An Asymptotic Analysis of Unlabeled k-Trees

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Motivation

- The notion of a $k$-tree originates from the parameter tree-width.
- A $k$-tree is the maximal graph with a fixed tree-width $k$ such that no more edges can be added without increasing its tree-width.
- Tree-width is important to the analysis of graphs with forbidden minors.
- Many NP-hard problems on graphs of bounded tree-width can be solved in polynomial time.
Unlabeled k-tree

Definition:
A $k$-tree is either a complete graph on $k$ vertices 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. In particular, a 1-tree is an unrooted tree.

Examples: 1-tree and 2-tree
Definition:

A \( k \)-tree is either a complete graph on \( k \) vertices 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. In particular, a 1-tree is an unrooted tree.

Examples: The rightmost ones are NOT \( k \)-trees.
Labeled k-tree

- Labeled $k$-trees have been already counted by Beineke, Pippert, Moon and Foata four decades ago. They showed that the number $B_n$ of $k$-trees having $n$ labeled vertices is

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


Generating function

Unlabeled k-tree

Basic definitions and facts:

- Let $g \in \mathcal{S}_m$ be a permutation of $\{1,2,\cdots,m\}$ that has $\ell_i$ cycles of size $i$, $1 \leq i \leq k$, in its cyclic decomposition. Then its cycle type $\lambda = (1^{\ell_1}2^{\ell_2} \cdots k^{\ell_k})$ is a partition of $m$ where $m = \sum_{i=1}^{k} i\ell_i$. We denote by $\lambda \vdash m$ that $\lambda$ is a partition of $m$.

- Let $z_{\lambda} = 1^{\ell_1}!2^{\ell_2}!\cdots k^{\ell_k}!\ell_k!$, then $\frac{m!}{z_{\lambda}}$ is the number of permutations in $\mathcal{S}_m$ of cycle type $\lambda$.

- A hedron is a $(k + 1)$-clique in a $k$-tree and a front is a $k$-clique in a $k$-tree. According to the inductive construction of a $k$-tree, the number of vertices in a $k$-tree having $n$ hedra is $n + k$.

- The size of a $k$-tree is $n$ if it has $n$ hedra.
Hedron-labeled k-tree

- A colored hedron-labeled $k$-tree of size $n$ is a $k$-tree that has each vertex colored from the set $\{1', 2', \ldots, (k+1)\}'$ so that any two adjacent vertices are colored differently, and each hedron is labeled with a distinct number from $\{1, 2, \ldots, n\}$.

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 and consider the hedron-labeled $k$-trees.

- Example: a hedron-labeled 2-tree (left)
Generating function

From a hedron-labeled $k$-tree to a $k$-coding tree

To construct a $k$-coding tree from a hedron-labeled $k$-tree, we color each front of a hedron with a distinct color from the set $\{1, 2, \cdots, k + 1\}$. The corresponding labeled $k$-coding tree has a black vertex labeled with $i$ representing a hedron of the $k$-tree with label $i$ and a $j$-colored vertex representing a front of the $k$-tree with color $j$. We connect a black vertex with a colored vertex if and only if the corresponding hedron contains the corresponding front.
The construction from a hedron-labeled, fronted colored \( k \)-tree of size \( n \) to a labeled \( k \)-coding tree of size \( n \) is a bijection.

Let \( G_1 \mapsto G_2 \) under this bijection, then for every \( \pi \in S_n \) and \( \sigma \in S_{k+1} \), \( \pi(G_1) \mapsto \pi(G_2) \) and \( \sigma(G_1) \mapsto \sigma(G_2) \).

Under the action of \( S_n \) and \( S_{k+1} \), the orbits of hedron-labeled, front-colored \( k \)-tree, which are unlabeled \( k \)-trees are in bijection with the orbits of unlabeled \( k \)-coding trees under the action \( S_{k+1} \).
The unlabeled $k$-trees are in bijection with the orbits of unlabeled $k$-coding trees under the action $\mathfrak{S}_{k+1}$.

