

# An Asymptotic Analysis of Labeled and Unlabeled $k$ -Trees

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**Abstract** In this paper we provide a systematic treatment of several shape parameters of (random)  $k$ -trees. Our research is motivated by many important algorithmic applications of  $k$ -trees in the context of tree-decomposition of a graph and graphs of bounded tree-width. On the other hand,  $k$ -trees are also a very interesting object from the combinatorial point of view. For both labeled and unlabeled  $k$ -trees, we prove that the number of *leaves* and more generally the number of *nodes* of given degree satisfy a central limit theorem with mean value and variance that are asymptotically linear in the size of the  $k$ -tree. In particular we solve the *asymptotic counting problem* for unlabeled  $k$ -trees. By applying a proper singularity analysis of generating functions we show that the numbers  $U_k(n)$  of unlabeled  $k$ -trees of size  $n$  are asymptotically given by  $U_k(n) \sim c_k n^{-5/2} \rho_k^{-n}$ , where  $c_k > 0$  and  $\rho_k > 0$  denotes the radius of convergence of the generating function  $U(z) = \sum_{n \geq 0} U_k(n) z^n$ .

**Keywords**  $k$ -trees · generating function · singularity analysis · central limit theorem

**Mathematics Subject Classification (2000)** MSC 05A16 · 05A15

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## 1 Introduction

A  $k$ -tree is a generalization of a tree and can be defined recursively: a  $k$ -tree is either a complete graph on  $k$  vertices (= a  $k$ -clique) or a graph obtained from a smaller  $k$ -tree by adjoining a new vertex together with  $k$  edges connecting it to a  $k$ -clique of the smaller  $k$ -tree (and thus forming a  $(k + 1)$ -clique). In particular, a 1-tree is a usual tree. Here the parameter  $k$  is fixed, not depending on the number of vertices in a  $k$ -tree.

A  $k$ -tree is an interesting graph from an algorithmic point of view since many NP-hard problems on graphs have polynomial, in fact usually linear, dynamic programming algorithms when restricted to  $k$ -trees and their subgraphs for fixed values of  $k$  [3, 28, 17]; subgraphs of  $k$ -trees are called partial  $k$ -trees. Such NP-hard problems include maximum independent set size, minimal dominating set size, chromatic number, Hamiltonian circuit, network reliability and minimum vertex removal forbidden subgraph [2, 5]. Several graphs which are important in practice [21], have been shown to be partial  $k$ -trees, among them are

1. Trees/ Forests (partial 1-trees)
2. Series parallel networks (partial 2-trees)
3. Outplanar graphs (partial 2-trees)
4. Halin graphs (partial 3-trees).

However, other interesting graph classes like planar graphs or bipartite graphs are not partial  $k$ -trees.

$k$ -trees are also very interesting from a combinatorial point of view. For example, the enumeration problem for  $k$ -trees has been studied in various ways, see [4, 23, 13, 8, 19, 20, 14–16]. The number of labeled  $k$ -trees has been determined by Beineke and Pippert [4], Moon [23], Foata [13], Darrasse and Soria [8]; as usual a  $k$ -tree on  $n$  vertices is called *labeled* if the integers from  $\{1, 2, \dots, n\}$  have been assigned to its vertices (one-to-one) and two labeled  $k$ -trees are considered to be different if the corresponding edge sets are different.

It turns out that it is convenient to consider the number of *hedra* instead of the number of vertices as the size of a  $k$ -tree. A *hedron* is a  $(k + 1)$ -clique in a  $k$ -tree, and by definition a  $k$ -tree with  $n$  hedra has  $n + k$  vertices. It was shown by [4, 23, 13, 8] that the number  $L_k(n)$  of labeled  $k$ -trees having  $n$  hedra is given by

$$L_k(n) = \binom{n+k}{k} (kn+1)^{n-2}. \quad (1)$$

The factor  $kn + 1$  has a nice interpretation in terms of *fronts*. A *front* of a  $k$ -tree is a  $k$ -clique (we adopt the notions from [16]). By definition it easily follows that a  $k$ -tree with  $n$  hedra has  $kn + 1$  fronts.

However, the counting problem of unlabeled  $k$ -trees is much more difficult. Only the case of 2-trees was already solved by Harary and Palmer [19, 20] and Fowler *et al.* [14] by using the dissimilarity characteristic theorem. The general case was a long-standing open problem and was solved just recently by Gainer-Dewar [15]. Subsequently both Gessel and Gainer-Dewar [16] simplified

the generating function approach for unlabeled  $k$ -trees by coloring the vertices of a  $k$ -tree in  $(k + 1)$  colors such that adjacent vertices have different colors. (This breaks the symmetry of  $k$ -trees and avoids the use of compatible cyclic orientation of each hedron in a  $k$ -tree.)

The purpose of this paper is to provide a systematic asymptotic analysis of  $k$ -trees. First we review the counting formula  $L_k(n)$  for labeled  $k$ -trees with the help of a generating function approach and Lagrange inversion formula [8]. Second, we consider unlabeled  $k$ -trees and provide the same kind of results. Instead of proving an explicit counting formula (which is maybe not easy to state, even for the case of trees there is no closed formula) we will solve the *asymptotic counting problem* and show (see Theorem 3) that the numbers  $U_k(n)$  of unlabeled  $k$ -trees of size  $n$  are asymptotically given by

$$U_k(n) \sim c_k n^{-5/2} \rho_k^{-n},$$

where  $c_k > 0$  and  $\rho_k > 0$  denotes the radius of convergence of the generating function  $U(z) = \sum_{n \geq 0} U_k(n) z^n$ . This is in complete accordance with Otter's result for trees [24], Labelle's *et al.* result for unlabeled 2-trees [22], and also with the corresponding results for labeled  $k$ -trees (recall that  $n^{n-2}/n! \sim (2\pi)^{-1/2} n^{-5/2} e^n$ ). We note that the subexponential term  $n^{-5/2}$  suggests  $k$ -tree is a "tree-like" structure.

Similarly to trees, where we can distinguish between leaves and internal vertices, we distinguish in  $k$ -trees between hedra that have only one front in common with other hedra (= *leaves* or *fringe* of a  $k$ -tree) and the other (internal) hedra. Furthermore we can generalize the *degree* of a tree vertex by considering the number of hedra that have a given front in common. Thus, if we consider a random  $k$ -tree (of given size), it is natural to ask the following questions:

1. What is the limiting distribution for the number of hedra that have only one front in common with other hedra in a uniformly chosen  $k$ -tree?
2. For a given integer  $d$ , what is the limiting distribution for the number of fronts that are contained in  $d$  distinct hedra in a uniformly chosen  $k$ -tree?

Actually the main purpose of this paper is to answer questions 1 and 2 for labeled and unlabeled  $k$ -trees and to prove they all satisfy a central limit theorem with mean value and variance that are asymptotically linear in the number of hedra (Theorems 1 and 2, Theorems 4 and 5). This is also a natural generalization of corresponding results for (unlabeled) trees, see [10].

We expect that labeled and unlabeled  $k$ -trees have many asymptotic properties in common with trees. For example, it is very likely that  $k$ -trees scaled by  $1/\sqrt{n}$  converge weakly to the so-called *continuum random tree* as it holds for labeled and unlabeled trees (see [1,18]). In this case it would follow that the diameter  $D_n$  scaled by  $1/\sqrt{n}$  has a limiting distribution. Further well-known "tree-like" graph classes are the subcritical graph classes, but it should be mentioned that  $k$ -trees are not subcritical for  $k \geq 2$ . Informally, a graph class is subcritical if for a graph, the average size of 2-connected components is bounded so that the block-decomposition looks tree-like. Recently Panagiotou

*et al.* [25] have proved that, for a uniform random graph  $C_n$  with  $n$  vertices drawn from a subcritical graph class of connected graphs, the rescaled graph  $C_n/\sqrt{n}$  converges weakly to the continuum random tree. As a consequence, the diameter of the graph  $C_n$  and the height of pointed graph  $C_n^\bullet$ , scaled by  $1/\sqrt{n}$ , satisfy a limit distribution.

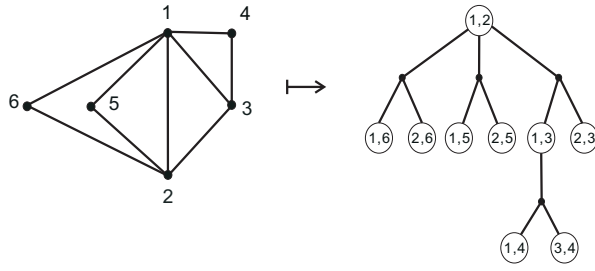
However, there are other parameters of interest – like the maximum degree – that cannot be characterized by a continuum tree property. Anyway, as in the case of trees (see [9]) we expect that the maximum degree of unlabeled  $k$ -trees should be concentrated at  $c \log n$  (for a proper constant  $c > 0$ ) and the maximum degree of labeled  $k$ -trees is concentrated at  $\log n / \log \log n$ . We plan to work on these (and related) questions in a follow-up paper. This corresponds to the fact that the tails of the degree distributions are different.

The plan of the paper is as follows. In Section 2 we study the numbers  $L_k(n)$  of labeled  $k$ -trees having  $n$  hedra, in Section 3 the number of leaves and in Section 4 the number of nodes of given degree for the labeled  $k$ -trees. Then in Section 5 we recall the combinatorial background for unlabeled  $k$ -trees from [16], in particular we present a system of equations for their generating functions. This system is then used to solve the asymptotic counting problem for unlabeled  $k$ -trees (Section 6). Finally, the number of leaves and the number of nodes of given degree for the unlabeled  $k$ -trees are discussed in Section 7 and 8.

## 2 Combinatorics of labeled $k$ -trees

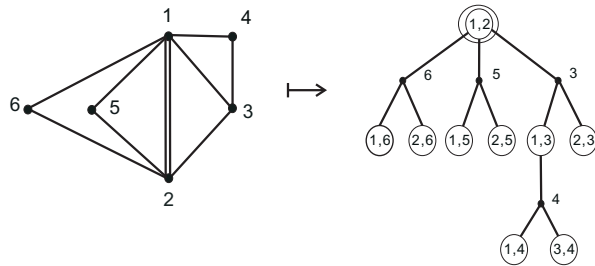
According to the inductive construction of a  $k$ -tree, the number of vertices in a  $k$ -tree having  $n$  hedra is  $k + 1 + (n - 1) = n + k$ . Since we will extend the counting problem to obtain the limit laws in Section 3 and 4, we present a detailed discussion of the counting problem. Here we use exponential generating functions for labeled  $k$ -trees to derive eq. (1), see [8]. We consider labeled  $k$ -trees having  $n$  hedra that are rooted at a front and translate labeled  $k$ -trees into  $k$ -front coding trees which are slightly different from the  $k$ -coding trees for unlabeled  $k$ -trees in Section 5.

First we introduce unlabeled  $k$ -front coding trees. An *unlabeled  $k$ -front coding tree* has unlabeled black nodes and labeled white nodes. To construct an unlabeled  $k$ -front coding tree from a labeled  $k$ -tree, an unlabeled black node in a  $k$ -front coding tree represents a hedron in the labeled  $k$ -tree. A white node labeled by the set  $\{i_1, i_2, \dots, i_k\}$  represents a front whose vertices are labeled by the integers  $i_1, i_2, \dots, i_k$  in the labeled  $k$ -tree. A black node connects with a white node if the corresponding hedron contains the corresponding front. It is clear that labeled  $k$ -trees having  $n$  hedra are in bijection with unlabeled  $k$ -front coding trees with  $n$  black nodes and  $kn + 1$  labeled white nodes. See Figure 1 for an example. Next we reduce the problem of counting unrooted trees to the problem of counting rooted trees. This can be done by rooting an unlabeled  $k$ -front coding tree at one of its fronts. Suppose that an unlabeled  $k$ -front coding tree is rooted at a white node labeled by the set  $\{i_1, i_2, \dots, i_k\}$ .



