bivariate generating functions and estimating parameters. Until now, our generating functions had only a single variable, z , recording the size of the objects we were counting. We now consider *multivariate* generating functions, where additional variables (x, y, \dots) record the value of other parameters of our objects. In our cases, we will consider at most two such parameters, which are numbers of certain "substructures" occurring in our objects. Namely, denoting $c_{n,k,m}$ the number of objects of size n in the combinatorial class \mathcal{C} such that the first parameter has value k and the second has value m , the multivariate exponential generating function we consider is $C(z, x, y) = \sum_{n,k,m} \frac{c_{n,k,m}}{n!} z^n x^k y^m$.

To continue our earlier example of binary trees, we could consider one additional parameter, which is the number of internal nodes. (Of course, we are aware that the number of internal nodes is always the number of leaves – *i.e.*, the size – minus one; but we keep this example just to illustrate definitions and tools available.) The coefficient of $z^n x^k$ in the generating function $B(z, x)$ is then the number of binary trees with n leaves and k internal nodes, divided by $n!$.

The "dictionary translating combinatorial specifications to equations satisfied by the generating function extends to multivariate series, and our earlier specification $\mathcal{B} = \bullet \uplus \begin{array}{c} \circ \\ \diagup \quad \diagdown \\ \mathcal{B} \quad \mathcal{B} \end{array}$ gives $B(z, x) = z + xB(z, x)^2$.

Here again, the Lagrange inversion formula may be used to derive a closed formula for the coefficients $c_{n,k,m}$. Indeed, assuming that our multivariate exponential generating function $C(z, x, y)$ satisfies an equation of the form $C(z, x, y) = z\phi(C(z), x, y)$ for $\phi(z, x, y) = \sum_{n \geq 0} \phi_n(x, y) z^n$ a formal power series such that $\phi_0 \neq 0$, then we have:

$$\frac{c_{n,k,m}}{n!} = [z^n x^k y^m] C(z, x, y) = \frac{1}{n} [z^{n-1} x^k y^m] \phi(z, x, y)^n.$$

Moreover, under some hypotheses, the following theorem (see [Drm09, Theorem 2.23]) allows to prove that the considered parameters are asymptotically normally distributed. The notation used in the statement of this theorem is as follows: if F is a function of several variables, including v , F_v denotes the partial derivative of F with respect to v ; as usual, \mathbb{E} and Var denote expectation and variance; $\mathcal{N}(0, 1)$ is the standard normal distribution; and \xrightarrow{d} denotes convergence in distribution.

Theorem 3.2. *Assume that $C(z, x)$ is a power series that is the (necessarily unique and analytic) solution of the functional equation $C = F(C, z, x)$, where $F(C, z, x)$ satisfies the following assumptions: $F(C, z, x)$ is analytic in C , z and x around 0, $F(C, 0, x) = 0$, $F(0, z, x) \neq 0$, and all coefficients $[z^n C^m] F(C, z, 1)$ are real and non-negative.*

Assume in addition that the region of convergence of $F(C, z, x)$ is large enough for having non-negative solutions $z = z_0$ and $C = C_0$ of the system of equations

$$\begin{aligned} C &= F(C, z, 1) \\ 1 &= F_C(C, z, 1) \end{aligned}$$

with $F_z(C_0, z_0, 1) \neq 0$ and $F_{CC}(C_0, z_0, 1) \neq 0$.

Then, if X_n is a sequence of random variables such that

$$\mathbb{E} x^{X_n} = \frac{[z^n] C(z, x)}{[z^n] C(z, 1)},$$

then X_n is asymptotically normally distributed.

More precisely, setting

$$\mu = \frac{F_x}{z_0 F_z}$$

$$\sigma^2 = \mu + \mu^2 + \frac{1}{z_0 F_z^3 F_{CC}} \left(F_z^2 (F_{CC} F_{xx} - F_{Cx}^2) - 2F_z F_x (F_{CC} F_{zx} - F_{Cz} F_{Cx}) + F_x^2 (F_{CC} F_{zz} - F_{Cz}^2) \right)$$

where all partial derivatives are evaluated at the point $(C_0, z_0, 1)$, we have

$$\mathbb{E}X_n = \mu n + O(1) \quad \text{and} \quad \text{Var}X_n = \sigma^2 n + O(1)$$

and if $\sigma^2 > 0$ then

$$\frac{X_n - \mathbb{E}X_n}{\sqrt{\text{Var}X_n}} \xrightarrow{d} \mathcal{N}(0, 1).$$

3.3. Implementation. Some of the computations used to obtain the results of this paper were programmed in Maple. A companion Maple document is available from the authors webpage².

4. COUNTING UNROOTED LEVEL-1 NETWORKS

4.1. Generating function and exact enumeration formula. Unrooted level-1 networks (also called unrooted galled trees) have been enumerated in [SS06]. The enumeration does not only consider the number of leaves of the galled trees, but is refined according to two parameters: the number of cycles (*i.e.*, level-1 generators) and the total number of edges which are part of a cycle (that we will call *inner edges*). We only reproduce in Theorem 4.1 and Proposition 4.2 a simplified version of the results of [SS06], taking into account the number of leaves only.

Theorem 4.1. *For any $n \geq 0$, let g_n denote the number of unrooted level-1 networks with $(n+1)$ leaves, and denote by $G(z) = \sum_{n \geq 0} g_n \frac{z^n}{n!}$ the corresponding generating function. Then G satisfies the following equation:*

$$G(z) = z + \frac{1}{2}G(z)^2 + \frac{1}{2} \frac{G(z)^2}{1 - G(z)},$$

or equivalently

$$G(z) = z\phi(G(z)) \quad \text{with} \quad \phi(z) = \frac{1}{1 - \frac{1}{2}z(1 + \frac{1}{1-z})}.$$

Proposition 4.2. *For any $n \geq 0$, let g_n denote the number of unrooted level-1 networks with $(n+1)$ leaves. We have:*

$$g_n = \frac{(2n-2)!}{2^{n-1}(n-1)!} + \sum_{1 \leq i \leq k \leq n-1} \frac{(n+i-1)!(n+k-i-2)!}{k!(k-1)!(i-k)!(n-i-1)!} 2^{-i}.$$

Notice that even if the formulas seem different, Proposition 4.2 can be recovered from Theorem 4 of [SS06] by summing over k and m and performing the change of variable $m = n - i + 3k - 1$. The first values of g_n have been included in Table 2.

Proof. We recall the main steps of the proofs of Theorem 4.1 and Proposition 4.2 given in [SS06]. To prepare the ground for future proofs, we emphasize their embedding in the context we presented in Section 3.

Since counting rooted objects is far easier than counting unrooted objects, we establish a bijective correspondence between unrooted level-1 networks, and a rooted version of these networks, that we call *pointed* level-1 networks. Pointed level-1 networks on a set of taxa X are simply unrooted level-1 networks on the set of taxa $X \uplus \{\#\}$, where we declare that the leaf labeled by $\{\#\}$ is the "root" of the network. This provides a bijection between unrooted level-1 networks on the set of taxa $X \uplus \{\#\}$ and pointed level-1 networks on X , that have a root labeled by $\{\#\}$. Therefore, there are as many unrooted level-1 networks on the set of taxa $X \uplus \{\#\}$ as pointed

²at <http://user.math.uzh.ch/bouvel/publications/BouvelGambetteMansouri.mw>

level-1 networks on X rooted in a leaf labeled by $\# \notin X$. Hence g_n is the number of pointed level-1 networks with n leaves in addition to the root.

In a pointed level-1 network N (with at least two leaves), we consider the other extremity of the edge to which the root belongs. This vertex may belong to a cycle or not. In the latter case, N is simply described as an unordered pair of two pointed level-1 networks. In the former case, it is described as a non-oriented sequence of at least two pointed level-1 networks. Taking into account the trivial pointed level-1 network with one leaf, a specification for the pointed level-1 networks is therefore the one shown in Figure 2, where the arrow labeled by *sym* indicates that there is a symmetry w.r.t. the vertical axis to take into account, and the dashed edge corresponds to an edge or a path with internal vertices that are incident with cut-edges, themselves identified with edges of other pointed level-1 networks, the vertex lying on the cycle being identified with a leaf of corresponding network.

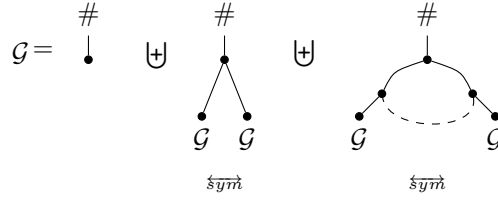


FIGURE 2. The combinatorial specification for unrooted level-1 networks (a.k.a. galled trees).

Thanks to the “dictionary”, the generating function therefore satisfies $G(z) = z + \frac{1}{2}G(z)^2 + \frac{1}{2} \frac{G(z)^2}{1-G(z)}$ as claimed by Theorem 4.1. The end of Theorem 4.1 is obtained by simple algebraic manipulations.