The number $U_n$ of unlabeled $k$-trees is equal to the number of the orbits of unlabeled $k$-coding trees under the action of $\mathfrak{S}_{k+1}$. 
Dissymmetry Theorem

The dissymmetry theorem transforms the problem of counting unrooted, unlabeled $k$-coding trees to that of counting rooted, unlabeled $k$-coding trees.

- $W_n$: the set of $k$-coding trees with black vertex set $[n]$.
- $W_n^\bullet$: the set of $\bullet$-rooted $k$-coding trees.
- $W_n^\circ$: the set of $\circ$-rooted $k$-coding trees.
- $W_n^{\circ\bullet}$: the set of $\circ$-$\bullet$ rooted $k$-coding trees.
Dissymmetry Theorem

Theorem (Dissymmetry Theorem)

There is a bijection \( \Theta : W_n^o \cup W_n^\bullet \rightarrow W_n \cup W_n^{o-\bullet} \) that commutes with the actions of \( S_n \) on vertex labels and of \( S_{k+1} \) on colors.

Ideas of the proof:

- Every longest path in the k-coding tree has a unique midpoint, we name it as a center point. This center point is either a labeled black vertex or a colored white vertex.

- Let \( T \) be a rooted tree in \( W_n^o \cup W_n^\bullet \). If \( T \) is rooted at its center point, \( \Theta( T) \) is the underlying unrooted tree of \( T \). Otherwise, we take \( \Theta( T) \) to be the underlying tree of \( T \) rooted at the first edge from the root of \( T \) to the center point.
Burnside’s Lemma

Lemma (Burnside)
Suppose that a finite group $G$ acts on the weighted set $S$ so that weights are constant on orbits. Let the weight of an orbit be the weight of any of its elements. For each $g \in G$, we denote by $\text{fix}(g)$ the sum of the weights of the elements of $S$ fixed by $g$. Then the sum of the weights of the orbits of $S$ under $G$ is equal to $\frac{1}{|G|} \sum_{g \in G} \text{fix}(g)$.

Lemma (Burnside’s lemma for $G = \mathfrak{S}_m$)
For each partition $\lambda$ of $m$, let $f_{\lambda}$ be the sum of the weights of the elements of $S$ fixed by a permutation of cycle type $\lambda$. Then the sum of the weights of the orbits of $S$ under $\mathfrak{S}_m$ is $\sum_{\lambda \vdash m} \frac{f_{\lambda}}{z_{\lambda}}$. 
Theorem (Gessel and Gainer-Dewar, 2013)

The generating function $U(z)$ for unlabeled $k$-trees is given by

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

where $B(z)$ (resp. $C(z)$, $E(z)$) is the generating function for color-orbits of •-rooted (resp. ◦-rooted, •-◦-rooted) unlabeled $k$-coding trees.

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

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

$$E(z) = \sum_{\mu \vdash k} \frac{B^*_\mu(z) C_\mu(z)}{z_\mu} \quad C_\mu(z) = \exp \left[ \sum_{m=1}^{\infty} \frac{B^*_\mu(z^m)}{m} \right]$$
The generating function $U(z)$ for unlabeled $k$-trees is given by

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

where

$$B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z^\lambda},$$

$$C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z^\mu},$$

$$E(z) = \sum_{\mu \vdash k} \frac{B_\mu^*(z) C_\mu(z)}{z^\mu}.$$

$B_\lambda(z)$ is the generating function for black-rooted tree that are fixed by $\pi$ where $\pi$ has cycle type $\lambda$. 
The generating function $U(z)$ for unlabeled $k$-trees is given by

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

where

$$B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z_\lambda},$$

$$C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z_\mu},$$

$$E(z) = \sum_{\mu \vdash k} \frac{B_\mu^*(z)C_\mu(z)}{z_\mu}.$$

$C_\mu(z)$ is the generating function for colored-rooted tree that are fixed by $\sigma$ where $\sigma$ has cycle type $\mu$. 
The generating function $U(z)$ for unlabeled $k$-trees is given by