**Fig. 1** The bijection between a labeled 2-tree (left) and an unlabeled 2-front coding tree (right).

Then we label the black nodes in this  $k$ -front coding tree as follows. For every hedron whose vertices are labeled by the integers  $j_1, j_2, \dots, j_{k+1}$  in a labeled  $k$ -tree, the corresponding black node connects with white nodes labeled by the  $k$ -subsets of  $\{j_1, j_2, \dots, j_{k+1}\}$  in the unlabeled  $k$ -front coding tree. We label this black node by an integer  $j_m$  if among all its neighbors, the white node labeled by the set  $\{j_1, j_2, \dots, j_{k+1}\} - \{j_m\}$  is closest to the root. In this way we get a  $k$ -front coding tree rooted at  $\{i_1, i_2, \dots, i_k\}$  with all black nodes labeled. So a labeled  $k$ -tree rooted at a front can be identified as a  $k$ -front coding tree rooted at a white node. See Figure 2 for an example. A



**Fig. 2** The bijection between a labeled 2-tree rooted at a front whose vertices are labeled by 1, 2 (left) and a 2-front coding tree rooted at a white node labeled by  $\{1, 2\}$  (right).

$j_m$ -reduced black-rooted tree is a  $k$ -front coding tree rooted at a black node with labeling  $j_m$  and if this black node represents the hedron whose vertices are labeled by  $j_1, j_2, \dots, j_{k+1}$ , then all the neighbors of this root are labeled by the  $k$ -subsets of  $\{j_1, j_2, \dots, j_{k+1}\}$  that contain  $j_m$ . For a permutation  $\pi$  of the set  $\{x_1, \dots, x_k\}$ , we write  $\pi(x_r) = i_r$  and  $\pi = i_1 \dots i_k$ . We further observe every  $j_m$ -reduced black-rooted tree is fixed by any permutation of the set  $\{j_1, j_2, \dots, j_{k+1}\} - \{j_m\}$  and every  $k$ -front coding tree rooted at a white node labeled by the set  $\{i_1, i_2, \dots, i_k\}$  is fixed by any permutation of the set  $\{i_1, i_2, \dots, i_k\}$ .

Let  $R_k(n)$  denote the number of labeled  $k$ -trees having  $n$  hedra that are rooted at a particular front whose vertices are labeled by  $i_1, i_2, \dots, i_k$ , which also counts  $k$ -front coding trees on  $n$  labeled black nodes and  $kn + 1$  labeled white nodes that are rooted at a white node labeled by the set  $\{i_1, i_2, \dots, i_k\}$ . Note that the number  $R_k(n)$  is independent of the choice of the particular root  $\{i_1, i_2, \dots, i_k\}$ . Let  $C_k(z)$  be the exponential generating function for  $\{i_1, i_2, \dots, i_k\}$ -rooted  $k$ -front coding trees where every black node has weight  $z$ , that is,

$$C_k(z) = \sum_{n=0}^{\infty} R_k(n) \frac{z^n}{n!}. \quad (2)$$

Let  $B_k(z)$  be the exponential generating function for  $j_m$ -reduced black-rooted  $k$ -front coding trees where every black node has weight  $z$ . In fact, every  $k$ -front coding tree rooted at a white node labeled by  $\{i_1, i_2, \dots, i_k\}$  can be identified as a set of reduced black-rooted trees that are fixed by any permutation of  $\{i_1, i_2, \dots, i_k\}$ . Thus according to the exponential formula for labeled structures, we have

$$C_k(z) = \exp(B_k(z)). \quad (3)$$

We observe that the black root  $j_m$  in a reduced black-rooted tree connects with  $k$  white-rooted coding trees. All these  $k$  white-rooted coding trees are respectively rooted at the white nodes labeled by the  $k$ -subsets of  $\{i_1, i_2, \dots, i_k, j_m\}$  except  $\{i_1, i_2, \dots, i_k\}$ . This yields

$$B_k(z) = z(C_k(z))^k.$$

In combination of eq. (3), we get

$$B_k(z) = z \exp(kB_k(z)). \quad (4)$$

By applying Lagrange inversion formula on eq. (4), we obtain the coefficients of  $B_k(z)$ :

$$[z^n]B_k(z) = \frac{1}{n} [z^{n-1}] \exp(knz) = \frac{(kn)^{n-1}}{n!}.$$

This implies that the number of  $j_m$ -reduced black rooted  $k$ -front coding trees having  $n$  black nodes is  $(kn)^{n-1}$ . Similarly we can derive the coefficients of  $C_k(z)$  from eq. (3) by using again Lagrange inversion formula:

$$[z^n]C_k(z) = \frac{1}{n} [z^{n-1}] \exp((kn+1)z) = \frac{(kn+1)^{n-1}}{n!}.$$

Equivalently,  $R_k(n) = (kn+1)^{n-1}$  counts the number of labeled  $k$ -trees having  $n$  hedra that are rooted at a particular front whose vertices are labeled by  $i_1, i_2, \dots, i_k$ . Since there are  $\binom{n+k}{k}$  ways to choose the set  $\{i_1, i_2, \dots, i_k\}$ , the number of labeled  $k$ -trees having  $n$  hedra that are rooted at a front is

$$(kn+1)L_k(n) = \binom{n+k}{k} R_k(n)$$

and the closed formula for  $L_k(n)$  given in eq. (1) follows.

### 3 Leaves of labeled $k$ -trees

In a  $k$ -front coding tree we call a black node a *leaf* if only one of its labeled white neighbors connects with other black nodes. Every hedron that has only one front in common with other hedra in a labeled  $k$ -tree therefore can be identified as a leaf of an unlabeled  $k$ -front coding tree. In Figure 1 only the hedron with nodes 1, 2, 3 has two fronts  $\{1, 2\}, \{1, 3\}$  in common with other hedra and therefore only the black node connecting with white nodes  $\{1, 2\}, \{2, 3\}, \{1, 3\}$  is not a leaf in the corresponding unlabeled 2-front coding tree.

Let  $L_k(n, m)$  denote the number of  $k$ -front coding trees having  $m$  leaves among  $n$  labeled black nodes and let  $R_k(n, m)$  denote the number of  $k$ -front coding trees having  $n$  labeled black nodes and  $m$  leaves that are rooted at a white node labeled by a particular set  $\{i_1, i_2, \dots, i_k\}$ . Since there are  $\binom{n+k}{k}$  ways to choose the set  $\{i_1, i_2, \dots, i_k\}$ , the number of  $k$ -front coding trees having  $n$  labeled black nodes and  $m$  leaves that are rooted at a white node is  $(kn + 1)L_k(n, m) = \binom{n+k}{k}R_k(n, m)$ . Hence  $L_k(n, m)/L_k(n) = R_k(n, m)/R_k(n)$ .

The main purpose of this section is to prove the following central limit theorem.

**Theorem 1** *Let  $\bar{X}_n$  be the random variable associated with the number of leaves of  $k$ -front coding trees given by*

$$\mathbb{P}(\bar{X}_n = m) = \frac{L_k(n, m)}{L_k(n)}.$$

*Then  $\mathbb{E}(\bar{X}_n) = (1/e)n + O(1)$  and  $\text{Var}(\bar{X}_n) = (1/e - 2/e^2)n + O(1)$  and  $\bar{X}_n$  satisfies a central limit theorem of type*

$$\frac{\bar{X}_n - \mathbb{E}(\bar{X}_n)}{\sqrt{\text{Var}(\bar{X}_n)}} \rightarrow N(0, 1).$$

*Proof* Let  $C_k(z, w)$  be the exponential generating function for  $\{i_1, i_2, \dots, i_k\}$ -rooted  $k$ -front coding trees where every black node has weight  $z$  and every leaf has weight  $w$ , that is,

$$C_k(z, w) = \sum_{n=0}^{\infty} \sum_{m=0}^n R_k(n, m) \frac{z^n w^m}{n!}. \quad (5)$$

With the help of this generating function we get

$$\mathbb{P}(\bar{X}_n = m) = \frac{L_k(n, m)}{L_k(n)} = \frac{R_k(n, m)}{R_k(n)} = \frac{[z^n w^m]C_k(z, w)}{[z^n]C_k(z, 1)}.$$

Recall that a  $j_m$ -reduced black-rooted tree is a  $k$ -front coding tree rooted at a black node with labeling  $j_m$  and if this black node represents the hedron whose vertices are labeled by  $j_1, j_2, \dots, j_{k+1}$ , then all the neighbors of this root are labeled by the  $k$ -subsets of  $\{j_1, j_2, \dots, j_{k+1}\}$  that contain  $j_m$ . Let  $B_k(z, w)$  be

the exponential generating function for  $j_m$ -reduced black rooted trees where every black node has weight  $z$  and every leaf has weight  $w$ . Then

$$\begin{aligned} C_k(z, w) &= \exp(B_k(z, w)), \\ B_k(z, w) &= z(C_k(z, w))^k - z + zw, \end{aligned}$$

which leads to

$$B_k(z, w) = z \exp(kB_k(z, w)) - z + zw. \quad (6)$$

We first analyze  $B_k(z) = B_k(z, 1)$  and  $C_k(z) = C_k(z, 1)$ . Let  $W(z)$  denote the classical tree function that is given by  $W(z) = z \exp(W(z))$ . It then follows that  $B_k(z) = B_k(z, 1) = \frac{1}{k}W(kz)$ . It is very well known that  $W(z)$  has radius of convergence  $\rho = 1/e$ , that it has a singular expansion of the form

$$W(z) = 1 - \sqrt{2}(1 - ez)^{1/2} + \frac{2}{3}(1 - ez) + \dots$$

around  $z = 1/e$  and that  $W(z)$  can be analytically continued to a region of the form  $\{z \in \mathbb{C} : |z| < 1/e + \eta\} \setminus [1/e, \infty)$  for some  $\eta > 0$ . In particular it follows that  $B_k(z)$  has corresponding properties, of course its radius of convergence equals  $1/(ke)$ . Actually, in what follows we will only need that  $B_k(z)$  is analytic in a so-called  $\Delta$ -domain

$$\Delta_\alpha(M, \phi) = \{z \mid |z| < M, z \neq \alpha, |\arg(z - \alpha)| > \phi\}$$

where  $0 < \phi < \frac{\pi}{2}$ . (Analyticity in  $\Delta$ -domains is used to *transfer* the singular expansion of the generating function into an asymptotic expansion for the coefficients, see Chapter VI.3 of [12].) In our case we know that  $B_k(z)$  is analytic in  $\Delta_{1/(ke)}(1/(ke) + \eta, \phi)$ . In view of  $B_k(z) = \frac{1}{k}W(kz)$ ,  $C_k(z) = (z^{-1}B_k(z))^{1/k}$  and the expansion of  $W(z)$ , we get the expansions of  $B_k(z)$  and  $C_k(z)$  around the dominant singularity  $\xi_k = (ke)^{-1}$ , too:

$$\begin{aligned} B_k(z) &= \frac{1}{k} - \frac{\sqrt{2}}{k}(1 - ekz)^{1/2} + \frac{2}{3k}(1 - ekz) + O(1 - ekz)^{3/2} \\ C_k(z) &= e^{1/k} - \frac{\sqrt{2}e^{1/k}}{k}(1 - ekz)^{1/2} + \frac{3 - k}{3k^2}e^{1/k}(1 - ekz) \\ &\quad + O(1 - ekz)^{3/2} \end{aligned}$$

Next we will analyze  $B_k(z, w)$  and  $C_k(z, w)$  based on eq. (6). We set

$$F(y, z, w) = z \exp(ky) + z(w - 1)$$

which is analytic for  $(y, z, w)$  around  $(0, 0, 0)$  and we have  $F(y, 0, w) \equiv 0$ ,  $F(0, z, w) \not\equiv 0$ . Furthermore, the coefficients of  $F(y, z, w)$  are all non-negative. Since  $B_k(z, w)$  is the unique solution of  $F(y, z, w) = y$  it can be expressed as

$$B_k(z, w) = \alpha_1(z, w) - \beta_1(z, w) \left[ 1 - \frac{z}{\xi_k(w)} \right]^{1/2},$$



where  $\xi_k(1) = (ek)^{-1}$  and  $\alpha_1(z, w), \beta_1(z, w), \xi_k(w)$  are analytic for  $|w - 1| \leq \epsilon$ ,  $|z - \xi_k(w)| < \epsilon$ ,  $|\arg(z - \xi_k(w))| > \phi$  (for some  $\phi \in (0, \pi/2)$ ) and  $\epsilon, \varepsilon$  are sufficiently small. Furthermore,  $\beta(\xi_k(w), w) \neq 0$  and  $B_k(\xi_k(w), w) = \alpha_1(\xi_k(w), w) = k^{-1} + (w - 1)\xi_k(w)$ . Since  $B_k(z, w) = zC_k(z, w)^k + z(w - 1)$ ,  $C_k(z, w)$  has a corresponding representation

$$C_k(z, w) = a_1(z, w) + b_1(z, w) \left[ 1 - \frac{z}{\xi_k(w)} \right]^{1/2} \quad (7)$$

where  $\xi_k(1) = (ek)^{-1}$  and  $a_1(z, w), b_1(z, w)$  are analytic functions around  $(z, w) = (\xi_k, 1)$ ,  $b(\xi_k(w), w) \neq 0$ ,  $C_k(\xi_k(w), w) = a_1(\xi_k(w), w) = (k\xi_k(w))^{-1/k}$ . By applying [9, Theorem 2.25] to eq. (7) and Lemma 4 of [11], it follows that  $\bar{X}_n$  satisfies the central limit theorem as stated.