From $G(z) = z\phi(G(z))$, where $\phi(z) = \frac{1}{1 - \frac{1}{2}z(1 + \frac{1}{1-z})}$, we can apply Lagrange inversion to find g_n . Indeed, $g_n = n![z^n]G(z) = (n-1)![z^{n-1}]\phi(z)^n$.

Recall the following development of $(1-z)^{-n}$, for any $n \geq 1$, which will be used here and several times later on:

$$\left(\frac{1}{1-z}\right)^n = \sum_{i \geq 0} \binom{n+i-1}{i} z^i.$$

Applying this identity twice and the binomial theorem, we get that

$$\begin{aligned} \phi(z)^n &= \sum_{i \geq 0} \binom{n+i-1}{i} \left(\frac{1}{2}z\left(1 + \frac{1}{1-z}\right)\right)^i \\ &= \sum_{i \geq 0} \binom{n+i-1}{i} \left(1 + \sum_{k=1}^i \sum_{p \geq 0} \binom{i}{k} \binom{k+p-1}{p} z^p\right) \frac{1}{2^i} z^i \\ &= \sum_{i \geq 0} \binom{n+i-1}{i} \frac{z^i}{2^i} + \sum_{i \geq 0} \sum_{k=1}^i \sum_{p \geq 0} \binom{n+i-1}{i} \binom{i}{k} \binom{k+p-1}{p} \frac{z^{i+p}}{2^i}. \end{aligned}$$

It follows that

$$\begin{aligned} [z^{n-1}]\phi(z)^n &= \binom{2n-2}{n-1} \frac{1}{2^{n-1}} + \sum_{i=0}^{n-1} \sum_{k=1}^i \frac{1}{2^i} \binom{n+i-1}{i} \binom{i}{k} \binom{n+k-i-2}{n-i-1} \\ \text{and } g_n &= \frac{(2n-2)!}{2^{n-1}(n-1)!} + \sum_{1 \leq k \leq i \leq n-1} \frac{(n+i-1)!(n+k-i-2)!}{k!(k-1)!(i-k)!(n-i-1)!} 2^{-i}. \quad \square \end{aligned}$$

4.2. Asymptotic evaluation. From Theorem 4.1, we can furthermore derive an asymptotic evaluation of the number g_n of unrooted level-1 networks on $(n + 1)$ leaves, using Theorem 3.1.

Proposition 4.3. *The number g_n of unrooted level-1 networks on $(n + 1)$ leaves is asymptotically equivalent to $c_1 \cdot c_2^n \cdot n^{n-1}$ for constants c_1 and c_2 such that $c_1 \approx 0.20748$ and $c_2 \approx 1.89004$.*

Proof. Recall that $G(z)$ satisfies $G(z) = z\phi(G(z))$, where $\phi(z) = \frac{1}{1 - \frac{1}{2}z(1 + \frac{1}{1-z})}$ is easily seen to satisfy the hypotheses of Theorem 3.1. Denoting by $\tau \approx 0.34270$ the unique solution of the characteristic equation $\phi(z) - z\phi'(z) = 0$ in the disk of convergence of ϕ , and $\rho = \frac{\tau}{\phi(\tau)} \approx 0.19464$, Theorem 3.1 gives:

$$[z^n]G(z) \sim \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)} \frac{\rho^{-n}}{\sqrt{\pi n^3}}}.$$

Using the Stirling estimate of the factorial $n! \sim \left(\frac{n}{e}\right)^n \sqrt{2\pi n}$, we get:

$$g_n \sim \left(\frac{n}{e}\right)^n \sqrt{2\pi n} \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)} \frac{\rho^{-n}}{\sqrt{\pi n^3}}} \sim \frac{n^{n-1}}{(e\rho)^n} \sqrt{\frac{\phi(\tau)}{\phi''(\tau)}}.$$

Replacing τ and ρ by their numerical approximations, we obtain the announced result. \square

4.3. Refined enumeration and asymptotic distribution of parameters. From the specification of pointed level-1 networks seen in the proof of Theorem 4.1, it follows easily, as done in [SS06], that the multivariate generating function $G(z, x, y) = \sum_{n,k,m} \frac{g_{n,k,m}}{n!} z^n x^k y^m$, where $g_{n,k,m}$ is the number of unrooted level-1 networks with $n + 1$ leaves, k cycles, and m inner edges, satisfies

$$(\star_G) \quad G(z, x, y) = z + \frac{1}{2}G(z, x, y)^2 + \frac{1}{2}xy^3 \frac{G(z, x, y)^2}{1 - yG(z, x, y)}.$$

This equation can be rewritten as $G(z, x, y) = z\phi(G(z, x, y), x, y)$ where ϕ is defined by $\phi(z, x, y) = \frac{1}{1 - \frac{1}{2}z\left(1 + \frac{xy^3}{1-yz}\right)}$. As done in [SS06], we can apply the Lagrange inversion formula to obtain an explicit expression for $g_{n,k,m}$ – see [SS06, Thm. 4].

Using Theorem 3.2, the above equation may also be used to prove that the parameters “number of cycles” and “number of inner edges” are both asymptotically normally distributed.

Proposition 4.4. *Let X_n (resp. Y_n) be the random variable counting the number of cycles (resp. inner edges) in unrooted level-1 networks with $n + 1$ leaves. Both X_n and Y_n are asymptotically normally distributed, and more precisely, we have*

$$\begin{aligned} \mathbb{E}X_n &= \mu_X n + O(1), & \text{Var}X_n &= \sigma_X^2 n + O(1) & \text{and} & & \frac{X_n - \mathbb{E}X_n}{\sqrt{\text{Var}X_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \\ \mathbb{E}Y_n &= \mu_Y n + O(1), & \text{Var}Y_n &= \sigma_Y^2 n + O(1) & \text{and} & & \frac{Y_n - \mathbb{E}Y_n}{\sqrt{\text{Var}Y_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \end{aligned}$$

where $\mu_X \approx 0.46$, $\sigma_X^2 \approx 0.18$, $\mu_Y \approx 1.61$ and $\sigma_Y^2 \approx 1.44$.

Proof. Consider first X_n . Defining $G(z, x) := G(z, x, 1)$, it holds that

$$\mathbb{E}x^{X_n} = \frac{[z^n]G(z, x)}{[z^n]G(z, 1)}.$$

It follows from the equation for $G(z, x, y)$ that $G(z, x) = F(G(z, x), z, x)$, where F is defined by $F(G, z, x) = z \frac{1}{1 - \frac{1}{2}G(1 + \frac{x}{1-G})}$. It is readily checked that F satisfies all hypotheses of Theorem 3.2.

The system

$$\begin{aligned} G &= F(G, z, 1) \\ 1 &= F_G(G, z, 1) \end{aligned}$$

admits a solution (G_0, z_0) such that $G_0 \approx 0.3427$ and $z_0 \approx 0.1946$, which satisfies the hypothesis of Theorem 3.2. The result then follows from Theorem 3.2, and the numerical estimates of μ_X and σ_X^2 are obtained plugging the numerical estimates for G_0 and z_0 into the explicit formulas

given by Theorem 3.2. The proof for Y_n follows the exact same steps, considering this time $G(z, y) := G(z, 1, y)$ instead, and adjusting the definition of F accordingly. As expected, the solution (G_0, z_0) of the associated system is the same as above. \square

5. COUNTING ROOTED LEVEL-1 NETWORKS

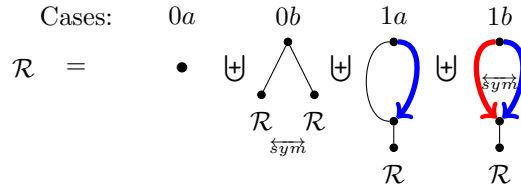
5.1. Combinatorial specification and generating function. As for unrooted level-1 networks, we start by a combinatorial specification that describes rooted level-1 networks (also called rooted galled trees). Because every cycle in a rooted level-1 network not only has a tree vertex above all other vertices of the cycle, but also a reticulation vertex which is below all vertices of the cycle, notice that these objects are different from the pointed level-1 networks that we considered in the proof of Theorem 4.1 and Proposition 4.2.

Recall that each cycle of a level-1 network has strictly more than one outgoing arc (otherwise there would be an infinite number of level-1 networks on n taxa).

Let us denote by \mathcal{R} the set of rooted level-1 networks. The size of a network of \mathcal{R} is the number of its leaves. Distinguishing on the level (0 or 1) of the bridgeless component containing its root, a network of \mathcal{R} is described in exactly one of the following ways. It may be:

- a single leaf (case 0a);
- a binary root vertex with two children that are roots of networks of \mathcal{R} , whose left-to-right order is irrelevant (case 0b);
- a cycle containing the root with at least two outgoing cut arcs leading to networks of \mathcal{R} . This last possibility splits into two subcases, since the reticulation vertex of the cycle may be a child of the root:
 - a cycle whose reticulation vertex is attached to a network of \mathcal{R} , is a child of the root and is the lowest vertex of a path coming from the root, where a sequence of at least one network of \mathcal{R} is attached (case 1a);
 - a cycle whose reticulation vertex is attached to a network of \mathcal{R} , and such that a sequence of at least one network of \mathcal{R} is attached to each path of this cycle, the left-to-right order of these two paths being irrelevant (case 1b).