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

where

$$B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z^\lambda},$$

$$C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z^\mu},$$

$$E(z) = \sum_{\mu \vdash k} \frac{B^*_\mu(z)C_\mu(z)}{z^\mu}.$$

A $j$-reduced black-rooted tree if it is a black-rooted unlabeled $k$-coding tree with all the neighbors of the root are colored by $[k + 1] - \{j\}$. $B^*_\mu(z)$ is the generating function for $j$-reduced black-rooted tree that are fixed by $\sigma$ where $\sigma$ has cycle type $\mu$. 
Generating function

\[ B_\lambda(z) = z \prod_i C_{\lambda_i}(z^i) = z \prod_c C_{\pi|c|}(z^{|c|}) \]

\[ B^*_\mu(z) = z \prod_i C_{\mu_i}(z^i) \]

Let \( T \) be a \( \bullet \)-rooted tree fixed by \( \pi \), then the root of \( T \) connects to the trees \( T_1, \ldots, T_{k+1} \) where \( T_j \) is a \( j \)-rooted tree. Suppose \( j \) is in a cycle of \( \pi \) of length \( i \), then tree \( T_j \) is fixed by \( \pi^i \) and an equivalent class under \( \pi \) consists of trees \( T_j, T_{\pi(j)}, \ldots, T_{\pi^{i-1}(j)} \). Then the generating function for this equivalent class of trees is \( C_{\pi^i}(z^i) \).
Generating function

Suppose that $T$ is a $(k + 1)$-rooted tree fixed by $\pi$, if we remove the root of $T$, we get a multiset of $(k + 1)$-reduced black rooted trees fixed by $\pi$. By applying the lemma below, the generating function $C_\mu(z)$ for these multisets is

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

We denote by $\rho_n[u]$ the result of replacing each variable in the formal power series $u$ by its $n$-th power.

**Lemma**

*Let $g$ be an element of $G$. Then the sum of the weights of the elements of $M(S)$ fixed by $g$ is $\exp \left( \sum_{m=1}^{\infty} \frac{\rho_m[\text{fix}(g^m)]}{m} \right)$.*
Generating function for $k = 3$

\[
B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{14}(z)}{4!}
\]

\[
C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{13}(z)}{6}
\]

\[
E(z) = \frac{B_3^*(z)C_3(z)}{3} + \frac{B_{2,1}^*(z)C_{2,1}(z)}{2} + \frac{B_{13}^*(z)C_{13}(z)}{6}
\]

\[
U(z) = B(z) + C(z) - E(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{13}(z)}{6}
\]

\[
- x\left[\frac{1}{8}(C_{13}(z))^4 + \frac{1}{4}C_{13}(z^2)(C_{2,1}(z))^2 - \frac{1}{8}(C_{13}(z^2))^2 - \frac{1}{4}C_{13}(z^4)\right].
\]
Generating function for $k = 3$

\[ B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{1^4}(z)}{4!} \]

\[ C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{1^3}(z)}{6} \]

\[ E(z) = \frac{B^*_3(z)C_3(z)}{3} + \frac{B^*_{2,1}(z)C_{2,1}(z)}{2} + \frac{B^*_{1^3}(z)C_{1^3}(z)}{6} \]

\[ B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z^\lambda} \]
Generating function for $k = 3$

\[
B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{1^4}(z)}{4!}
\]

\[
C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{1^3}(z)}{6}
\]

\[
E(z) = \frac{B_{3^*}(z)C_3(z)}{3} + \frac{B_{2,1^*}(z)C_{2,1}(z)}{2} + \frac{B_{1^3}(z)C_{1^3}(z)}{6}
\]

\[
C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z_\mu}
\]
Generating function for $k = 3$

\[
B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{1,1,1,1}(z)}{4!}
\]

\[
C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{1,1,1}(z)}{6}
\]

\[
E(z) = \frac{B^*_3(z)C_3(z)}{3} + \frac{B^*_{2,1}(z)C_{2,1}(z)}{2} + \frac{B^*_{1,1,1}(z)C_{1,1,1}(z)}{6}
\]