It also follows that  $\mathbb{E}(\bar{X}_n) = \bar{\mu}n + O(1)$  and  $\text{Var}(\bar{X}_n) = \sigma^2 n + O(1)$ , where  $\bar{\mu}$  and  $\sigma^2$  can be computed by

$$\bar{\mu} = -\frac{\xi'_k(1)}{\xi_k(1)} = \frac{F_w}{zF_z} = \frac{1}{e}$$

and

$$\begin{aligned} \sigma^2 &= -\frac{\xi''_k(1)}{\xi_k(1)} + \frac{\xi'_k(1)^2}{\xi_k(1)^2} - \frac{\xi'_k(1)}{\xi_k(1)} \\ &= \bar{\mu} + \bar{\mu}^2 + \frac{1}{z_0 F_z^3 F_{yy}} \left( F_z^2 (F_{yy} F_{ww} - F_{yw}^2) - 2F_z F_w (F_{yy} F_{zw} - F_{yz} F_{yw}) \right. \\ &\quad \left. + F_w^2 (F_{yy} F_{zz} - F_{yz}^2) \right), \end{aligned}$$

where all partial derivatives are evaluated at the point  $(y_0, z_0, w_0) = (1/k, 1/(ek), 1)$ . See Theorem 2.23 in [9]. More precisely, we compute  $F_z = \exp(ky) + w - 1$  and  $F_w = z$ . It follows that  $\bar{\mu} = (F_z(y_0, z_0, w_0))^{-1} = 1/e$ . Furthermore,  $F_{yy} = zk^2 \exp(ky)$  and  $F_{yy}(y_0, z_0, w_0) = k$ ,  $F_{ww} = 0$ ,  $F_{yw} = 0$ ,  $F_{zw} = 1$ ,  $F_{zz} = 0$ ,  $F_w = z$  and  $F_w(y_0, z_0, w_0) = 1/(ek)$ ,  $F_y = kz \exp(ky)$ ,  $F_{yy} = zk^2 \exp(ky)$  and  $F_{yy}(y_0, z_0, w_0) = k$ ,  $F_{yz} = k \exp(ky)$  and  $F_{yz}(y_0, z_0, w_0) = ek$ . This gives

$$\bar{\mu} = \frac{1}{e} \quad \text{and} \quad \sigma^2 = \frac{1}{e} - \frac{2}{e^2}$$

and completes the proof of the theorem.  $\square$

#### 4 The degree distribution of labeled $k$ -trees

In order to quantify the number of “neighbors” in  $k$ -trees we refer to the corresponding  $k$ -front coding trees and consider the degree distribution of white nodes (since every black node in the  $k$ -front coding tree has degree  $k + 1$ ). It is convenient to change the underlying statistics by measuring the size of a  $k$ -tree

according to the number of white labeled nodes. Let  $\tilde{C}_k(x)$  be the exponential generating function for  $\{i_1, i_2, \dots, i_k\}$ -rooted  $k$ -front coding trees, that is:

$$\tilde{C}_k(x) = \sum_{n=0}^{\infty} R_k(n) \frac{x^{kn+1}}{n!} = xC_k(x^k).$$

Let  $\tilde{B}_k(x)$  be the exponential generating function for  $j_m$ -reduced black rooted trees where every white node has weight  $x$ . Then we have

$$\tilde{C}_k(x) = x \exp(\tilde{B}_k(x)), \quad \tilde{B}_k(x) = (\tilde{C}_k(x))^k.$$

That leads to  $\tilde{B}_k(x) = x^k \exp(k\tilde{B}_k(x))$ . By using the same techniques shown in Section 3, we conclude that the dominant singularity  $x = \zeta_k = (ek)^{-1/k}$  of  $\tilde{B}_k(x)$  satisfying  $\tilde{B}_k(\zeta_k) = 1/k$ , is of square root type, i.e.,

$$\begin{aligned} \tilde{B}_k(x) &= k^{-1} - \sqrt{\frac{2}{k}} \left(1 - x(ek)^{1/k}\right)^{1/2} + O(1 - x(ek)^{1/k}), \\ \tilde{C}_k(x) &= k^{-1/k} - \sqrt{\frac{2}{k^{1+2/k}}} \left(1 - x(ek)^{1/k}\right)^{1/2} + O(1 - x(ek)^{1/k}). \end{aligned}$$

Since  $\tilde{B}_k(x) = B_k(x^k)$  and  $\tilde{C}_k(x) = xC_k(x^k)$ , the corresponding local singular expansions hold for  $x = (ek)^{-1/k} e^{2\pi i \ell/k}$  and  $\ell = 1, 2, \dots, k-1$ .

Now we give each labeled white node of degree  $d_i$  a weight  $u_i$ . Let  $\mathbf{u} = (u_1, \dots, u_M)$ ,  $\mathbf{m} = (m_1, \dots, m_M)$  where  $m_i \geq 0$  and  $\mathbf{d} = (d_1, \dots, d_M)$  where  $d_i > 0$ , and the coefficient of  $x^{kn+1} \mathbf{u}^{\mathbf{m}}/n!$  in the exponential generating function  $\tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u})$  is  $R_k^{(\mathbf{d})}(n, \mathbf{m})$ , which counts the number of  $\{i_1, i_2, \dots, i_k\}$ -rooted  $k$ -front coding trees having  $n$  black nodes and there are  $m_i$  white nodes out of  $kn+1$  total white nodes having degree  $d_i$  for every  $i$ ,  $1 \leq i \leq M$ :

$$\tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u}) = \sum_{n \geq 0} \sum_{\mathbf{m}} R_k^{(\mathbf{d})}(n, \mathbf{m}) \frac{x^{kn+1} \mathbf{u}^{\mathbf{m}}}{n!}.$$

Let  $L_k^{(\mathbf{d})}(n, \mathbf{m})$  denote the number of labeled  $k$ -trees having  $kn+1$  fronts and there are  $m_i$  fronts that are contained in  $d_i$  hedra for every  $i$ ,  $1 \leq i \leq M$ . Then the number of white-rooted  $k$ -front coding trees on  $kn+1$  white nodes is

$$(kn+1)L_k^{(\mathbf{d})}(n, \mathbf{m}) = \binom{n+k}{k} R_k^{(\mathbf{d})}(n, \mathbf{m}).$$

The main result of this section is a multivariate central limit theorem for the joint distribution of the number of white nodes with given degrees. It certainly applies for one given degree, i.e., the case  $M = 1$ .

**Theorem 2** Let  $\bar{Y}_{n,\mathbf{d}} = (\bar{Y}_{n,d_1}^{(1)}, \dots, \bar{Y}_{n,d_M}^{(M)})$  be the random vector of the number of white nodes in a  $k$ -front coding tree that have degrees  $d_1, \dots, d_M$ , respectively, that is,

$$\mathbb{P}(\bar{Y}_{n,\mathbf{d}} = \mathbf{m}) = \frac{L_k^{(\mathbf{d})}(n, \mathbf{m})}{L_k(n)}.$$

Set

$$\mu_d = e^{-1/k} \frac{k^{-d+1}}{(d-1)!},$$

$$\sigma_{d,t} = \begin{cases} -\mu_d \mu_t \left(1 + \frac{(dk-k-1)(tk-k-1)}{k}\right) & \text{if } d \neq t, \\ \mu_d - \mu_d^2 \left(1 + \frac{(dk-k-1)^2}{k}\right) & \text{if } d = t \end{cases}$$

and

$$\mathbf{M} = (\mu_{d_1}, \dots, \mu_{d_M}) \quad \text{and} \quad \mathbf{S} = (\sigma_{d_i, d_j})_{1 \leq i, j \leq M}.$$

Then  $\mathbb{E}(\bar{Y}_{n,\mathbf{d}}) = \mathbf{M}kn + O(1)$  and  $\text{Cov}(\bar{Y}_{n,\mathbf{d}}) = \mathbf{S}kn + O(1)$ . Furthermore  $\bar{Y}_{n,\mathbf{d}}$  satisfies a central limit theorem of the form

$$\frac{\bar{Y}_{n,\mathbf{d}} - \mathbb{E}(\bar{Y}_{n,\mathbf{d}})}{\sqrt{kn}} \rightarrow N(0, \mathbf{S}).$$

*Proof* In terms of the generating function, we have

$$\mathbb{P}(\bar{Y}_{n,\mathbf{d}} = \mathbf{m}) = \frac{L_k^{(\mathbf{d})}(n, \mathbf{m})}{L_k(n)} = \frac{R_k^{(\mathbf{d})}(n, \mathbf{m})}{R_k(n)} = \frac{[x^{kn+1} \mathbf{u}^{\mathbf{m}}] \tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u})}{[x^{kn+1}] \tilde{C}_k(x)}.$$

Let  $\tilde{P}_k^{(\mathbf{d})}(x, \mathbf{u})$  denote the exponential generating function for  $k$ -front coding trees whose root only connects to the root of a white-rooted  $k$ -front coding tree. So that  $\tilde{P}_k^{(\mathbf{d})}(x, \mathbf{1}) = \tilde{C}_k^{(\mathbf{d})}(x, \mathbf{1})$ . We use  $\tilde{P}_k^{(\mathbf{d})}(x, \mathbf{u})$  to distinguish the case that the white node root has degree  $d_i$  for some  $i$ ,  $1 \leq i \leq M$ . Furthermore, let  $\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})$  be the exponential generating function for  $j_m$ -reduced black rooted trees that each white node of degree  $d_i$  has weight  $u_i$  for  $1 \leq i \leq M$ . We get the functions

$$\begin{aligned} \tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u}) &= (P_k^{(\mathbf{d})}(x, \mathbf{u}))^k \\ \tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u}) &= x \exp(\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})) + \sum_{j=1}^M x(u_j - 1) \frac{\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})^{d_j}}{d_j!} \\ \tilde{P}_k^{(\mathbf{d})}(x, \mathbf{u}) &= x \exp(\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})) + \sum_{j=1}^M x(u_j - 1) \frac{\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})^{d_j-1}}{(d_j - 1)!} \end{aligned} \quad (8)$$

and we consider

$$\bar{S}(x, y, \mathbf{u}) = \left( x e^y + \sum_{j=1}^M x(u_j - 1) \frac{\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})^{d_j-1}}{(d_j - 1)!} \right)^k.$$

Since  $\bar{S}(0, y, \mathbf{u}) \equiv 0$ ,  $\bar{S}(x, 0, \mathbf{u}) \neq 0$  and all coefficients of  $\bar{S}(x, y, \mathbf{1})$  are real and positive, then  $y(x, \mathbf{u}) = \tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})$  is the unique solution of the functional equation  $\bar{S}(x, y, \mathbf{u}) = y$ . Furthermore,  $(x, y) = (\zeta_k, 1/k)$  is the only solution of  $\bar{S}(x, y, \mathbf{1}) = 0$  and  $\bar{S}_y(x, y, \mathbf{1}) = 1$  with  $\bar{S}_x(\zeta_k, 1/k, \mathbf{1}) \neq 0$ ,  $\bar{S}_{yy}(\zeta_k, 1/k, \mathbf{1}) \neq 0$ . Consequently,  $\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u})$  can be represented as

$$\tilde{B}_k^{(\mathbf{d})}(x, \mathbf{u}) = \bar{g}(x, \mathbf{u}) - \bar{h}(x, \mathbf{u}) \left[ 1 - \frac{x}{\zeta_k(\mathbf{u})} \right]^{1/2}$$

which holds locally around  $(x, \mathbf{u}) = (\zeta_k, \mathbf{1})$  and  $\bar{h}(\zeta_k(\mathbf{u}), \mathbf{u}) \neq 0$ . In view of eq. (8),  $\tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u})$  also has expansion of square root type, i.e.,

$$\tilde{C}_k^{(\mathbf{d})}(x, \mathbf{u}) = \bar{s}(x, \mathbf{u}) - \bar{t}(x, \mathbf{u}) \left[ 1 - \frac{x}{\zeta_k(\mathbf{u})} \right]^{1/2} \quad (9)$$

where  $\bar{t}(\zeta_k(\mathbf{u}), \mathbf{u}) \neq 0$  since  $\bar{t}(\zeta_k(\mathbf{1}), \mathbf{1}) \neq 0$  and  $t$  is an analytic function around  $(x, \mathbf{u}) = (\zeta_k, \mathbf{1})$ . Of course there are corresponding representations locally around  $(x, \mathbf{u}) = (\zeta_k e^{2\pi i \ell/k}, \mathbf{1})$  for  $\ell = 1, 2, \dots, k-1$ .