The specification for \mathcal{R} is therefore given by (all arcs are directed downwards, the thick arcs each represent a directed path which contains at least one internal vertex incident with a cut arc):



Denoting r_n the number of rooted level-1 networks on n leaves, and $R(z) = \sum_{n \geq 0} r_n \frac{z^n}{n!}$ the associated exponential generating function, we deduce from the specification that

$$R = z + \frac{1}{2}R^2 + \frac{R^2}{1-R} + \frac{R}{2} \left(\frac{R}{1-R} \right)^2 .$$

Unlike for the other generating functions considered in this paper, the above equation for R allows to find a closed formula for R . Indeed, the above equation has four solutions that can be made explicit with the help of a solver. We can further notice that evaluating the generating function $R(z)$ at $z = 0$, we must obtain $R(0) = r_0 = 0$. Among the four candidate solutions for R , we therefore select the only one which has value 0 for $z = 0$ and obtain an explicit form for $R(z)$, given in Theorem 5.1.

Theorem 5.1. *The exponential generating function $R(z)$ of rooted level-1 networks is expressed as*

$$R(z) = -\frac{\sqrt{2}\sqrt{-4(\sqrt{1-8z}-2)z+9\sqrt{1-8z}-1}}{4(1-8z)^{\frac{1}{4}}} - \frac{1}{4}\sqrt{1-8z} + \frac{5}{4}$$

within its disk of convergence of radius $\frac{1}{8}$.

5.2. Exact enumeration formula. The first terms of the sequence (r_0, r_1, r_2, \dots) can be read on the Taylor expansion of $R(z)$, and have been collected in Table 2:

$$R(z) = z + 3\frac{z^2}{2!} + 36\frac{z^3}{3!} + 723\frac{z^4}{4!} + 20280\frac{z^5}{5!} + o(z^5).$$

More generally, we have:

Proposition 5.2. *For any $n \geq 1$, the number r_n of rooted level-1 networks with n leaves is given by*

$$\frac{(2n-2)!}{2^{n-1}(n-1)!} + \sum_{\substack{1 \leq k \leq i \leq n-1 \\ 0 \leq p \leq k}} \frac{(n+i-1)!(n+k-i-2)!}{(i-k)!(k-p)!p!(n-1-i-k+p)!(2k-p-1)!} 2^{p-i}.$$

Proof. To obtain a generic formula for r_n , we apply the Lagrange inversion formula, rewriting $R(z)$ as $R(z) = z\phi(R(z))$ where $\phi(z) = \frac{1}{1-\frac{1}{2}z-\frac{z}{1-z}-\frac{1}{2}\left(\frac{z}{1-z}\right)^2}$.

Using twice the usual development of $(1-z)^{-n}$ (for $n \geq 1$) and twice the binomial theorem, we obtain that

$$\begin{aligned} \phi(z)^n &= \sum_{i \geq 0} \binom{n+i-1}{i} \frac{z^i}{2^i} \\ &+ \sum_{i \geq 0} \sum_{k=1}^i \sum_{p=0}^k \sum_{j \geq 0} \binom{n+i-1}{i} \binom{i}{k} \binom{k}{p} \binom{2k-p+j-1}{j} \frac{z^{i+k-p+j}}{2^{i-p}}, \end{aligned}$$

and we deduce that

$$\begin{aligned} r_n &= n![z^n]R(z) = n! \frac{1}{n} [z^{n-1}] \phi(z)^n = (n-1)! [z^{n-1}] \phi(z)^n \\ &= \frac{(2n-2)!}{2^{n-1}(n-1)!} \\ &+ \sum_{\substack{1 \leq k \leq i \leq n-1 \\ 0 \leq p \leq k}} \frac{(n+i-1)!(n+k-i-2)!}{(i-k)!(k-p)!p!(n-1-i-k+p)!(2k-p-1)!} 2^{p-i} \end{aligned}$$

as announced. \square

5.3. Asymptotic evaluation. The equation for $R(z)$ also enables us to derive an asymptotic estimate of r_n .

Proposition 5.3. *The number r_n of rooted level-1 networks on n leaves is asymptotically equivalent to $c_1 \cdot c_2^n \cdot n^{n-1}$ for $c_1 = \frac{\sqrt{34}(\sqrt{17}-1)}{136} \approx 0.1339$ and $c_2 = \frac{8}{e} \approx 2.943$.*

Proof. Recall that $R(z) = z\phi(R(z))$ where $\phi(z) = \frac{1}{1-\frac{1}{2}z-\frac{z}{1-z}-\frac{1}{2}\left(\frac{z}{1-z}\right)^2}$ so that we can apply the Singular Inversion Theorem. Unlike in the case of unrooted level-1 networks, the solution τ of the characteristic equation $\phi(z) - z\phi'(z) = 0$ to be considered has a nice explicit expression here, and we have $\tau = \frac{5-\sqrt{17}}{4}$. We obtain $\rho = \frac{\tau}{\phi(\tau)} = \frac{1}{8}$ and $\sqrt{\frac{\phi(\tau)}{2\phi'(\tau)}} = \frac{\sqrt{17}(\sqrt{17}-1)}{136}$. Consequently, from Theorem 3.1 we have:

$$[z^n]R(z) \sim \frac{\sqrt{17}(\sqrt{17}-1)}{136} \frac{8^n}{\sqrt{\pi n^3}}.$$

Since $r_n = n![z^n]R(z)$, using the Stirling estimate of the factorial, we finally get:

$$r_n \sim \frac{\sqrt{34}(\sqrt{17}-1)}{136} \left(\frac{8}{e}\right)^n n^{n-1}. \quad \square$$

Notice that with the explicit expression of the generating function $R(z)$ in Theorem 5.1, another way of proving Proposition 5.3 would have been to use the Transfer Theorem (Corollary VI.1 of [FS08]). We do not enter the details of this other method here, but we can check that it gives the same result.

5.4. Refined enumeration formula. As in the work of Semple and Steel [SS06], we can refine the enumeration of rooted level-1 networks according to two additional parameters, which are typical of the “level-1” nature of our networks: their number of cycles and their total number of arcs among cycles. To do so, let us introduce the multivariate generating function $R(z, x, y) = \sum \frac{r(n, k, m)}{n!} z^n x^k y^m$, where $r(n, k, m)$ is the number of rooted level-1 networks with n leaves, k cycles and m inner arcs (i.e. the total number of arcs inside those k cycles is m). The specification for \mathcal{R} translates into the following equation for $R = R(z, x, y)$:

$$(\star_R) \quad R = z + \frac{1}{2}R^2 + x \frac{R^2 y^3}{1 - yR} + xR \frac{1}{2} \left(\frac{Ry^2}{1 - yR} \right)^2.$$

The equation can be rewritten as follows:

$$R = z\phi(R, x, y) \text{ where } \phi(z, x, y) = \frac{1}{1 - \frac{1}{2}z - x \frac{zy^3}{1-yz} - \frac{1}{2}xy^4 \left(\frac{z}{1-yz} \right)^2}.$$

Applying the Lagrange inversion formula again, we have

$$\frac{r(n, k, m)}{n!} = [z^n x^k y^m]R(z, x, y) = \frac{1}{n} [z^{n-1} x^k y^m] \phi(z, x, y)^n,$$

and by the exact same steps of computation as in the proof of Proposition 5.2, we get:

Proposition 5.4. *The number $r(n, k, m)$ of level-1 networks with n leaves, k cycles and m inner arcs (with $k \geq 1$ and $m \geq 1$) is*

$$r(n, k, m) = \sum_{p=0}^k \frac{(2n + 3k - m - 2)!(m - 2k - 1)!2^{p+m+1-n-3k}}{(n + 2k - m - 1)!p!(k - p)!(m - 4k + p)!(2k - p - 1)!}.$$

Notice that from $r_n = r(n, 0, 0) + \sum_{k=1}^{n-1} \sum_{m=3k}^{n+2k-1} r(n, k, m)$ and the above theorem, we can recover Proposition 5.2 by the change of variable $m = n + 3k - i - 1$.

5.5. Asymptotic distribution of parameters. As we have seen with Proposition 4.4, the equation for the refined generating function does not only give access to the explicit formula of Proposition 5.4 above, but also allows to prove that the two parameters of interest are each asymptotically normally distributed.