\[
E(z) = \sum_{\mu \vdash k} \frac{B^*_\mu(z)C_\mu(z)}{z_\mu}
\]
Generating function for $k = 3$

\[
B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{14}(z)}{4!}
\]

\[
C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{13}(z)}{6}
\]

\[
E(z) = \frac{B_3^*(z)C_3(z)}{3} + \frac{B_{2,1}^*(z)C_{2,1}(z)}{2} + \frac{B_{13}^*(z)C_{13}(z)}{6}
\]

\[
B_4(z) = zC_{14}(z^4) = zC_{13}(z^4)
\]

\[
B_{3,1}(z) = zC_3(z)C_{13}(z^3)
\]

\[
B_{2,1,1}(z) = z(C_{2,1}(z))^2C_{13}(z^2)
\]

\[
B_{14}(z) = z(C_{14}(z))^4 = z(C_{13}(z))^4
\]

\[
B_\lambda(z) = z \prod_{i} C_{\lambda i}(z^i)
\]
Generating function for $k = 3$

$B(z) = \frac{B_4(z)}{4} + \frac{B_{3,1}(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1,1}(z)}{4} + \frac{B_{14}(z)}{4!}$

$C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{13}(z)}{6}$

$E(z) = \frac{B_3^*(z) C_3(z)}{3} + \frac{B_{2,1}^*(z) C_{2,1}(z)}{2} + \frac{B_{13}^*(z) C_{13}(z)}{6}$

$B_3^*(z) = zC_{13}(z^3)$

$B_{2,1}^*(z) = zC_{2,1}(z)C_{13}(z^2)$

$B_{13}^*(z) = z(C_{13}(z))^3$

$B_{\mu}^*(z) = z \prod_i C_{\mu i}(z^i)$
Generating function for \( k = 3 \)

\[
B(z) = \frac{B_4(z)}{4} + \frac{B_3(z)}{3} + \frac{B_{2,2}(z)}{8} + \frac{B_{2,1}(z)}{4} + \frac{B_{1^3}(z)}{4!}
\]

\[
C(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{1^3}(z)}{6}
\]

\[
E(z) = \frac{B_3^*(z)C_3(z)}{3} + \frac{B_{2,1}^*(z)C_{2,1}(z)}{2} + \frac{B_{1^3}^*(z)C_{1^3}(z)}{6}
\]

\[
U(z) = B(z) + C(z) - E(z) = \frac{C_3(z)}{3} + \frac{C_{2,1}(z)}{2} + \frac{C_{1^3}(z)}{6}
\]

\[
- x\left[\frac{1}{8}(C_{1^3}(z))^4 + \frac{1}{4}C_{1^3}(z^2)(C_{2,1}(z))^2\right]
\]

\[
- \frac{1}{8}(C_{1^3}(z^2))^2 - \frac{1}{4}C_{1^3}(z^4)].
\]
Asymptotic analysis

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

**Theorem**

The numbers of unlabeled $k$-trees are asymptotically given by

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

where $m(z) = z \exp \left[ k \sum_{m=2}^{\infty} B^*_{1k}(z^m)/m \right]$, $B^*_{1k}(z) = m(z)e^{kB^*_{1k}(z)}$ and $\rho_k$ is the unique real positive solution of $m(z) = (ek)^{-1}$. 
Asymptotic analysis

Sketch of the proof:

▷ Step 1: Let $\rho_k$ be the unique dominant singularity of $B_{1k}^*(z)$, then the dominant singularity $z = \rho_k$ of $B_{1k}^*(z)$ is of square root type.