Finally by applying [9, Theorem 2.25] (as in the proof of Theorem 1) and setting  $\bar{A}(\mathbf{u}) = \log \zeta_k(\mathbf{1}) - \log \zeta_k(\mathbf{u})$ ,  $\mathbf{M} = (\bar{A}_{u_j}(\mathbf{1}))_{1 \leq j \leq M}$  and  $\mathbf{S} = (\bar{A}_{u_i u_j}(\mathbf{1}) + \delta_{i,j} \bar{A}_{u_j}(\mathbf{1}))_{1 \leq j \leq M}$  then  $\mathbb{E}(\bar{Y}_{n, \mathbf{d}}) = \mathbf{M} kn + O(1)$ ,  $\text{Cov}(\bar{Y}_{n, \mathbf{d}}) = \mathbf{S} kn + O(1)$ , and the central limit theorem follows. It is a simply exercise to compute  $\mathbf{M}$  and  $\mathbf{S}$  explicitly (compare with the proof of Theorem 1).  $\square$

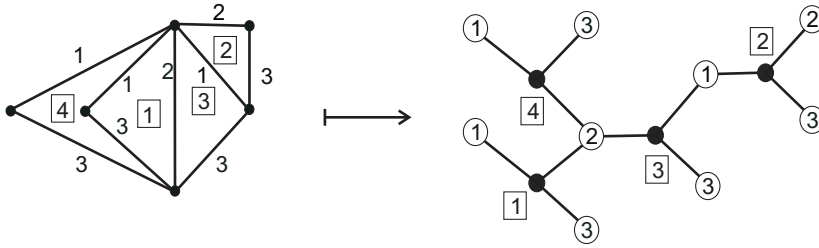
## 5 Combinatorics of unlabeled $k$ -trees

In this section we recall the combinatorial background for counting unlabeled  $k$ -trees. More precisely we shall use the terminology introduced in [15, 16] to formulate a system of equations for the generating functions.

Let  $g \in \mathfrak{S}_m$  be a permutation of  $\{1, 2, \dots, m\}$  that has  $\ell_i$  cycles of size  $i$ ,  $1 \leq i \leq k$ , in its cyclic decomposition. Then its cycle type  $\lambda = (1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k})$  is a partition of  $m$  where  $m = \ell_1 + 2\ell_2 + \dots + k\ell_k$ . (In what follows we will denote by  $\lambda \vdash m$  that  $\lambda$  is a partition of  $m$ .) Furthermore we set  $z_\lambda = 1^{\ell_1} \ell_1! 2^{\ell_2} \ell_2! \dots k^{\ell_k} \ell_k!$  and note that  $\frac{m!}{z_\lambda}$  is the number of permutations in  $\mathfrak{S}_m$  of cycle type  $\lambda$ .

We recall that a *hedron* is a  $(k+1)$ -clique in a  $k$ -tree and a *front* is a  $k$ -clique in a  $k$ -tree. The number of vertices in a  $k$ -tree having  $n$  hedra is  $k+1 + (n-1) = n+k$ . A *colored hedron-labeled  $k$ -tree* is a  $k$ -tree that has each vertex colored from the set  $\{1', 2', \dots, (k+1)'\}$  so that any two adjacent vertices are colored differently, and each hedron is labeled with a distinct number from  $\{1, 2, \dots, n\}$ . The only automorphism that preserves hedra and colors of a colored hedron-labeled  $k$ -tree is the identity automorphism, for which we can ignore the colors of vertices. We now introduce  $k$ -coding trees. A  *$k$ -coding tree* has labeled black nodes and colored nodes. Each edge connects

a labeled black node with a colored node from colors  $\{1, 2, \dots, k + 1\}$ . To construct a  $k$ -coding tree from a colored hedron-labeled  $k$ -tree, we color each front of a hedron with a distinct color from  $\{1, 2, \dots, k + 1\}$ . The corresponding  $k$ -coding tree has a black node labeled with  $i$  representing a hedron of the  $k$ -tree with label  $i$  and a  $j$ -colored node representing a front of the  $k$ -tree with color  $j$ . We connect a black node with a colored node if and only if the corresponding hedron contains the corresponding front. As a result, the colored hedron-labeled  $k$ -trees are in bijection with the  $k$ -coding trees. Under the action of  $\mathfrak{S}_n$  and  $\mathfrak{S}_{k+1}$ , the orbits of colored hedron-labeled  $k$ -tree, which are unlabeled  $k$ -trees are in bijection with the orbits of unlabeled  $k$ -coding trees under the action of  $\mathfrak{S}_{k+1}$ . See Figure 3 for an example. In [16] the following



**Fig. 3** The bijection between a colored hedron-labeled 2-tree (left) and a 2-coding tree (right).

system of equations was set up that determines the generating function  $U(z)$  for unlabeled  $k$ -trees by

$$U(z) = B(z) + C(z) - E(z),$$

where

$$B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z_\lambda} \quad B_\lambda(z) = z \prod_i C_{\lambda^i}(z^i) \quad (10)$$

$$C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z_\mu} \quad \bar{B}_\mu(z) = z \prod_i C_{\mu^i}(z^i) \quad (11)$$

$$E(z) = \sum_{\mu \vdash k} \frac{\bar{B}_\mu(z) C_\mu(z)}{z_\mu} \quad C_\mu(z) = \exp \left[ \sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m} \right]. \quad (12)$$

Here  $B(z)$  is the generating function for color-orbits of black-rooted unlabeled  $k$ -coding trees,  $C(z)$  is the generating function for color-orbits of colored-rooted unlabeled  $k$ -coding trees and  $E(z)$  is the generating function for color-orbits of unlabeled  $k$ -coding trees rooted at an edge. We call an unlabeled  $k$ -coding tree a  $j$ -reduced black-rooted tree if it is a black-rooted  $k$ -coding tree with all the neighbors of the root are colored by the integers  $1, 2, \dots, j - 1, j + 1, \dots, k + 1$ .  $\bar{B}(z)$  is the generating function for  $j$ -reduced black-rooted trees. For any  $\pi \in \mathfrak{S}_{k+1}$ ,  $B_\lambda(z)$  is the generating function for

black-rooted trees that are fixed by  $\pi$  where  $\pi$  has cycle type  $\lambda$ . For any  $\sigma \in \mathfrak{S}_k$ ,  $\bar{B}_\mu(z)$  (resp.  $C_\mu(z)$ ) is the generating function for  $j$ -reduced black-rooted trees (resp. colored-rooted trees) that are fixed by  $\sigma$  where  $\sigma$  has cycle type  $\mu$ . The generating functions  $\bar{B}_\mu(z), C_\mu(z)$  are related to the unlabeled  $k$ -coding trees for a fixed  $k$ . For any  $\sigma \in \mathfrak{S}_k$ ,  $\bar{B}_\mu(z)$  (resp.  $C_\mu(z)$ ) is the generating function for  $j$ -reduced black-rooted trees (resp. colored-rooted trees) that are fixed by  $\sigma$  where  $\sigma$  has cycle type  $\mu$ . Here note that  $\sigma \in \mathfrak{S}_k$  is equivalent to say,  $\sigma \in \mathfrak{S}_{k+1}$  and  $\sigma$  has an element  $j$  fixed. We need this condition since every  $j$ -reduced black-rooted tree has one color  $j$  fixed and every color-rooted tree has the color on its root fixed. Consequently  $\bar{B}_\mu(z) = \bar{B}_\lambda(z), C_\mu(z) = C_\lambda(z)$  if  $\lambda$  is obtained from  $\mu$  by adding a part 1 and  $\mu \vdash k$ . If  $\lambda \vdash (k+1)$  has no part of size 1, then  $\bar{B}_\lambda(z) = C_\lambda(z) = 0$ . In particular, the functions  $\bar{B}_{1^k}(z) = \bar{B}_{1^{k+1}}(z)$  and  $C_{1^k}(z) = C_{1^{k+1}}(z)$  hold in the context of  $k$ -trees.  $C_{\lambda^i}(z)$  is the generating function for color-rooted trees that are fixed by  $\pi^i$  and  $\lambda^i$  denotes the cycle type of permutation  $\pi^i$  where  $\pi \in \mathfrak{S}_{k+1}$  has cycle type  $\lambda$  and  $i$  is a part of  $\lambda$ . Finally, the above products over  $i$  range over all parts  $i$  of  $\lambda$  or  $\mu$ , respectively, that is, if  $i$  is contained  $m$  times in  $\lambda$  then it appears  $m$  times in the product. For simplicity, we write  $B_\lambda(z) = B_{1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k}}(z)$ ,  $\bar{B}_\lambda(z) = \bar{B}_{1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k}}(z)$ ,  $C_\lambda(z) = C_{1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k}}(z)$  and  $z_\lambda = z_{1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k}}$  if  $\lambda = (1^{\ell_1} 2^{\ell_2} \dots k^{\ell_k})$ .

## 6 Asymptotics of unlabeled $k$ -trees

Let  $U_k(n) = [z^n]U(z)$  denote the number of unlabeled  $k$ -trees having  $n$  hedra. Then we have the following asymptotic property.

**Theorem 3** *The number of unlabeled  $k$ -trees with  $n$  hedra is asymptotically given by*

$$U_k(n) = \frac{1}{k!} \frac{(k\rho_k)^{-\frac{1}{k}}}{\sqrt{2\pi k^2}} \left[ \frac{\rho_k m'(\rho_k)}{m(\rho_k)} \right]^{3/2} n^{-5/2} \rho_k^{-n} (1 + O(n^{-1})), \quad (13)$$

where  $m(z) = z \exp \left[ k \sum_{m=2}^{\infty} \bar{B}_{1^k}(z^m)/m \right]$ ,  $\bar{B}_{1^k}(z) = m(z) e^{k\bar{B}_{1^k}(z)}$  and  $\rho_k$  is the unique real positive solution of  $m(z) = (ek)^{-1}$ . More precisely, we have  $(4k)^{-1} \leq \rho_k \leq (ek)^{-1}$  and the asymptotic expansion

$$\rho_k = \frac{1}{ek} - \frac{1}{2e^3 k^2} + O(k^{-3}), \quad k \rightarrow \infty.$$

Furthermore,  $\rho_k m'(\rho_k)/m(\rho_k) = 1 + O(k^{-1})$  as  $k \rightarrow \infty$ .