Proposition 5.5. *Let X_n (resp. Y_n) be the random variable counting the number of cycles (resp. inner arcs) in rooted level-1 networks with n leaves. Both X_n and Y_n are asymptotically normally distributed, and more precisely, we have*

$$\begin{aligned} \mathbb{E}X_n &= \mu_X n + O(1), & \text{Var}X_n &= \sigma_X^2 n + O(1) & \text{and} & & \frac{X_n - \mathbb{E}X_n}{\sqrt{\text{Var}X_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \\ \mathbb{E}Y_n &= \mu_Y n + O(1), & \text{Var}Y_n &= \sigma_Y^2 n + O(1) & \text{and} & & \frac{Y_n - \mathbb{E}Y_n}{\sqrt{\text{Var}Y_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \end{aligned}$$

where $\mu_X \approx 0.56$, $\sigma_X^2 \approx 0.18$, $\mu_Y \approx 1.93$ and $\sigma_Y^2 \approx 1.24$.

Proof. Recall that, defining $\phi(z, x, y) = \frac{1}{1 - \frac{1}{2}z - x\frac{zy^3}{1-yz} - \frac{1}{2}xy^4\left(\frac{z}{1-yz}\right)^2}$, $R(z, x, y)$ satisfies $R = z\phi(R, x, y)$. We focus first on X_n , setting $y = 1$, and we consider $R(z, x) := R(z, x, 1)$. It holds that

$$\mathbb{E}x^{X_n} = \frac{[z^n]R(z, x)}{[z^n]R(z, 1)}.$$

Defining the function F by $F(R, z, x) = z\phi(R, x, 1)$, it also holds that $R(z, x) = F(R(z, x), z, x)$. It is readily checked that F satisfies all hypotheses of Theorem 3.2. Moreover, the system

$$\begin{aligned} R &= F(R, z, 1) \\ 1 &= F_R(R, z, 1) \end{aligned}$$

admits a solution (R_0, z_0) with $z_0 = 1/8$ and $R_0 \approx 0.2192$, which satisfies the hypothesis of Theorem 3.2. The result and numerical estimates of μ_X and σ_X^2 then follow from Theorem 3.2.

For Y_n instead of X_n , the proof works in the exact same way, considering this time $R(z, y) := R(z, 1, y)$ instead, and adjusting the definition of F accordingly. As in the proof of Proposition 4.4, we find the same solution (R_0, z_0) of the associated system, as it should be. \square

6. COUNTING UNROOTED LEVEL-2 NETWORKS

6.1. Combinatorial specification. First of all, let us recall that any bridgeless component in an unrooted level-2 network has at least three outgoing cut-edges (since otherwise there would be an infinite number of such networks with a given number of leaves).

As in the case of level-1 unrooted networks, we consider *pointed* level-2 networks, that are unrooted level-2 networks equipped with a fictitious root, which is a new leaf labeled by the special taxa $\#$. This provides a bijection between unrooted level-2 networks on the set of taxa $X \uplus \{\#\}$ and pointed level-2 networks on X . Therefore, there are as many unrooted level-2 networks of the set of taxa $X \uplus \{\#\}$ as pointed level-2 networks on X rooted in a leaf labeled by $\# \notin X$. Notice that pointed level-2 networks do not correspond to classical rooted level-2 networks. Indeed, every bridgeless component in a pointed level-2 network has a distinguished vertex which could be considered as the equivalent of a root, but no reticulation vertices, whereas it has both in the usual definition of rooted level-2 networks.

Let us denote by \mathcal{U} the set of such pointed level-2 networks, the size of a network of \mathcal{U} being the number of its leaves different from the root. Denoting u_n the number of networks of size n in \mathcal{U} , the above argument shows that u_n counts the number of unrooted level-2 networks on $(n+1)$ leaves. We introduce $U(z) = \sum_{n \geq 0} u_n \frac{z^n}{n!}$ the associated exponential generating function.

To obtain a combinatorial specification for \mathcal{U} , and hence an equation satisfied by $U(z)$, we describe the possible shapes of a network N of \mathcal{U} , depending on the level (0, 1 or 2) of the bridgeless component that contains the neighbouring vertex of the fictitious root.

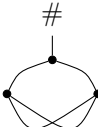
- Of course, we must start with the trivial case in which the fictitious root is attached directly to a leaf.

For the remaining cases, denote by v the vertex at the other extremity of the edge incident to the fictitious root.

- If v does not belong to a cycle nor to a bridgeless component of level 2, then N is described as an unordered pair of two pointed level-2 networks.
- If v belongs to a cycle but not to a bridgeless component of level 2, then N is described as an unoriented sequence of at least two pointed level-2 networks.

(These first three cases are the same as in Section 5.)

- The last possibility is that v belongs to a bridgeless component of level 2. The underlying

level-2 generator, G , is necessarily of the shape . In this case, we distinguish

many cases in Section 8.1 of the Appendix, depending on whether each edge of the level-2 generator contains exactly one vertex incident with a cut-edge, several or none.

6.2. Generating function. The specification is directly translated into the following equation for the generating function U (see the Appendix for details):

$$U = z + \frac{U^2}{2} + \frac{U^2}{2(1-U)} + \frac{3U^2}{2(1-U)} + 2U^2 + \frac{7U^3}{2(1-U)} + \frac{7U^4}{4(1-U)^2} + U^3 + \frac{3U^4}{1-U} \\ + \frac{3U^5}{(1-U)^2} + \frac{U^6}{(1-U)^3} + \frac{U^4}{4} + \frac{U^5}{1-U} + \frac{3U^6}{2(1-U)^2} + \frac{U^7}{(1-U)^3} + \frac{U^8}{4(1-U)^4}.$$

This equation for the generating function allows to derive the first coefficients of the series expansion of $U(z)$, namely:

$$U(z) = z + \frac{9}{2}z^2 + 47z^3 + \frac{4899}{8}z^4 + \frac{35725}{4}z^5 + \dots.$$

The corresponding first values of u_n have been included in Table 2. (Recall indeed that $U(z) = \sum_{n \geq 0} u_n \frac{z^n}{n!}$ and that u_n is the number of unrooted level-2 networks on $(n+1)$ leaves).

The above equation for $U(z)$ can also be rewritten as follows:

Theorem 6.1. *The generating function $U(z)$ satisfies:*

$$U(z) = z\phi(U(z)) \text{ where } \phi(z) = \frac{1}{1 - \frac{3z^5 - 20z^4 + 46z^3 - 46z^2 + 18z}{4(1-z)^4}}.$$

Proof. This is simply obtained from the above equation for U by algebraic manipulations. \square

6.3. Exact enumeration formula. To obtain a closed form for u_n , we start from the equation for U given in Theorem 6.1. By the Lagrange inversion formula we obtain that:

$$u_n = n![z^n]U(z) = \frac{n!}{n}[z^{n-1}]\phi^n(z) = (n-1)![z^{n-1}]\phi^n(z),$$

so, to compute the first values of u_n , we can compute the Taylor expansions of $\phi^n(z)$ and get the values in Table 2.

As for the case of level-1 networks, we may also deduce with routine algebra an explicit formula for u_n .

Proposition 6.2. *For any $n \geq 1$, the number u_n of unrooted level-2 phylogenetic networks with $(n+1)$ leaves is given by*

$$u_n = (n-1)! \sum_{\substack{0 \leq s \leq q \leq p \leq k \leq i \leq n-1 \\ j = n-1-i-k-p-q-s \geq 0 \\ i \neq 0}} \binom{n+i-1}{i} \binom{4i+j-1}{j} \binom{i}{k} \binom{k}{p} \binom{p}{q} \binom{q}{s} \\ \times \left(\frac{9}{2}\right)^i \left(\frac{-23}{9}\right)^k (-1)^p \left(\frac{-10}{23}\right)^q \left(\frac{-3}{20}\right)^s.$$

Proof sketch. Recall that $U(z) = z\phi(U(z))$ with $\phi(z) = \frac{1}{1 - \frac{3z^5 - 20z^4 + 46z^3 - 46z^2 + 18z}{4(1-z)^4}}$. Using first the classical development of $(1-z)^{-n}$ in series, and then the binomial theorem, we have

$$\phi(z)^n = \sum_{i \geq 0} \binom{n+i-1}{i} \left(\frac{18z}{4(1-z)^4} + \frac{-46z^2 + 46z^3 - 20z^4 + 3z^5}{4(1-z)^4} \right)^i \\ = \sum_{i \geq 0} \sum_{k=0}^i \binom{n+i-1}{i} \binom{i}{k} \left(\frac{18z}{4(1-z)^4} \right)^{i-k} \left(\frac{-46z^2 + 46z^3 - 20z^4 + 3z^5}{4(1-z)^4} \right)^k.$$

We continue applying the binomial theorem inside the above formula, isolating each time the term with the lowest degree in the numerator (that is, first $\frac{-46z^2}{4(1-z)^4}$, second $\frac{46z^3}{4(1-z)^4}$, ...). This yields

$$\begin{aligned} \phi(z)^n &= \sum_{i \geq 0} \sum_{k=0}^i \sum_{p=0}^k \sum_{q=0}^p \sum_{s=0}^q \binom{n+i-1}{i} \binom{i}{k} \binom{k}{p} \binom{p}{q} \binom{q}{s} \\ &\quad \left(\frac{18z}{4(1-z)^4} \right)^{i-k} \left(\frac{-46z^2}{4(1-z)^4} \right)^{k-p} \left(\frac{46z^3}{4(1-z)^4} \right)^{p-q} \left(\frac{-20z^4}{4(1-z)^4} \right)^{q-s} \left(\frac{3z^5}{4(1-z)^4} \right)^s \\ &= \sum_{i \geq 0} \sum_{k=0}^i \sum_{p=0}^k \sum_{q=0}^p \sum_{s=0}^q \binom{n+i-1}{i} \binom{i}{k} \binom{k}{p} \binom{p}{q} \binom{q}{s} \frac{\left(\frac{9}{2}\right)^i \left(\frac{-23}{9}\right)^k (-1)^p \left(\frac{-10}{23}\right)^q \left(\frac{-3}{20}\right)^s}{(1-z)^{4i}} z^{i+k+p+q+s}. \end{aligned}$$

The result then follows from developing of $(1-z)^{-4i}$ in series as $(1-z)^{-4i} = \sum_{j \geq 0} \binom{4i+j-1}{j} z^j$ and using the Lagrange inversion formula. \square

6.4. Asymptotic evaluation. From Theorem 6.1, we can furthermore derive an asymptotic evaluation of the number u_n of unrooted level-2 networks on $(n+1)$ leaves, using Theorem 3.1.

Proposition 6.3. *The number u_n of unrooted level-2 networks on $(n+1)$ leaves is asymptotically equivalent to $c_1 \cdot c_2^n \cdot n^{n-1}$ for constants c_1 and c_2 such that $c_1 \approx 0.0590$ and $c_2 \approx 7.662$.*

Proof. Denoting by $\tau \approx 0.08965$ the unique solution of the characteristic equation $\phi(z) - z\phi'(z) = 0$ in the disk of convergence of ϕ , and $\rho = \frac{\tau}{\phi(\tau)} \approx 0.04801$, we have:

$$[z^n]U(z) \sim \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)}} \frac{\rho^{-n}}{\sqrt{\pi n^3}}.$$

Using the Stirling estimate of the factorial, we get:

$$u_n \sim \left(\frac{n}{e}\right)^n \sqrt{2\pi n} \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)}} \frac{\rho^{-n}}{\sqrt{\pi n^3}} \sim \frac{n^{n-1}}{(e\rho)^n} \sqrt{\frac{\phi(\tau)}{\phi''(\tau)}}.$$

Replacing τ and ρ by their numerical approximations, we get the announced result. \square

6.5. Refined enumeration formula and asymptotic distribution of parameters. Consider the refined generating function $U(z, x, y)$ for unrooted level-2 networks, where the variable z counts the size as before, the variable x counts the number of bridgeless components of level 1 or 2 (or equivalently, the number of level-1 or level-2 generators in the decomposition of these networks), and the variable y counts the number of inner edges, defined as the total number of edges across all level-1 and level-2 bridgeless components. The specification provided in the Appendix can be refined for these statistics, yielding the following equation for $U := U(z, x, y)$:

$$\begin{aligned} U &= z + \frac{U^2}{2} + \frac{xy^3U^2}{2(1-yU)} + \frac{3xy^6U^2}{2(1-yU)} + 2xy^6U^2 + \frac{7xy^7U^3}{2(1-yU)} + \frac{7xy^8U^4}{4(1-yU)^2} + xy^7U^3 + \frac{3xy^8U^4}{1-yU} \\ (\star_U) \quad &+ \frac{3xy^9U^5}{(1-yU)^2} + \frac{xy^{10}U^6}{(1-yU)^3} + \frac{xy^8U^4}{4} + \frac{xy^9U^5}{1-yU} + \frac{3xy^{10}U^6}{2(1-yU)^2} + \frac{xy^{11}U^7}{(1-yU)^3} + \frac{xy^{12}U^8}{4(1-yU)^4}. \end{aligned}$$

From the above equation, and similarly to Proposition 5.4, it would be possible (although computations and result are not reported in this paper) to derive an explicit formula for the number of unrooted level-2 networks with n leaves, k bridgeless components of level 1 or 2, and m edges across them. Furthermore, some information on the asymptotic behavior of these parameters can be obtained from Equation (\star_U) .

Proposition 6.4. *Let X_n (resp. Y_n) be the random variable counting the number of level-1 or level-2 bridgeless components (resp. the number of edges across them) in unrooted level-2 networks*

with $n + 1$ leaves. Both X_n and Y_n are asymptotically normally distributed, and more precisely, we have

$$\begin{aligned} \mathbb{E}X_n &= \mu_X n + O(1), & \text{Var}X_n &= \sigma_X^2 n + O(1) & \text{and} & & \frac{X_n - \mathbb{E}X_n}{\sqrt{\text{Var}X_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \\ \mathbb{E}Y_n &= \mu_Y n + O(1), & \text{Var}Y_n &= \sigma_Y^2 n + O(1) & \text{and} & & \frac{Y_n - \mathbb{E}Y_n}{\sqrt{\text{Var}Y_n}} &\xrightarrow{d} \mathcal{N}(0, 1), \end{aligned}$$

where $\mu_X \approx 0.7835$, $\sigma_X^2 \approx 0.1462$, $\mu_Y \approx 4.5580$ and $\sigma_Y^2 \approx 4.3711$.

Proof. Consider first X_n . Defining $U(z, x) := U(z, x, 1)$, it holds that

$$\mathbb{E}x^{X_n} = \frac{[z^n]U(z, x)}{[z^n]U(z, 1)}.$$

It follows from the equation for $U(z, x, y)$ that $U(z, x) = F(U(z, x), z, x) = z \frac{1}{1 - A(U(z, x), z, x)}$ with

$$\begin{aligned} A(U, z, x) &= \frac{U}{2} + \frac{xU}{2(1-U)} + \frac{3xU}{2(1-U)} + 2xU + \frac{7xU^2}{2(1-U)} + \frac{7xU^3}{4(1-U)^2} + xU^2 + \frac{3xU^3}{1-U} \\ &\quad + \frac{3xU^4}{(1-U)^2} + \frac{xU^5}{(1-U)^3} + \frac{xU^3}{4} + \frac{xU^4}{1-U} + \frac{3xU^5}{2(1-U)^2} + \frac{xU^6}{(1-U)^3} + \frac{xU^7}{4(1-U)^4}. \end{aligned}$$

It is readily checked that F satisfies all hypotheses of Theorem 3.2. The system

$$\begin{aligned} U &= F(U, z, 1) \\ 1 &= F_U(U, z, 1) \end{aligned}$$

admits a solution (U_0, z_0) such that $U_0 \approx 0.0897$ and $z_0 \approx 0.04801$, which satisfies the hypothesis of Theorem 3.2. The result then follows from Theorem 3.2, and the numerical estimates of μ_X and σ_X^2 are obtained plugging the numerical estimates for U_0 and z_0 into the explicit formulas given by Theorem 3.2. The proof for Y_n follows the exact same steps, considering this time $U(z, y) := U(z, 1, y)$ instead, and adjusting the definition of F accordingly. Again, as expected, the solution (U_0, z_0) of the associated system is the same as above. \square

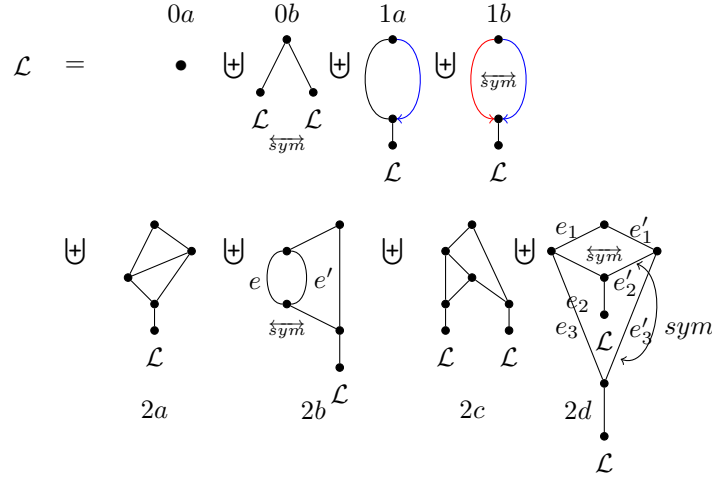
7. COUNTING ROOTED LEVEL-2 NETWORKS

7.1. Combinatorial specification and generating function. To derive a specification for rooted level-2 networks, we distinguish cases depending on the level (0, 1 or 2) of the generator to which the root belongs. The cases corresponding to levels 0 and 1 will be the same as in Section 5. When the root of a rooted level-2 network belongs to a level-2 generator, we have to remember that these generators have one vertex which is above all their other vertices (which is the root of the network) and not just one but two reticulation vertices. As for rooted level-1 networks, it is important to keep in mind that any bridgeless component of level 2 in a rooted level-2 network has at least two outgoing cut-arcs (since otherwise there would be an infinite number of such networks with a given number of leaves).