We will prove Theorem 3 in the following way:

1. The dominant singularity  $z = \rho_k$  of  $\bar{B}_{1^k}(z)$  and  $C_{1^k}(z)$  are of square root type.
2. For any  $k \geq 2$  and  $\mu \neq (1^k)$ ,  $\bar{B}_\mu(z)$  and  $C_\mu(z)$  are analytic at  $z = \rho_k$ .
3. The coefficient for the term  $(\rho_k - z)^{1/2}$  in the singular expansion of  $U(z)$  is zero and the coefficient for  $(\rho_k - z)^{3/2}$  is positive.

4. Asymptotic behavior of  $\rho_k$  as  $k \rightarrow \infty$ .

Each step of the proof will be described below with more details explained.

*Proof Step 1: The dominant singularity  $z = \rho_k$  of  $\bar{B}_{1^k}(z)$  and  $C_{1^k}(z)$  are of square root type.*

For  $\mu = (1^k)$ , from eq. (11) and (12), we have

$$\bar{B}_{1^k}(z) = z \exp \left[ k \sum_{m=1}^{\infty} \frac{\bar{B}_{1^k}(z^m)}{m} \right] = \exp(k\bar{B}_{1^k}(z)) \cdot z \cdot \exp \left[ k \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m)}{m} \right]. \quad (14)$$

Setting

$$m(z) = z \exp \left[ k \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m)}{m} \right], \quad (15)$$

and  $\bar{B}_{1^k}(z) = T(m(z))$  for some power series  $T(z)$  we thus obtain  $T(z) = z \exp(kT(z))$ . Recall that in Section 2,  $W(z)$  denotes the classical tree function that is given by  $W(z) = z \exp(W(z))$  it follows that  $T(z) = \frac{1}{k}W(kz)$  and we can expand  $T(z)$  in the region  $\Delta_{1/(ke)}(1/(ke) + \eta, \phi)$  based on the expansion of  $W(z)$ .

Let  $\rho_k$  be the unique dominant singularity of  $\bar{B}_{1^k}(z)$ , within this step we shall prove that the dominant singularity  $z = \rho_k$  of  $\bar{B}_{1^k}(z)$  is of square root type, too. Since  $m(z)$  has radius of convergence  $\sqrt{\rho_k} > \rho_k$  it follows that it is analytic at  $z = \rho_k$ . More precisely the singular expansion of  $\bar{B}_{1^k}(z)$  close to  $z = \rho_k$  comes from composing the singular expansion of  $T(z)$  at  $1/(ek)$  with the analytic expansion of  $m(z)$  at  $\rho_k$ . In this context we also observe that  $m(\rho_k) = (ek)^{-1}$  and  $m'(\rho_k) > 1$ . According to this we get the local expansion

$$\begin{aligned} \bar{B}_{1^k}(z) &= \frac{1}{k} - \frac{\sqrt{2}}{k} \left[ 1 - \frac{m(z)}{m(\rho_k)} \right]^{1/2} + \frac{2}{3k} \left[ 1 - \frac{m(z)}{m(\rho_k)} \right] + \sum_{i \geq 3} (-1)^i m_i \left[ 1 - \frac{m(z)}{m(\rho_k)} \right]^{i/2} \\ &= \frac{1}{k} - \frac{\sqrt{2}}{k} \left[ \frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)} \right]^{1/2} + \frac{2}{3k} \left[ \frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)} \right] + O(\rho_k - z)^{3/2}. \end{aligned}$$

Henceforth  $C_{1^k}(z) = z^{-1/k} \bar{B}_{1^k}(z)^{1/k}$  has  $z = \rho_k$  as dominant singularity of square root type, too, and a local expansion of the form

$$C_{1^k}(z) = (k\rho_k)^{-1/k} + a(\rho_k - z)^{1/2} + b(\rho_k - z) + c(\rho_k - z)^{3/2} + O(\rho_k - z)^2 \quad (16)$$

where  $a, b$  are given by

$$a = -\frac{\sqrt{2}(k\rho_k)^{(k-1)/k}}{k^2\rho_k} \left[ \frac{m'(\rho_k)}{m(\rho_k)} \right]^{1/2}, \quad b = \frac{3 - k(k\rho_k)^{(k-1)/k}}{3k^3\rho_k} \left[ \frac{m'(\rho_k)}{m(\rho_k)} \right].$$

Recall that  $\bar{B}_\mu(z) = \bar{B}_\lambda(z)$ ,  $C_\mu(z) = C_\lambda(z)$  if  $\lambda$  is obtained from  $\mu$  by adding a part 1 and  $\mu \vdash k$ . If  $\lambda \vdash (k+1)$  has no part of size 1, then  $\bar{B}_\lambda(z) = C_\lambda(z) = 0$ . In particular, the functions  $\bar{B}_{1^k}(z) = \bar{B}_{1^{k+1}}(z)$  and  $C_{1^k}(z) = C_{1^{k+1}}(z)$  hold in

the context of  $k$ -trees. Therefore, in view of eq. (16), it follows that  $B_{1^{k+1}}(z)$  have the same radius of convergence  $\rho_k$  (which is a square-root singularity).

*Step 2: For any  $k \geq 2$  and  $\mu \neq (1^k)$ ,  $\bar{B}_\mu(z)$  and  $C_\mu(z)$  are analytic at  $z = \rho_k$ .*

Let  $\tau_\mu$  be the unique dominant singularity of  $\bar{B}_\mu(z)$  for  $\mu \neq (1^k)$ . Since the number of black-rooted trees that are fixed by the permutation of type  $\mu \neq (1^k)$  is less than or equal to those fixed by the identity permutation, i.e.,  $[z^n]\bar{B}_\mu(z) \leq [z^n]\bar{B}_{1^k}(z)$  it follows that  $\tau_\mu \geq \rho_k$ . Therefore it remains to prove  $\tau_\mu \neq \rho_k$ . If  $\mu$  has exactly  $j$  parts of size 1, where  $0 < j < k$ , then we have

$$\bar{B}_\mu(z) = zC_\mu(z)^j \prod_{i \neq 1} C_{\mu^i}(z^i) \quad \text{and} \quad C_\mu(z) = \exp(\bar{B}_\mu(z)) \exp \left[ \sum_{m=2}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m} \right] \quad (17)$$

which lead to

$$\bar{B}_\mu(z) = z \prod_{i \neq 1} C_{\mu^i}(z^i) \exp(j\bar{B}_\mu(z)) \exp \left[ j \sum_{m=2}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m} \right]. \quad (18)$$

By setting  $\bar{B}_\mu(z) = y$ , it follows that  $(\tau_\mu, \bar{B}_\mu(\tau_\mu))$  is the unique solution of

$$M(z, y) = z \prod_{i \neq 1} C_{\mu^i}(z^i) \exp(jy) \exp \left[ j \sum_{m=2}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m} \right] = y,$$

$$M_y(z, y) = jz \prod_{i \neq 1} C_{\mu^i}(z^i) \exp(jy) \exp \left[ j \sum_{m=2}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m} \right] = 1,$$

consequently  $\bar{B}_\mu(\tau_\mu) = 1/j$ . Recall that  $\bar{B}_{1^k}(\rho_k) = 1/k$ , thus, we have  $k\bar{B}_{1^k}(\rho_k) = j\bar{B}_\mu(\tau_\mu) = 1$ . If  $\tau_\mu = \rho_k$ , then  $k\bar{B}_{1^k}(\rho_k) > j\bar{B}_\mu(\rho_k) = 1$ , which contradicts the relation  $k\bar{B}_{1^k}(\rho_k) = 1$ . Therefore we can conclude that  $\rho_k < \tau_\mu$  and from eq. (17), eq. (18),  $C_\mu(z)$  also has dominant singularity  $\tau_\mu$ . If  $\mu$  has no part of size 1, then  $\bar{B}_\mu(z)$  is a product of  $C_{\mu^i}(z^i)$  where  $i \geq 2$  and  $\mu^i$  has part of size 1. Consequently we have  $\tau_\mu > \min\{\tau_{\mu^i} : i \in \mu\} > \rho_k$ . Now we can conclude for any  $k \geq 2$  and  $\mu \neq (1^k)$ ,  $\rho_k < \tau_\mu$ , namely  $\bar{B}_\mu(z)$  and  $C_\mu(z)$  are analytic at  $z = \rho_k$ . Furthermore, we observe that the dominant singularity of  $B_\lambda(z)$  is determined by  $C_\lambda(z)$  where  $\lambda$  has at least one part of size 1. It follows that  $B_\lambda(z)$  is also analytic at  $z = \rho_k$  for any  $\lambda \neq (1^{k+1})$ .

*Step 3: The coefficient for the term  $(\rho_k - z)^{1/2}$  in the singular expansion of  $U(z)$  is zero and the coefficient for  $(\rho_k - z)^{3/2}$  is positive.*

Since  $B_{1^{k+1}}(z) = zC_{1^k}(z)^{k+1}$  has a square-root singularity at  $z = \rho_k$  and  $B_\lambda$  for any  $\lambda \neq (1^{k+1})$  is analytic at  $\rho_k$ , the dominant term in the singular expansion of  $U(z)$  comes from

$$\frac{B_{1^{k+1}}(z)}{z_{1^{k+1}}} + \frac{C_{1^k}(z)}{z_{1^k}} - \frac{C_{1^k}(z)\bar{B}_{1^k}(z)}{z_{1^k}} = \frac{-kzC_{1^k}(z)^{k+1}}{(k+1)!} + \frac{C_{1^k}(z)}{k!}.$$



All the other terms are all analytic at  $z = \rho_k$ . Together with the singular expansion of  $C_{1^k}(z)$  shown in eq. (16), we can calculate the coefficient for the term  $(\rho_k - z)^{1/2}$  in the singular expansion of  $U(z)$ , which is  $\frac{-k\rho_k}{(k+1)!} \binom{k+1}{1} \frac{a}{k\rho_k} + \frac{a}{k!} = 0$ . Similarly the coefficient for the term  $(\rho_k - z)^{3/2}$  in the singular expansion of  $U(z)$  is

$$\frac{-k\rho_k}{(k-1)!} a(b(k\rho_k)^{-\frac{1}{k}} + \frac{k-1}{3!} a^2)(k\rho_k)^{-\frac{k-2}{k}} = \frac{2\sqrt{2}}{k!} \frac{(k\rho_k)^{-\frac{1}{k}}}{3k^2} \left[ \frac{m'(\rho_k)}{m(\rho_k)} \right]^{3/2}$$

which is positive. Now we have derived the singular expansion of  $U(z)$  at  $z = \rho_k$ :

$$U(z) = U(\rho_k) + \frac{2\sqrt{2}}{k!} \frac{(k\rho_k)^{-\frac{1}{k}}}{3k^2} \left[ \frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)} \right]^{3/2} \quad (19)$$

$$+ c_1(\rho_k - z) + c_2(\rho_k - z)^2 + O(\rho_k - z)^{5/2}.$$

By applying the transfer theorem ([12, Theorem VI.3] or [9, Corollary 2.15]), we get eq. (13) and the proof of the asymptotic expansion is complete.

*Step 4: Asymptotic behavior of  $\rho_k$  as  $k \rightarrow \infty$ .*

We first show  $(4k)^{-1} \leq \rho_k \leq (ek)^{-1}$ . Since  $[z^n]\bar{B}_{1^k}(z) > 0$ ,  $[z^n]T(z) > 0$  and  $\bar{B}_{1^k}(z) = T(m(z))$  where  $m(z) = z + \dots$  has non-negative coefficients, then we have  $[z^n]\bar{B}_{1^k}(z) \geq [z^n]T(z)$  which indicates the radius of convergence for  $\bar{B}_{1^k}(z)$  is at most that for  $T(z)$  which is  $(ek)^{-1}$ . On the other hand, the radius of convergence for  $\bar{B}_{1^k}(z)$  is at least that for  $M(z)$  where  $M(z) = z(1 - kM(z))^{-1}$  and accordingly  $\rho_k \geq (4k)^{-1}$ .