We denote by \mathcal{L} the set of rooted level-2 networks, where the size corresponds to the number of leaves. And we denote by $L(z)$ the corresponding exponential generating function. Distinguishing on the level (0, 1 or 2) of the bridgeless component containing the root, we can see that any network N of \mathcal{L} satisfies exactly one of the following (see Fig. 3).

- N is just a leaf. This contributes z to the generating function (case 0a).
- The root of N belongs to a bridgeless component of level 0, that is to say it is a binary root vertex. Its children are themselves networks of \mathcal{L} whose left-to-right order is irrelevant. This contributes $\frac{L^2}{2}$ to the generating function (case 0b).
- The root of N belongs to a bridgeless component of level 1. This case splits into two subcases, just as in Section 5.
 - Either N consists of a cycle whose reticulation vertex is attached to a network of \mathcal{L} , is a child of the root and is the lowest vertex of a path from the root where a sequence of at least one network of \mathcal{L} is attached. This contributes $\frac{L^2}{1-L}$ to the generating function (case 1a).

- Or N consists of a cycle whose reticulation vertex is attached to a network of \mathcal{L} , and a sequence of at least one network of \mathcal{L} is attached to each path of this cycle (case 1b). This contributes $\frac{L}{2} \left(\frac{L}{1-L} \right)^2$.
- The root of N belongs to a bridgeless component of level 2. The level-2 generators are displayed in Fig. 3, cases 2a to 2d. From these generators, the networks whose root belong to a bridgeless component of level 2 are obtained attaching networks of \mathcal{L} to their reticulation vertex or vertices with out-degree 0, and possibly replacing their arcs with sequences of at least one network of \mathcal{L} . Note that in cases 2b and 2d, depending on our choices for such arcs, we may have to cope with horizontal and vertical symmetry. We study these cases in order, and find their contribution to the generating function $L(z)$.

FIGURE 3. The specification of the class \mathcal{L} .

- We first deal with the case where the level-2 generator to which the root belongs is of type 2a. This generator has 5 internal arcs, all distinguished from each other by the structure of the generator. A network of \mathcal{L} is attached to its reticulation vertex of out-degree 0. Moreover, recalling that each bridgeless component must have at least two outgoing cut-arcs, at least one of the five internal arcs of the generator must carry a non-empty sequence of networks of \mathcal{L} . Therefore, the contribution of case 2a to the generating function of \mathcal{L} is

$$L \cdot \sum_{i=1}^5 \binom{5}{i} \left(\frac{L}{1-L} \right)^i.$$

- In the case where the level-2 generator to which the root belongs is of type 2b, we similarly have 5 internal arcs in the generator, at least one of which must be replaced by a non-empty sequence of networks of \mathcal{L} . However, the two arcs e and e' are not distinguishable. The contribution to the generating function is therefore more subtle to analyze, and we perform this detailed analysis in the Section 8.2 of the Appendix. The overall contribution of case 2b to the generating function of \mathcal{L} is then shown to be

$$4L \frac{L}{1-L} + \frac{13}{2} L \left(\frac{L}{1-L} \right)^2 + \frac{11}{2} L \left(\frac{L}{1-L} \right)^3 + \frac{5}{2} L \left(\frac{L}{1-L} \right)^4 + \frac{1}{2} L \left(\frac{L}{1-L} \right)^5.$$

- We now consider the case where the level-2 generator to which the root belongs is of type 2c. This generator has 6 internal arcs, all distinguished from each other by the structure of the generator. Moreover, two networks of \mathcal{L} are attached to its

reticulation vertices, so that the condition that each bridgeless component must be have at least two outgoing cut-arcs is already satisfied. Therefore, all 6 internal arcs of the generator carry possibly empty sequences of networks of \mathcal{L} . As a consequence, the contribution of case $2c$ to the generating function of \mathcal{L} is

$$L^2 \left(\frac{1}{1-L} \right)^6.$$

- Similarly, when the root belongs to a level-2 generator of type $2d$, the 6 arcs of the generator carry possibly empty sequences of networks of \mathcal{L} . However, this generator enjoys both a horizontal symmetry (mapping e_i to e'_i for $i = 1, 2, 3$) and a vertical symmetry (exchanging the indices 2 and 3 and the corresponding pending networks of \mathcal{L}). In case all arcs carry empty sequences, the horizontal symmetry is actually the identity, so that only the vertical symmetry applies, yielding a factor $\frac{1}{2}$. Otherwise, both the horizontal and the vertical symmetry need to be taken into account, yielding a factor $\frac{1}{4}$. The total contribution of case $2d$ to the generating function of \mathcal{L} is therefore

$$\frac{1}{2}L^2 + \frac{1}{4}L^2 \cdot \sum_{i=1}^6 \binom{6}{i} \left(\frac{L}{1-L} \right)^i.$$

Following this case analysis we obtain an equation characterizing the generating function of \mathcal{L} .

Theorem 7.1. *The exponential generating function $L(z)$ of rooted level-2 networks counted by number of leaves satisfies*

$$\begin{aligned} L = z + L^2 + \frac{10L^2}{1-L} + \frac{3L^3}{2(1-L)} + \frac{17L^3}{(1-L)^2} + \frac{15L^4}{4(1-L)^2} + \frac{31L^4}{2(1-L)^3} + \frac{5L^5}{(1-L)^3} \\ + \frac{15L^5}{2(1-L)^4} + \frac{15L^6}{4(1-L)^4} + \frac{3L^6}{2(1-L)^5} + \frac{3L^7}{2(1-L)^5} + \frac{L^2}{(1-L)^6} + \frac{L^8}{4(1-L)^6}, \end{aligned}$$

or equivalently

$$L(z) = z\phi(L(z)) \quad \text{where} \quad \phi(z) = \frac{1}{1 - \frac{48z - 150z^2 + 235z^3 - 208z^4 + 105z^5 - 28z^6 + 3z^7}{4(1-z)^6}}.$$

We therefore obtain the first terms of the series expansion of $L(z)$,

$$L(z) = z + 12z^2 + \frac{645}{2}z^3 + \frac{43183}{4}z^4 + \frac{1618247}{4}z^5 + \frac{129927717}{8}z^6 + \dots,$$

as reported in Table 2.

7.2. Exact enumeration formula. As in the previous sections, Theorem 7.1 allows to derive an explicit formula for the number ℓ_n of rooted level-2 phylogenetic networks with n leaves.

Proposition 7.2. *For any $n \geq 1$, the number ℓ_n of rooted level-2 phylogenetic networks with n leaves is given by*

$$\ell_n = (n-1)! \sum_{\substack{0 \leq t \leq m \leq s \leq q \leq p \leq k \leq i \leq n-1 \\ j=n-1-i-k-p-q-s-m-t \geq 0 \\ i \neq 0}} \binom{n+i-1}{i} \binom{6i+j-1}{j} \binom{i}{k} \binom{k}{p} \binom{p}{q} \binom{q}{s} \binom{s}{m} \binom{m}{t} \times (12)^i \left(\frac{-25}{8} \right)^k \left(\frac{-47}{30} \right)^p \left(\frac{-208}{235} \right)^q \left(\frac{-105}{208} \right)^s \left(\frac{-28}{105} \right)^m \left(\frac{-3}{28} \right)^t.$$

Proof sketch. This follows again from the Lagrange inversion formula, using the equation $L(z) = z\phi(L(z))$ for the function ϕ given in Theorem 7.1. The computations involve the usual development of $(1-z)^{-n}$ and the binomial formula, applied following exactly the same steps as in the proof of Proposition 6.2. Details of the computations are left to the reader. \square

7.3. Asymptotic evaluation. Similarly, from Theorem 7.1, we can also derive the asymptotic behavior of ℓ_n .

Proposition 7.3. *The number ℓ_n of rooted level-2 phylogenetic networks with n leaves behaves asymptotically as*

$$\ell_n \sim c_1 c_2^n n^{n-1},$$

where $c_1 \approx 0.02386$ and $c_2 \approx 19.687$.

Proof. Recall that

$$L(z) = z\phi(L(z)) \quad \text{where} \quad \phi(z) = \frac{1}{1 - \frac{48z - 150z^2 + 235z^3 - 208z^4 + 105z^5 - 28z^6 + 3z^7}{4(1-z)^6}}.$$

Denoting by $\tau \approx 0.0355$ the unique solution of the characteristic equation $\phi(z) - z\phi'(z) = 0$ in the disk of convergence of ϕ , and $\rho = \frac{\tau}{\phi(\tau)} \approx 0.0187$, the Singular Inversion Theorem gives:

$$[z^n]L(z) \sim \sqrt{\frac{\phi(\tau)}{2\phi''(\tau)}} \frac{\rho^{-n}}{\sqrt{\pi n^3}}.$$

Like before, we get the claimed result from $\ell_n = n![z^n]L(z)$ and the Stirling estimate of the factorial. \square

7.4. Refined enumeration formula and asymptotic distribution of parameters. Let $L(z, x, y) = \sum_{n,k,m} \ell_{n,k,m} \frac{z^n}{n!} x^k y^m$ be the multivariate generating function counting rooted level-2 networks w.r.t. their number of leaves (variable z), their number of bridgeless components of level 1 or 2 (variable x) and their number of arcs across all these (variable y). From the specification of \mathcal{L} discussed earlier, $L(z, x, y) = L$ is easily seen to satisfy the following equation:

$$\begin{aligned} L &= z + \frac{L^2}{2} + x \left(\frac{y^6 L^2}{2} + (y^3 + 9y^6) \frac{L^2}{1-yL} + \frac{3y^7 L^3}{2(1-yL)} + \left(\frac{y^4}{2} + \frac{33y^7}{2} \right) \frac{L^3}{(1-yL)^2} \right. \\ &\quad + \frac{15y^8 L^4}{4(1-yL)^2} + \frac{31y^8 L^4}{2(1-yL)^3} + \frac{5y^9 L^5}{(1-yL)^3} + \frac{15y^9 L^5}{2(1-yL)^4} + \frac{15y^{10} L^6}{4(1-yL)^4} \\ (\star_L) \quad &\quad \left. + \frac{3y^{10} L^6}{2(1-yL)^5} + \frac{3y^{11} L^7}{2(1-yL)^5} + \frac{y^6 L^2}{(1-yL)^6} + \frac{y^{12} L^8}{4(1-yL)^6} \right). \end{aligned}$$

From the above equation, an explicit formula for $\ell_{n,k,m}$ could routinely be derived, as in Proposition 5.4, although the computations are more involved. We decided not to report this formula here. Equation (\star_L) also allows to study the asymptotic behavior of the considered parameters.

Proposition 7.4. *Let X_n (resp. Y_n) be the random variable counting the number of bridgeless components of level 1 or 2 (resp. the number of edges across them) in rooted level-2 networks with n leaves. Both X_n and Y_n are asymptotically normally distributed, and more precisely, we have*

$$\mathbb{E}X_n = \mu_X n + O(1), \quad \text{Var}X_n = \sigma_X^2 n + O(1)$$

$$\mathbb{E}Y_n = \mu_Y n + O(1), \quad \text{Var}Y_n = \sigma_Y^2 n + O(1)$$

where $\mu_X \approx 0.8671$, $\sigma_X^2 \approx 0.1027$, $\mu_Y \approx 5.0877$ and $\sigma_Y^2 \approx 3.0973$.

Proof. To prove the result for X_n (resp. Y_n), we specialize Equation (\star_L) for $y = 1$ (resp. $x = 1$) and rewrite it as $L(z, x, 1) = F(L(z, x, 1), z, x)$ for some explicit function F (resp. $L(z, 1, y) = F(L(z, 1, y), z, y)$, for an explicit different F). It is readily checked that F satisfies all hypotheses of Theorem 3.2, as well as the solutions (L_0, z_0) of the system

$$L = F(L, z, 1)$$

$$1 = F_L(L, z, 1)$$

whose approximate values are $L_0 \approx$ and $z_0 \approx$. The result then follows from Theorem 3.2, and the numerical estimates of μ_X and σ_X^2 (resp. μ_Y and σ_Y^2) are obtained plugging the numerical estimates for L_0 and z_0 into the explicit formulas given by Theorem 3.2. \square

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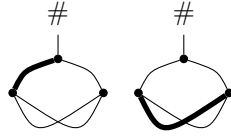
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8. APPENDIX

8.1. Case analysis for unrooted level-2 generators. In the pictures below, we use thick lines to represent paths containing at least 2 internal nodes incident with a cut-edge which is incident with another pointed unrooted level-2 network. We use $\#$ to represent the fictitious root in the pointed network, v to denote its neighbour, and \mathcal{U} to represent any pointed network.

8.1.1. *Case 1: One edge with no attached networks.* One edge of the generator carries a sequence of at least two outgoing arcs. It can either be one of the two edges incident to v (these two are not distinguished), or one of the two edges not incident to v (there are not distinguished either). In the second case, the sequence is unordered, because of symmetry, explaining the factor $\frac{1}{2}$ below.

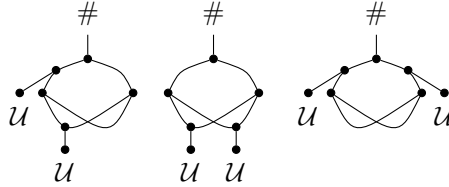
$$\frac{U^2}{1-U} + \frac{1}{2} \frac{U^2}{1-U} = \frac{3U^2}{2(1-U)}$$



8.1.2. *Case 2: Two edges with no attached networks.*

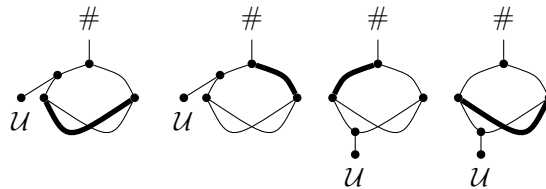
Case 2A - Two edges of the generator carry exactly one outgoing arc. It can either be one edge incident to v and one not, or both edges incident to v , or both edges not incident to v . In the latter two cases, the two edges should not be distinguished, hence the factor $\frac{1}{2}$.

$$U^2 + \frac{U^2}{2} + \frac{U^2}{2} = 2U^2$$



Case 2B - One edge of the generator carries a single outgoing arc and another edge carries a sequence of at least two outgoing arcs. The only case where symmetries need to be taken care of is when the two edges are those not incident to v : in this case, the sequence is not oriented, hence the factor $\frac{1}{2}$. In all other cases, the orientation of the sequence is determined by the presence of the fictitious root or the outgoing arc from the other edge with no attached networks.

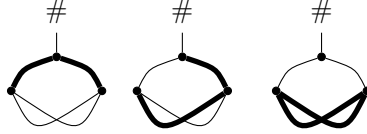
$$\frac{U^3}{1-U} + \frac{U^3}{1-U} + \frac{U^3}{1-U} + \frac{U^3}{2(1-U)} = \frac{7U^3}{2(1-U)}$$



Case 2C - Two edges of the generator carry a sequence of at least two outgoing arcs. If both edges are those incident to v , then both sequences are oriented, but we have a factor $\frac{1}{2}$ for symmetry reason. If one arc is incident to v and the other not, then both sequences are oriented and there is no symmetry factor. If the two arcs are those not incident to v , then the two sequences they carry

can be seen as an unordered pair of oriented sequences, seen up to symmetry w.r.t. the vertical axis. This yields a factor $\frac{1}{2}$ since the pair is unordered, and another factor $\frac{1}{2}$ to account for the symmetry w.r.t. the vertical axis.

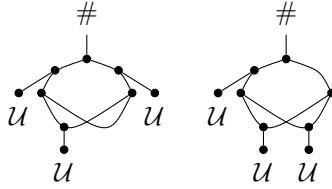
$$\frac{U^4}{2(1-U)^2} + \frac{U^4}{(1-U)^2} + \frac{U^4}{4(1-U)^2} = \frac{7U^4}{4(1-U)^2}$$



8.1.3. Case 3: Three edges with no attached networks.

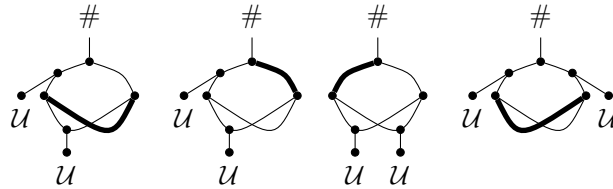
Case 3A - Three edges of the generator carry exactly one outgoing arc. The unused edge can either be incident with v or not. In both cases, we have a factor $\frac{1}{2}$ because of symmetry.

$$\frac{U^3}{2} + \frac{U^3}{2} = U^3$$



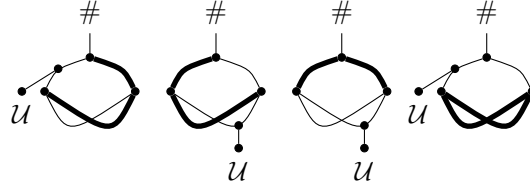
Case 3B - Two edges of the generator carry a single outgoing arc and one carries a sequence of at least two outgoing arcs. The only cases where a symmetry comes into play here are when the edges carrying single outgoing arcs are either the two edges incident to v or the two edges not incident to v . This yield the factor $\frac{1}{2}$ in these two cases. Moreover, all sequences are oriented, because of the presence of the fictitious root or the single outgoing arcs.

$$\frac{U^4}{1-U} + \frac{U^4}{1-U} + \frac{U^4}{2(1-U)} + \frac{U^4}{2(1-U)} = \frac{3U^4}{1-U}$$



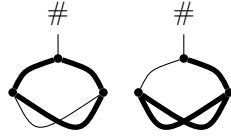
Case 3C - One edge of the generator carries a single outgoing arc and two edges carry a sequence of at least two outgoing arcs. Similarly to the previous case, we obtain a factor $\frac{1}{2}$ for symmetry reasons when the two edges carrying sequences are either the two edges incident to v or the two edges not incident to v . Moreover, all sequences are oriented, because of the presence of the fictitious root or the single outgoing arc.

$$\frac{U^5}{(1-U)^2} + \frac{U^5}{(1-U)^2} + \frac{U^5}{2(1-U)^2} + \frac{U^5}{2(1-U)^2} = \frac{3U^5}{(1-U)^2}$$



Case 3D - Three edges of the generator carry a sequence of at least two outgoing arcs. In both cases, we have a factor $\frac{1}{2}$ for symmetry reason, but all sequences are oriented by the presence of the fictitious root, or of the sequence on the edge(s) incident to v .