It remains to consider the radius of convergence  $\rho_k$  in a more precise way. If we set  $A_k(z) = k\bar{B}_{1^k}(z/k)$  then  $A_k(z)$  satisfies the equation

$$A_k(z) = z \exp(A_k(z)) \exp\left(\sum_{m=2}^{\infty} \frac{A_k(z^m/k^{m-1})}{m}\right). \quad (20)$$

By definition the radius of convergence of  $A_k(z)$  is given by  $\alpha_k = k\rho_k$ . Furthermore by (20) it follows that  $A_{k+1}(z) \leq_c A_k(z)$ , where  $\leq_c$  means that the inequality is satisfied for all coefficients. Of course this implies that  $\alpha_{k+1} \geq \alpha_k$  and has, thus, a limit. By using the uniform estimate  $A_k(z) = z + O(A_k(z) - z) = z + O(A_1(z) - z) = z + O(z^2)$ , the representation

$$\alpha_k = \exp\left(-1 - \sum_{m=2}^{\infty} \frac{A_k(\alpha_k^m/k^{m-1})}{m}\right),$$

and a simple boots-trapping procedure it follows that

$$\alpha_k = \exp\left(-1 - \frac{\alpha_k^2}{2k} + O(k^{-2})\right) = \frac{1}{e} - \frac{1}{2e^3k} + O(k^{-2}),$$

which proves the asymptotic expansion for  $\rho_k = \alpha_k/k$ . It is also easy to show that  $m'(\rho_k) = 1 + O(k^{-1})$  which proves  $\rho_k m'(\rho_k)/m(\rho_k) = 1 + O(k^{-1})$  as  $k \rightarrow \infty$ .

□

It is worthwhile to mention that the coefficients for the asymptotics of  $[z^n]\bar{B}_{1^k}(z)$ ,  $[z^n]C_{1^k}(z)$  and  $[z^n]U(z)$  are determined by  $m(z)$  and  $\rho_k$  where the value of  $\rho_k$  can be computed by following Otter's work on 1-trees [24]. More precisely, let  $T_n = [z^n]\bar{B}_{1^k}(z)$  and  $m_n = [z^n]m(z)$ . Then by taking the derivative of eq. (14), eq. (15) and equating the coefficients, we get the recurrences for  $T_n$  and  $m_n$ , namely

$$T_n = \frac{k}{n-1} \sum_{i=1}^{n-1} T_{n-i} \sum_{m|i} m T_m \quad \text{for } n > 1 \text{ and } T_1 = 1.$$

$$m_n = \frac{k}{n-1} \sum_{i=2}^{n-1} m_{n-i} \sum_{m|i, m \neq i} m T_m \quad \text{for } n > 2 \text{ and } m_1 = 1, m_2 = 0.$$

From these two recurrences we can compute the exact value of  $m_n$ . Then the value of  $\rho_k$  is obtained by solving numerically the equation  $m(z) = 1/(ek)$ . The series  $m(z)$  can be estimated by its first 20 terms in its expansion at  $z = 0$  since the resulting error term is exponentially small. For  $k = 2$ ,  $\rho_2$  is already computed in [14] and turns out to be approximately 0.177.

## 7 Leaves of unlabeled $k$ -trees

As we have explained in Section 5 unlabeled  $k$ -trees are in bijection with the orbits of unlabeled  $k$ -coding tree under the action of  $\mathfrak{S}_{k+1}$ . In an unlabeled  $k$ -coding tree we call a black node a *leaf* if only one of its colored neighbors connects with other black nodes.

In the sequel we shall weight each black node by  $z$  and each leaf by  $w$ . Let  $U(z, w)$  be the generating function for color-orbits of unlabeled  $k$ -coding trees, then we have:

**Theorem 4** *Let  $X_n$  be the random variable associated with the number of leaves of unlabeled  $k$ -coding trees, that is*

$$\mathbb{P}(X_n = r) = \frac{[z^n w^r]U(z, w)}{[z^n]U(z, 1)}.$$

*Then there exist positive constants  $\mu_k$  and  $\sigma_k^2$  such that  $\mathbb{E}(X_n) = \mu_k n + O(1)$ ,  $\text{Var}(X_n) = \sigma_k^2 n + O(1)$ , and that  $X_n$  satisfies a central limit theorem of type*

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

*Furthermore, we have, as  $k \rightarrow \infty$ ,*

$$\mu_k = \frac{1}{e} + O\left(\frac{1}{k}\right) \quad \text{and} \quad \sigma_k^2 = \frac{1}{e} - \frac{2}{e^2} + O\left(\frac{1}{k}\right)$$

*Remark 1* Note that for large  $k$  the mean value  $\mu_k n + O(1)$  is quite close to the mean value  $(1/e)n + O(1)$  in the labeled case, and the variance  $\sigma_k^2 n + O(1)$  is quite close to the variance  $(1/e - 2/e^2)n + O(1)$  in the labeled case.

We will prove Theorem 4 in the following way:

1. Derivation of the generating function  $U(z, w)$ .
2. For  $m \geq 2$  and  $\mu \neq (1^k)$ ,  $\bar{B}_{1^k}(z^m, w^m)$ ,  $\bar{B}_\mu(z, w)$ ,  $C_\mu(z, w)$  and  $C_{1^k}(z^m, w^m)$  are analytic if  $(z, w)$  is close to  $(\rho_k, 1)$ .
3. The singular expansion of  $\bar{B}_{1^k}(z, w)$  and  $C_{1^k}(z, w)$  for  $w$  close to 1 and  $z$  close to  $\rho_k(w)$ .
4. Reformulate as for the Step 4 in the proof of Theorem 3.
5. Asymptotic behaviors of  $\mu_k$  and  $\sigma_k^2$  as  $k \rightarrow \infty$ .

Each step of the proof will be described below with more details explained.

*Proof Step 1: Derivation of the generating function  $U(z, w)$ .*

Let  $B(z, w)$  be the generating function for color-orbits of black-rooted unlabeled  $k$ -coding trees, let  $C(z, w)$  be the generating function for color-orbits of color-rooted unlabeled  $k$ -coding trees and let  $E(z, w)$  be the generating function for color-orbits of unlabeled  $k$ -coding trees rooted at an edge, then according to the dissymmetry theorem and Cauchy-Frobenius theorem, we have  $U(z, w) = B(z, w) + C(z, w) - E(z, w)$  where

$$B(z, w) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z, w)}{z_\lambda}, \quad C(z, w) = \sum_{\mu \vdash k} \frac{C_\mu(z, w)}{z_\mu},$$

$$E(z, w) = \sum_{\mu \vdash k} \frac{(\bar{B}_\mu(z, w) - zw + z)C_\mu(z, w) + z(w-1)}{z_\mu}$$

$$B_\lambda(z, w) = z \prod_i C_{\lambda^i}(z^i, w^i) + z(w-1) \quad (21)$$

$$\bar{B}_\mu(z, w) = z \prod_i C_{\mu^i}(z^i, w^i) + z(w-1) \quad (22)$$

$$C_\mu(z, w) = \exp \left[ \sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}(z^m, w^m)}{m} \right]. \quad (23)$$

*Step 2: For  $m \geq 2$  and  $\mu \neq (1^k)$ ,  $\bar{B}_{1^k}(z^m, w^m)$ ,  $\bar{B}_\mu(z, w)$ ,  $C_\mu(z, w)$  and  $C_{1^k}(z^m, w^m)$  are analytic if  $(z, w)$  is close to  $(\rho_k, 1)$ .*

For  $\mu = (1^k)$ , from eq. (22) and (23), we obtain

$$\bar{B}_{1^k}(z, w) = z \exp \left[ k \sum_{m=1}^{\infty} \frac{\bar{B}_{1^k}(z^m, w^m)}{m} \right] + z(w-1). \quad (24)$$

We first show for  $\mu \neq (1^k)$  and  $m \geq 2$ ,  $\bar{B}_\mu(z, w)$  and  $\bar{B}_{1^k}(z^m, w^m)$  are analytic if  $(z, w)$  is close to  $(\rho_k, 1)$ . For sufficiently small  $\epsilon > 0$ , we consider  $|w| \leq \frac{\rho_k}{\rho_k + \epsilon}$  and  $|z| \leq \rho_k + \epsilon$ , then for  $m \geq 2$ ,

$$|\bar{B}_\mu(z, w)| \leq \bar{B}_\mu(|zw|, 1) \leq \bar{B}_\mu(\rho_k, 1) \leq K\rho_k,$$

$$|\bar{B}_{1^k}(z^m, w^m)| \leq \bar{B}_{1^k}(|zw|^m, 1) \leq \bar{B}_{1^k}(\rho_k^m, 1) \leq M\rho_k^m.$$

The last inequality holds because  $\bar{B}_\mu(z, 1)$  and  $\bar{B}_{1^k}(z, 1)$  are convex for  $z \in [0, \rho_k]$  and  $z \in [0, \rho_k^2]$ , respectively. This implies for  $\mu \neq (1^k)$  and  $m \geq 2$ ,  $\bar{B}_\mu(z, w)$  and  $\bar{B}_{1^k}(z^m, w^m)$  are analytic if  $(z, w)$  is close to  $(\rho_k, 1)$ . Analogous to  $\bar{B}_{1^k}(z, w)$ , for  $m \geq 2$  and  $\mu \neq (1^k)$ ,  $C_\mu(z, w)$  and  $C_{1^k}(z^m, w^m)$  are analytic if  $(z, w)$  is close to  $(\rho_k, 1)$ .

*Step 3: The singular expansion of  $\bar{B}_{1^k}(z, w)$  and  $C_{1^k}(z, w)$  for  $w$  close to 1 and  $z$  close to  $\rho_k(w)$ .*

We set

$$F(y, z, w) = z \exp \left[ ky + k \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m, w^m)}{m} \right] + z(w-1) \quad (25)$$

which is analytic for  $(y, z, w)$  around  $(0, 0, 0)$  and we have  $F(y, 0, w) \equiv 0$ ,  $F(0, z, w) \neq 0$ . Furthermore, the coefficients of  $F(y, z, w)$  are all non-negative. Since  $\bar{B}_{1^k}(z, w)$  is the unique solution of  $F(y, z, w) = y$  it can be expressed as

$$\bar{B}_{1^k}(z, w) = \alpha(z, w) - \beta(z, w) \left[ 1 - \frac{z}{\rho_k(w)} \right]^{1/2},$$

where  $\alpha(z, w), \beta(z, w), \rho_k(w)$  are analytic for  $|w-1| \leq \epsilon$ ,  $|z - \rho_k(w)| < \epsilon$ ,  $|\arg(z - \rho_k(w))| > \phi$  (for some  $\phi \in (0, \pi/2)$ ) and  $\epsilon, \varepsilon$  are sufficiently small. Furthermore,  $\beta(\rho_k(w), w) \neq 0$  and  $\bar{B}_{1^k}(\rho_k(w), w) = \alpha(\rho_k(w), w) = k^{-1} + (w-1)\rho_k(w)$ . Since  $\bar{B}_{1^k}(z, w) = zC_{1^k}(z, w)^k + z(w-1)$ ,  $C_{1^k}(z, w)$  has a corresponding representation

$$C_{1^k}(z, w) = a(z, w) + b(z, w) \left[ 1 - \frac{z}{\rho_k(w)} \right]^{1/2}, \quad (26)$$

where  $a(z, w), b(z, w)$  are analytic functions around  $(z, w) = (\rho_k, 1)$ ,  $b(\rho_k(w), w) \neq 0$ ,  $C_{1^k}(\rho_k(w), w) = a(\rho_k(w), w) = (k\rho_k(w))^{-1/k}$ .

*Step 4: Reformulate as for the Step 4 in the proof of Theorem 3.*

For  $|w-1| \leq \epsilon$ ,  $|z - \rho_k(w)| < \varepsilon$ ,  $|\arg(z - \rho_k(w))| > \phi$  and  $\epsilon, \varepsilon$  are sufficiently small,  $U(z, w)$  has the expansion

$$U(z, w) = -\frac{kz}{(k+1)!} C_{1^k}(z, w)^{k+1} + \frac{1}{k!} C_{1^k}(z, w) + H_1(z, w)$$

where  $H_1(z, w)$  is an analytic function around  $(z, w) = (\rho_k, 1)$ . By substituting  $C_{1^k}(z, w)$  by its singular expansion in eq. (26),  $U(z, w)$  can be expanded locally around  $z = \rho_k(w)$ , i.e.,

$$U(z, w) = g(z, w) + \left[ -\frac{za^k(z, w)}{(k-1)!} + \frac{1}{k!} + O(\rho_k(w) - z) \right] b(z, w) \left[ 1 - \frac{z}{\rho_k(w)} \right]^{1/2},$$

Since  $-\rho_k(w) \frac{a^k(\rho_k(w), w)}{(k-1)!} + \frac{1}{k!} = 0$ , together with the fact  $a(z, w) = a(\rho_k(w), w) + O(\rho_k(w) - z)$  and  $b(\rho_k(w), w) \neq 0$ , we can conclude

$$U(z, w) = g(z, w) + f(z, w) \left[ 1 - \frac{z}{\rho_k(w)} \right]^{3/2} \quad (27)$$

where  $f(\rho_k, 1) \neq 0$  from Section 6 and therefore  $f(\rho_k(w), w) \neq 0$  for  $|w-1| \leq \epsilon$ . By applying [9, Theorem 2.25] to eq. (27), there is a central limit theorem for  $(X_n - \mathbb{E}(X_n))/(\sigma_k \sqrt{n})$ . More precisely there exist  $\mu_k$  and  $\sigma_k^2$  with  $\mathbb{E}(X_n) = \mu_k n + O(1)$  and  $\text{Var}(X_n) = \sigma_k^2 n + O(1)$ . By applying Lemma 4 of [11] it actually follows that  $\sigma_k^2 > 0$  and  $X_n$  satisfies a central limit theorem as stated.

*Step 5: Asymptotic behaviors of  $\mu_k$  and  $\sigma_k^2$  as  $k \rightarrow \infty$ .*

In order to compute  $\mu_k$  and  $\sigma_k^2$  we proceed similarly to the proof of Theorem 1. We just have to replace  $F(y, z, w) = z \exp(ky) + z(w-1)$  by  $F(y, z, w)$  given in (25). Furthermore we have  $y_0 = 1/k$ ,  $z_0 = 1/(ek) + O(k^{-2})$ , and  $w_0 = 1$ . From this and the approximation  $\bar{B}_{1^k}(z, w) = zw + O(z^2/k)$  (for  $z \rightarrow 0$  and  $w$  close to 1) we obtain (for  $(y, z, w) = (y_0, z_0, w_0)$ )  $F_y = 1$ ,  $F_{yy} = k$ ,  $F_w = 1/(ke) + O(k^{-2})$ ,  $F_z = e + O(k^{-1})$ ,  $F_{ww} = 1/(k^2 e^2) + O(k^{-3})$ ,  $F_{yw} = 1/(ke^2) + O(k^{-2})$ ,  $F_{zw} = 1 + O(k^{-1})$ ,  $F_{yz} = ke + O(1)$ , and  $F_{zz} = 2 + O(k^{-2})$ . From this it directly follows that  $\mu_k = 1/e + O(k^{-1})$  and  $\sigma_k^2 = 1/e - 2/e^2 + O(k^{-1})$ .

We just present the details for the  $F_z$ . The other cases can be handled in the same way. By (25) we have

$$F_z = \exp \left[ ky + k \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m, w^m)}{m} \right] + (w-1) \\ + kz \exp \left[ ky + k \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m, w^m)}{m} \right] \sum_{m=2}^{\infty} \bar{B}_{1^k, z}(z^m, w^m) z^{m-1}$$

and consequently for  $(y, z, w) = (y_0, z_0, w_0)$

$$F_z = \frac{y_0}{z_0} + ky_0 \sum_{m=2}^{\infty} \bar{B}_{1^k, z}(z_0^m, 1) z_0^{m-1}.$$

Since  $\bar{B}_{1^k, z}(z, 1) = 1 + O(z/k)$  as  $z \rightarrow 0$  it follows that

$$\sum_{m=2}^{\infty} \bar{B}_{1^k, z}(z_0^m, 1) z_0^{m-1} = \frac{1}{ek} + O(k^{-2}).$$

Summing up this implies

$$F_z = e + O(k^{-1})$$

as proposed. □

## 8 The degree distribution of unlabeled $k$ -trees

We again refer to the unlabeled  $k$ -coding trees and consider here the degree distribution. Clearly every black node in the  $k$ -coding tree has degree  $k+1$ . So we concentrate on the degree distribution of colored nodes. If an unlabeled  $k$ -coding tree has  $n$  black nodes, then it has  $kn+1$  colored nodes. As in the

labeled case we change the statistics slightly by measuring the size according to the number of colored nodes. Formally the variable  $x$  (instead of  $z$ ) takes care of the number of colored nodes. Now let  $\tilde{U}(x) = xU(x^k)$  be the generating function for color-orbits of unlabeled  $k$ -coding trees, let  $\tilde{B}(x)$  be the generating function for color-orbits of black-rooted unlabeled  $k$ -coding trees, let  $\tilde{C}(x)$  be the generating function for color-orbits of color-rooted unlabeled  $k$ -coding trees and let  $\tilde{E}(x)$  be the generating function for color-orbits of unlabeled  $k$ -coding trees rooted at an edge, then we have similarly to the above:  $\tilde{U}(x) = \tilde{B}(x) + \tilde{C}(x) - \tilde{E}(x)$  where

$$\begin{aligned} \tilde{B}(x) &= \sum_{\lambda \vdash k+1} \frac{\tilde{B}_\lambda(x)}{z_\lambda} & \tilde{B}_\lambda(x) &= \prod_i \tilde{C}_{\lambda^i}(x^i) \\ \tilde{C}(x) &= \sum_{\mu \vdash k} \frac{\tilde{C}_\mu(x)}{z_\mu} & \tilde{B}_\mu(x) &= \prod_i \tilde{C}_{\mu^i}(x^i) \\ \tilde{E}(x) &= \sum_{\mu \vdash k} \frac{\tilde{B}_\mu(x)\tilde{C}_\mu(x)}{z_\mu} & \tilde{C}_\mu(x) &= x \exp \left[ \sum_{m=1}^{\infty} \frac{\tilde{B}_{\mu^m}(x^m)}{m} \right]. \end{aligned}$$

In completely the same way as in Section 6, we can find the singular expansion of  $\tilde{U}(x)$  given by

$$\tilde{U}(x) = \tilde{U}(\gamma_k) + \bar{c}_1(\gamma_k - x) + r(\gamma_k - x)^{3/2} + \bar{c}_2(\gamma_k - x)^2 + O((\gamma_k - x)^{5/2})$$

for some positive constant  $r$  and some constants  $\bar{c}_1, \bar{c}_2$ . Furthermore  $\tilde{B}_{1^k}(\gamma_k) = 1/k$ . As in the labeled case there are similar expansions at  $x = \gamma_k e^{2\pi i \ell/k}$ ,  $\ell = 1, 2, \dots, k-1$ .

Now we give each colored node of degree  $d_i$  with weight  $u_i$ . Let  $\mathbf{u} = (u_1, \dots, u_M)$ ,  $\mathbf{m} = (m_1, \dots, m_M)$  where  $m_i \geq 0$  and  $\mathbf{d} = (d_1, \dots, d_M)$  where  $d_i > 0$ , then the coefficient of  $x^{kn+1} \mathbf{u}^{\mathbf{m}}$  in the generating function  $U^{(\mathbf{d})}(x, \mathbf{u})$  is the number of unlabeled  $k$ -coding trees on  $n$  black nodes and there are  $m_i$  colored nodes out of  $kn+1$  total colored nodes having degree  $d_i$  for every  $i$ ,  $1 \leq i \leq M$ . Then we have

**Theorem 5** *Let  $Y_{n,\mathbf{d}} = (Y_{n,d_1}^{(1)}, \dots, Y_{n,d_M}^{(M)})$  be the random vector of the number of colored nodes in an unlabeled  $k$ -tree that have degrees  $(d_1, \dots, d_M)$ , that is,*

$$\mathbb{P}(Y_{n,\mathbf{d}} = \mathbf{m}) = \frac{[x^{kn+1} \mathbf{u}^{\mathbf{m}}]U^{(\mathbf{d})}(x, \mathbf{u})}{[x^{kn+1}]U^{(\mathbf{d})}(x, \mathbf{1})}.$$

*Then there exist an  $M$ -dimensional vector  $\tilde{\mathbf{M}}$  and a  $M \times M$  positive semidefinite matrix  $\tilde{\mathbf{S}}$  such that  $\mathbb{E}(Y_{n,\mathbf{d}}) = \tilde{\mathbf{M}}kn + O(1)$  and  $\text{Cov}(Y_{n,\mathbf{d}}) = \tilde{\mathbf{S}}kn + O(1)$ . Furthermore  $Y_{n,\mathbf{d}}$  satisfies a central limit theorem of the form*

$$\frac{Y_{n,\mathbf{d}} - \mathbb{E}(Y_{n,\mathbf{d}})}{\sqrt{kn}} \rightarrow N(0, \tilde{\mathbf{S}}).$$

*Remark 2* The case of trees, that is, the case  $k = 1$ , has been discussed in [26, 10]. There it was proved that the number of vertices  $Y_{n,d}$  of degree  $d$  satisfy  $\mathbb{E}(Y_{n,d}) = \tilde{\mu}_d n + O(1)$  and  $\text{Var}(Y_{n,d}) = \tilde{\sigma}_d^2 n + O(1)$ , where  $\tilde{\mu}_d$  and  $\tilde{\sigma}_d^2$  are asymptotically given by

$$\tilde{\mu}_d \sim \tilde{\sigma}_d^2 \sim C\rho_1^d,$$

as  $d \rightarrow \infty$ , where  $C \approx 6.380045$  (and  $\rho_1 = 0.338219$ ). A similar result holds for  $k$ -trees. The corresponding constants  $\tilde{\mu}_{k,d}$ ,  $\tilde{\sigma}_{k,d}^2$  are asymptotically given by

$$\tilde{\mu}_{k,d} \sim \tilde{\sigma}_{k,d}^2 \sim C\rho_k^d$$

for fixed  $k$  and  $d \rightarrow \infty$ . The proof is very similar to that given in [26, 10] but quite technical. So we do not present the details.

We will prove Theorem 5 in the following way:

1. Derivation of the generating function  $U^{(\mathbf{d})}(x, \mathbf{u})$ .
2. For  $\mu \neq (1^k)$  and  $m \geq 2$ ,  $\bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})$  and  $\bar{B}_{1^k}^{(\mathbf{d})}(x^m, \mathbf{u}^m)$  are analytic if  $(x, \mathbf{u})$  is close to  $(\gamma_k, \mathbf{1})$ .
3. The singular expansion of  $\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  and  $C_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$ .
4. Reformulate as for the Step 4 in the proof of Theorem 3.

Each step of the proof will be described below with more details explained.