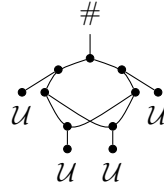
$$\frac{U^6}{2(1-U)^3} + \frac{U^6}{2(1-U)^3} = \frac{U^6}{(1-U)^3}$$



8.1.4. Case 4: Four edges with no attached networks.

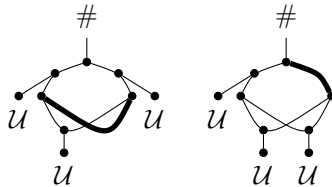
Case 4A - The four edges of the generator each carry exactly one outgoing arc. In this case, the two edges incident to v can be exchanged without modifying the network, and the same holds for the two edges not incident to v . This yields a factor $\frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$ due to symmetries.

$$\frac{U^4}{4}$$



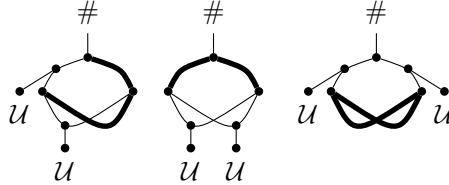
Case 4B - Three edges of the generator carry a single outgoing arc and the fourth one carries a sequence of at least two outgoing arcs. If this fourth edge is one incident to v , then the sequence it carries is oriented by the presence of the fictitious root, but the two arcs pending on the edges not incident to v are symmetric, hence a factor $\frac{1}{2}$. If on the contrary the edge carrying the sequence is not incident to v , then the sequence is also oriented, this time because of the arcs attached to the edges incident to v . Moreover, the picture has a symmetry w.r.t. the vertical axis, hence a factor $\frac{1}{2}$.

$$\frac{U^5}{2(1-U)} + \frac{U^5}{2(1-U)} = \frac{U^5}{1-U}$$



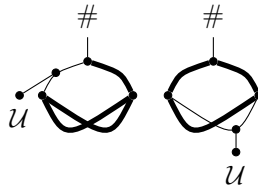
Case 4C - Two edges carry a single outgoing arc and the two others carry a sequence of at least two outgoing arcs. In all cases, the sequences are oriented, by the presence of either the fictitious root or of the single arcs attached to edges. If the edges carrying sequences are one incident to v and the other not incident to v , all edges are in addition distinguished from each other. In the other two cases, both edges incident to v form an unordered pair, as well as the two edges not incident to v . In each case, we therefore have a factor $\frac{1}{4}$.

$$\frac{U^6}{(1-U)^2} + \frac{U^6}{4(1-U)^2} + \frac{U^6}{4(1-U)^2} = \frac{3U^6}{2(1-U)^2}$$



Case 4D - One edge of the generator carries a single outgoing arc and three edges carry a sequence of at least two outgoing arcs. As in the previous case, all sequences are oriented. However, if the two edges incident to v carry a sequence, the picture has a symmetry w.r.t. the vertical axis, hence a factor $\frac{1}{2}$. If on the contrary the two edges not incident to v carry a sequence, these two edges are indistinguishable, hence a factor $\frac{1}{2}$ also in this case.

$$\frac{U^7}{2(1-U)^3} + \frac{U^7}{2(1-U)^3} = \frac{U^7}{(1-U)^3}$$



Case 4E - All four edges of the generator carry a sequence of at least two outgoing arcs. Then all sequences are oriented, but the two edges not incident to v are indistinguishable. The picture has in addition a symmetry w.r.t. the vertical axis. This yields a factor $\frac{1}{4}$.

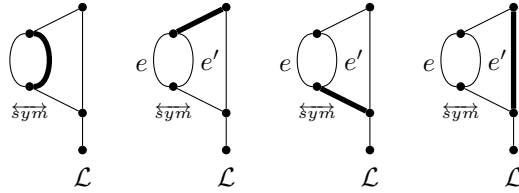
$$\frac{U^8}{4(1-U)^4}$$



8.2. Case analysis for the rooted level-2 generator 2b. In the pictures below, we use thick lines to represent paths containing at least one internal node incident with a cut-arc which is incident with the root of another rooted level-2 network. All arcs are directed downwards. We use \mathcal{L} to represent any rooted level-2 network.

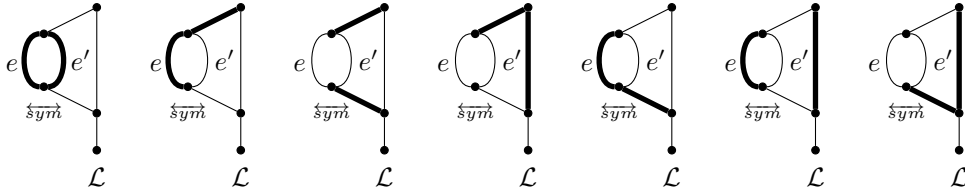
8.2.1. *Case 1:* Only one arc of the generator carries a sequence of at least one outgoing arc. This arc can be e (or e' , which is symmetric), or any arc of the generator other than e or e' , so there are 4 distinct choices for this arc.

$$4L \frac{L}{1-L}$$



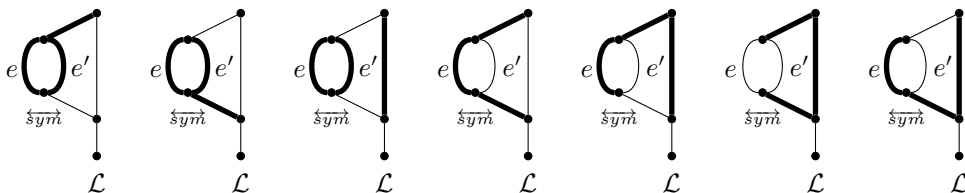
8.2.2. *Case 2:* Exactly two arcs of the generator carry a sequence of at least one outgoing arc. Either these two arcs are e and e' (and those two arcs are symmetric, hence the factor $\frac{1}{2}$), or it is any (unordered) pair of arcs among a total of 4 arcs: the arcs of the generator other than e and e' , and e (as e' is symmetric to e).

$$\frac{1}{2}L \left(\frac{L}{1-L} \right)^2 + \binom{4}{2}L \left(\frac{L}{1-L} \right)^2 = \frac{13}{2}L \left(\frac{L}{1-L} \right)^2$$



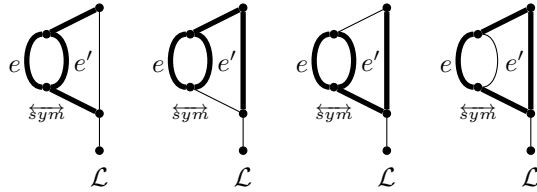
8.2.3. *Case 3:* Exactly three arcs of the generator carry a sequence of at least one outgoing arc. Either both e and e' are among those three arcs (and those two arcs are symmetric, hence the factor $\frac{1}{2}$), so the last one is any of the three other arcs of the generator. Or we choose any three arcs among a total of 4 arcs: the arcs of the generator other than e and e' , and e (as e' is symmetric to e).

$$\frac{3}{2}L \left(\frac{L}{1-L} \right)^3 + \binom{4}{3}L \left(\frac{L}{1-L} \right)^3 = \frac{11}{2}L \left(\frac{L}{1-L} \right)^3$$



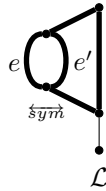
8.2.4. *Case 4:* Exactly four arcs of the generator carry a sequence of at least one outgoing arc. Either both e and e' are among those four arcs (and those two arcs are symmetric, hence the factor $\frac{1}{2}$), so the last two are chosen among the three other arcs of the generator. Or we choose the three arcs of the generator other than e and e' , and e (as e' is symmetric to e).

$$\frac{\binom{3}{2}}{2}L\left(\frac{L}{1-L}\right)^4 + L\left(\frac{L}{1-L}\right)^4 = \frac{5}{2}L\left(\frac{L}{1-L}\right)^4$$



8.2.5. *Case 5:* All five arcs of the generator carry a sequence of at least one outgoing arc. The fact that e and e' are symmetric explains the factor $\frac{1}{2}$.

$$\frac{1}{2}L\left(\frac{L}{1-L}\right)^5$$



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