*Proof Step 1: Derivation of the generating function  $U^{(\mathbf{d})}(x, \mathbf{u})$ .*

Let  $C^{(\mathbf{d})}(x, \mathbf{u})$  be the generating function for color-orbits of colored-rooted trees that have each colored node of degree  $d_i$  weighted by  $u_i$ . Let  $P^{(\mathbf{d})}(x, \mathbf{u})$  be the generating function for the trees whose root is only connected with the root of a color-orbit of color-rooted unlabeled  $k$ -coding tree, so that  $C^{(\mathbf{d})}(x, \mathbf{1}) = P^{(\mathbf{d})}(x, \mathbf{1})$ . Let  $B^{(\mathbf{d})}(x, \mathbf{u})$  be the generating function for color-orbits of black-rooted unlabeled  $k$ -coding trees that have each node of degree  $d_i$  weighted by  $u_i$ .  $E^{(\mathbf{d})}(x, \mathbf{u})$  be the generating function for color-orbits of unlabeled  $k$ -coding trees rooted at an edge that have each node of degree  $d_i$  weighted by  $u_i$ . Here we introduce  $P^{(\mathbf{d})}(x, \mathbf{u})$  to distinguish the case that the colored root has degree  $d_i$  for some  $1 \leq i \leq M$ . Let  $Z(\mathfrak{S}_p, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u}))$  represent the generating function for the forest consisting of exactly  $k$  reduced black-rooted unlabeled  $k$ -coding trees:

$$\begin{aligned} Z(\mathfrak{S}_p, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})) &= Z(\mathfrak{S}_p, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u}), \bar{B}_{\mu^2}^{(\mathbf{d})}(x^2, \mathbf{u}^2), \dots, \bar{B}_{\mu^p}^{(\mathbf{d})}(x^p, \mathbf{u}^p)) \\ &= \sum_{\lambda \vdash p} \frac{1}{z_\lambda} \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})^{\lambda_1} \bar{B}_{\mu^2}^{(\mathbf{d})}(x^2, \mathbf{u}^2)^{\lambda_2} \dots \bar{B}_{\mu^p}^{(\mathbf{d})}(x^p, \mathbf{u}^p)^{\lambda_p} \end{aligned}$$

where  $\lambda = (1^{\lambda_1} 2^{\lambda_2} \dots p^{\lambda_p})$ . Then the generating function  $U^{(\mathbf{d})}(x, \mathbf{u})$  for unlabeled  $k$ -trees with colored nodes of degree  $\mathbf{d}$  is given by  $U^{(\mathbf{d})}(x, \mathbf{u}) = B^{(\mathbf{d})}(x, \mathbf{u}) +$

$C^{(\mathbf{d})}(x, \mathbf{u}) - E^{(\mathbf{d})}(x, \mathbf{u})$  where

$$\begin{aligned} B^{(\mathbf{d})}(x, \mathbf{u}) &= \sum_{\lambda \vdash k+1} \frac{B_\lambda^{(\mathbf{d})}(x, \mathbf{u})}{z_\lambda}, \quad C^{(\mathbf{d})}(x, \mathbf{u}) = \sum_{\mu \vdash k} \frac{C_\mu^{(\mathbf{d})}(x, \mathbf{u})}{z_\mu}, \\ E^{(\mathbf{d})}(x, \mathbf{u}) &= \sum_{\mu \vdash k} \frac{\bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u}) P_\mu^{(\mathbf{d})}(x, \mathbf{u})}{z_\mu}, \\ B_\lambda^{(\mathbf{d})}(x, \mathbf{u}) &= \prod_i P_{\lambda^i}^{(\mathbf{d})}(x^i, \mathbf{u}^i), \quad \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u}) = \prod_i P_{\mu^i}^{(\mathbf{d})}(x^i, \mathbf{u}^i), \end{aligned} \quad (28)$$

$$C_\mu^{(\mathbf{d})}(x, \mathbf{u}) = x \exp \left[ \sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}^{(\mathbf{d})}(x^m, \mathbf{u}^m)}{m} \right] + \sum_{j=1}^M x(u_j - 1) Z(\mathfrak{S}_{d_j}, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})), \quad (29)$$

$$P_\mu^{(\mathbf{d})}(x, \mathbf{u}) = x \exp \left[ \sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}^{(\mathbf{d})}(x^m, \mathbf{u}^m)}{m} \right] + \sum_{j=1}^M x(u_j - 1) Z(\mathfrak{S}_{d_j-1}, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})). \quad (30)$$

*Step 2: For  $\mu \neq (1^k)$  and  $m \geq 2$ ,  $\bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})$  and  $\bar{B}_{1^k}^{(\mathbf{d})}(x^m, \mathbf{u}^m)$  are analytic if  $(x, \mathbf{u})$  is close to  $(\gamma_k, \mathbf{1})$ .*

The dominant singularity for  $\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{1})$  is  $\gamma_k$ . As before, for  $\mu \neq (1^k)$ ,  $\bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})$  and for  $m \geq 2$ ,  $\bar{B}_{1^k}^{(\mathbf{d})}(x^m, \mathbf{u}^m)$  are analytic if  $(x, \mathbf{u})$  is close to  $(\gamma_k, \mathbf{1})$ .

*Step 3: The singular expansion of  $\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  and  $C_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$ .*

Next we consider

$$\begin{aligned} S(x, y, \mathbf{u}) &= \left( x e^y \exp \left( \sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}^{(\mathbf{d})}(x^m, \mathbf{u}^m)}{m} \right) \right. \\ &\quad \left. + \sum_{j=1}^M x(u_j - 1) Z(\mathfrak{S}_{d_j-1}, y, \bar{B}_{1^k}^{(\mathbf{d})}(x^2, \mathbf{u}^2), \dots, \bar{B}_{1^k}^{(\mathbf{d})}(x^{d_j-1}, \mathbf{u}^{d_j-1})) \right)^k. \end{aligned}$$

Since  $S(0, y, \mathbf{u}) \equiv 0$ ,  $S(x, 0, \mathbf{u}) \not\equiv 0$  and all coefficients of  $S(x, y, \mathbf{1})$  are real and positive, then  $y(x, \mathbf{u}) = \bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  is the unique solution of the functional equation  $S(x, y, \mathbf{u}) = y$ . Furthermore,  $(x, y) = (\gamma_k, 1/k)$  is the only solution of  $S(x, y, \mathbf{1}) = 0$  and  $S_y(x, y, \mathbf{1}) = 1$  with  $S_x(\gamma_k, 1/k, \mathbf{1}) \neq 0$ ,  $S_{yy}(\gamma_k, 1/k, \mathbf{1}) \neq 0$ . Consequently,  $\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  can be represented as

$$\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u}) = g(x, \mathbf{u}) - h(x, \mathbf{u}) \left[ 1 - \frac{x}{\gamma_k(\mathbf{u})} \right]^{1/2} \quad (31)$$

which holds locally around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$  and  $h(\gamma_k(\mathbf{u}), \mathbf{u}) \neq 0$ . In view of  $\bar{B}_{1^k}^{(\mathbf{d})}(x, \mathbf{u}) = P_{1^k}^{(\mathbf{d})}(x, \mathbf{u})^k$ ,  $P_{1^k}^{(\mathbf{d})}(x, \mathbf{u})$  also has the expansion of square root



type, i.e.,

$$P_{1^k}^{(\mathbf{d})}(x, \mathbf{u}) = s(x, \mathbf{u}) - t(x, \mathbf{u}) \left[ 1 - \frac{x}{\gamma_k(\mathbf{u})} \right]^{1/2} \quad (32)$$

where  $t(\gamma_k(\mathbf{u}), \mathbf{u}) \neq 0$ . From eq. (29) and eq. (30), we have

$$C_\mu^{(\mathbf{d})}(x, \mathbf{u}) = P_\mu^{(\mathbf{d})}(x, \mathbf{u}) + \sum_{j=1}^M x(u_j - 1) \left[ Z(\mathfrak{S}_{d_j}, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})) - Z(\mathfrak{S}_{d_j-1}, \bar{B}_\mu^{(\mathbf{d})}(x, \mathbf{u})) \right].$$

*Step 4: Reformulate as for the Step 4 in the proof of Theorem 3.*

Based on Step 3, we shall next compute the dominant term in the singular expansion of  $U^{(\mathbf{d})}(x, \mathbf{u})$ .

For simplicity we will omit variables  $(x, \mathbf{u})$  and degree  $\mathbf{d}$ .

$$\begin{aligned} U(x, \mathbf{u}) &= \frac{P_{1^k}^{k+1}}{(k+1)!} + \frac{C_{1^k}}{k!} - \frac{P_{1^k}^{k+1}}{k!} + M_1 \\ &= \frac{P_{1^k}^{k+1}}{(k+1)!} + \frac{1}{k!}(1 - P_{1^k}^k)P_{1^k} + \frac{1}{k!}(C_{1^k} - P_{1^k}) + M_1 \\ &= -\frac{kP_{1^k}^{k+1}}{(k+1)!} + \frac{P_{1^k}}{k!} + \frac{1}{k!} \sum_{j=1}^M x(u_j - 1) \left[ Z(\mathfrak{S}_{d_j}, \bar{B}_{1^k}) - Z(\mathfrak{S}_{d_j-1}, \bar{B}_{1^k}) \right] + M_1 \end{aligned}$$

where  $M_1$  is an analytic function around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$ . It is now convenient to write  $U(x, \mathbf{u}) = f(x, \mathbf{u}) + \bar{h}(x, \mathbf{u}) \left[ 1 - \frac{x}{\gamma_k(\mathbf{u})} \right]^{1/2}$ . Then by substituting  $P_{1^k}, \bar{B}_{1^k}$  with its representation in eq. (32) and eq. (31), we obtain

$$\begin{aligned} \bar{h}(x, \mathbf{u}) &= \frac{s^k t}{(k-1)!} - \frac{t}{k!} \\ &\quad + \frac{h}{k!} \sum_{j=1}^M x(u_j - 1) \left[ Z'(\mathfrak{S}_{d_j-1}, g, X_2, \dots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j}, g, X_2, \dots, X_{d_j}) \right] \end{aligned}$$

where  $X_i$  are analytic functions around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$  and  $Z'$  is the derivative w.r.t. the first variable of  $Z(\mathfrak{S}_k, x_1, \dots, x_k)$ , namely  $Z'(\mathfrak{S}_k, x_1, \dots, x_k) = Z(\mathfrak{S}_{k-1}, x_1, \dots, x_{k-1})$ . Furthermore, by replacing  $s, t$  by  $g = s^k$  and  $h = ks^{k-1}t$ , we can further simplify  $\bar{h}(x, \mathbf{u})$ , that is

$$\begin{aligned} \bar{h}(x, \mathbf{u}) &= \frac{h}{k!} \frac{g - \frac{1}{k}}{g^{1-\frac{1}{k}}} \\ &\quad + \frac{h}{k!} \sum_{j=1}^M x(u_j - 1) \left[ Z'(\mathfrak{S}_{d_j-1}, g, X_2, \dots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j}, g, X_2, \dots, X_{d_j}) \right]. \end{aligned}$$

Now we use the fact that  $y = g(\gamma_k(\mathbf{u}), \mathbf{u})$  and  $x = \gamma_k(\mathbf{u})$  is the solution of  $S(x, y, \mathbf{u}) = y$  and  $S_y(x, y, \mathbf{u}) = 1$ , which yields

$$g(\gamma_k(\mathbf{u}), \mathbf{u}) = \frac{1}{k} + g(\gamma_k(\mathbf{u}), \mathbf{u})^{\frac{k-1}{k}} \sum_{j=1}^M x(u_j - 1) \\ \times [Z(\mathfrak{S}_{d_j-1}, g, X_2, \dots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j-1}, g, X_2, \dots, X_{d_j-1})]$$

and consequently  $\bar{h}(\gamma_k(\mathbf{u}), \mathbf{u}) \equiv 0$  and  $U(x, \mathbf{u})$  has a local expansion around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$  of the form

$$U(x, \mathbf{u}) = w(x, \mathbf{u}) + r(x, \mathbf{u}) \left[ 1 - \frac{x}{\gamma_k(\mathbf{u})} \right]^{3/2}. \quad (33)$$

where  $r(\gamma_k(\mathbf{u}), \mathbf{u}) \neq 0$  since  $r(\gamma_k, \mathbf{1}) = r \neq 0$  and  $w(x, \mathbf{u}), r(x, \mathbf{u})$  are analytic function around  $(x, \mathbf{u}) = (\gamma_k, \mathbf{1})$ . Thus a central limit theorem follows. More precisely by setting  $A(\mathbf{u}) = \log \gamma_k(\mathbf{1}) - \log \gamma_k(\mathbf{u})$ ,  $\mu_2 = (A_{u_j}(\mathbf{1}))_{1 \leq j \leq M}$  and  $\Sigma_2 = (A_{u_i u_j}(\mathbf{1}) + \delta_{i,j} A_{u_j}(\mathbf{1}))_{1 \leq j \leq M}$  then  $\mathbb{E}(Y_{n,\mathbf{d}}) = \mu_2(kn) + O(1)$  and  $\text{Cov}(Y_{n,\mathbf{d}}) = \Sigma_2(kn) + O(1)$ .  $\square$

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