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

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

The value of $\rho_k$ can be computed by following Otter’s work on 1-trees, cf. [Otter, 1948]. For $k = 2$, $\rho_2$ is already computed in [Fowler, Gessel, Labelle, Leroux, 2002] and turns out to be $\approx 0.177$. 
Asymptotic analysis

We will use $k = 3$ as an example to show the strategy of the proof. Step 1 of the proof:

From the generating functions

$$B_{\mu}^*(z) = z \prod_i C_{\mu_i}(z^i)$$

$$C_{\mu}(z) = \exp\left(\sum_{m=1}^{\infty} \frac{B_{\mu m}(z^m)}{m}\right)$$

we consider the case $\mu = (1^3)$, then

$$B_{13}^*(z) = z (C_{13}(z))^3 = z \exp(3 \sum_{m=1}^{\infty} \frac{B_{13}(z^m)}{m})$$

$$= \exp(3B_{13}^*(z)) z \exp(3 \sum_{m=2}^{\infty} \frac{B_{13}(z^m)}{m})$$

$$= m(z)$$
Step 1 of the proof:

and $B^*_1(z) = T(m(z))$ for some power series $T(z)$ that satisfies $T(z) = z \exp(3T(z))$. We denote by $W(z)$ the Cayley function given by $W(z) = z \exp(W(z))$. It follows that $T(z) = \frac{1}{3} W(3z)$. It is very well known $W(z)$ has radius of convergence $\rho = 1/e$ that it has a singular expansion of the form

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

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 $\eta > 0$. That implies $T(z)$ has corresponding properties, of course its radius of convergence equals $1/(3e)$ and $T(z)$ is analytic in $\Delta_{1/(3e)}(1/(3e) + \eta, \phi)$. 
Asymptotic analysis

Step 1 of the proof:

Since \( m(z) \) has radius of convergence \( \sqrt{\rho_3} > \rho_3 \) it follows that it is analytic at \( z = \rho_3 \). More precisely the singular expansion of \( B_{13}^*(z) \) close to \( z = \rho_3 \) comes from composing the singular expansion of \( T(z) \) at \( 1/(3e) \) with the analytic expansion of \( m(z) \) at \( \rho_3 \). In this context we also observe that \( m(\rho_3) = (3e)^{-1} \) and \( m'(\rho_3) > 1 \). According to this we get the local expansion

\[
B_{13}^*(z) = \frac{1}{3} - \frac{\sqrt{2}}{3} \left[ \frac{(\rho_3 - z)m'(\rho_3)}{m(\rho_3)} \right]^{1/2} + \frac{2}{9} \left[ \frac{(\rho_3 - z)m'(\rho_3)}{m(\rho_3)} \right] + O((\rho_3 - z)^{3/2}).
\]
Asymptotic analysis

Step 1 of the proof:

Henceforth $C_{13}(z) = z^{-1/3} B_{13}^*(z)^{1/3}$ has $z = \rho_3$ as dominant singularity of square root type, too, and a local expansion of the form

$$C_{13}(z) = (3\rho_3)^{-1/3} + a(\rho_3 - z)^{1/2} + b(\rho_3 - z) + c(\rho_3 - z)^{3/2} + O(\rho_3 - z)^2$$

where $a, b$ are given by

$$a = -\sqrt{2}(3\rho_3)^{2/3} \left[ \frac{m'(\rho_3)}{m(\rho_3)} \right]^{1/2}$$

$$b = 0.$$

Actually the functions $B_{13}^*(z) = B_{14}^*(z)$, $C_{13}(z) = C_{14}(z)$, and $B_{14}(z)$ have the same radius of convergence $\rho_3$. 
Asymptotic analysis

- Step 2 of the proof:

\[ B_3^*(z) = zC_{13}(z^3) \]
\[ B_{2,1}^*(z) = zC_{2,1}(z)C_{13}(z^2) \]
\[ B_{13}^*(z) = z(C_{13}(z))^3 \]

We only need to show \( B_{2,1}^*(z) \) is analytic at \( z = \rho_3 \). Let \( \tau_{2,1} \) be the unique dominant singularity of \( B_{2,1}^*(z) \). Since the number of black-rooted trees that are fixed by permutation of type \( \mu \) is less than or equal to those fixed by identity permutation, i.e., \([z^n]B_{(2,1)}^*(z) \leq [z^n]B_{13}^*(z)\) it follows that \( \tau_{(2,1)} \geq \rho_3 \). Therefore it remains to prove \( \tau_{(2,1)} \neq \rho_3 \).
Step 2 of the proof:

From the generating functions

\[
B_{(2,1)}^*(z) = zC_{(2,1)}(z)C_1^3(z^3)
\]

(1)

\[
C_{(2,1)}(z) = \exp(B_{(2,1)}^*(z)) \exp\left[ \sum_{m=2}^{\infty} \frac{B_{(2,1)}^*(z^m)}{m} \right]
\]

(2)

we have

\[
B_{(2,1)}^*(z) = zC_1^3(z^3) \exp(B_{(2,1)}^*(z)) \exp\left[ \sum_{m=2}^{\infty} \frac{B_{(2,1)}^*(z^m)}{m} \right].
\]
Asymptotic analysis

Step 2 of the proof:

By setting $B_{(2,1)}^*(z) = y$, it follows that $(\tau_{(2,1)}, B_{(2,1)}^*(\tau_{(2,1)}))$ is the unique solution of

$$M(z, y) = zC_{13}(z^3) \exp(y) \exp \left[ \sum_{m=2}^{\infty} \frac{B_{(2,1)}^*(z^m)}{m} \right] = y$$

$$M_y(z, y) = zC_{13}(z^3) \exp(y) \exp \left[ \sum_{m=2}^{\infty} \frac{B_{(2,1)}^*(z^m)}{m} \right] = 1,$$

and consequently $B_{(2,1)}^*(\tau_{(2,1)}) = 1$.

Recall that $B_{13}^*(\rho_3) = 1/3$, thus, we have $3B_{13}^*(\rho_3) = B_{(2,1)}^*(\tau_{(2,1)}) = 1$. If $\tau_{(2,1)} = \rho_3$, then $3B_{13}^*(\rho_3) > B_{(2,1)}^*(\rho_3) = 1$, which contradicts the relation $3B_{13}^*(\rho_3) = 1$. Therefore we can conclude that $\rho_3 < \tau_{(2,1)}$ and therefore $C_{(2,1)}(z)$ also has dominant singularity $\tau_{(2,1)}$. 
Asymptotic analysis

Step 3 of the proof:

Summing up, since $B_{14}(z) = zC_{13}(z)^4$ has a square-root singularity at $z = \rho_3$ and $B_\lambda$ for any $\lambda \neq (1^4)$ is analytic at $\rho_3$, the dominant term in the singular expansion of $U(z)$ comes from

$$\frac{B_{14}(z)}{z_{14}} + \frac{C_{13}(z)}{z_{13}} - \frac{C_{13}(z)B_{13}^*(z)}{z_{13}} = -\frac{zC_{13}(z)^4}{8} + \frac{C_{13}(z)}{6}.$$

All the other terms are all analytic at $z = \rho_3$. Together with the singular expansion of $C_{13}(z)$, we can derive the singular expansion of $U(z)$ at $z = \rho_3$:

$$U(z) = U(\rho_k) + \frac{2\sqrt{2}}{9} \frac{(3\rho_3)^{-\frac{1}{3}}}{27} \left[ \frac{(\rho_3 - z)m'(\rho_3)}{m(\rho_3)} \right]^{3/2} + c_1(\rho_3 - z) + c_2(\rho_3 - z)^2 + O((\rho_3 - z)^{5/2}).$$
Asymptotic analysis

Compute the value of \( \rho_k \) for specific \( k \)

Let \( T_n = [z^n]B_{1,k}^*(z) \) and \( m_n = [z^n]m(z) \). Then by taking the derivative of equations

\[
B_{1,k}^*(z) = z \exp \left[ k \sum_{m=1}^{\infty} \frac{B_{1,k}^*(z^m)}{m} \right], \quad m(z) = z \exp \left[ k \sum_{m=2}^{\infty} \frac{B_{1,k}^*(z^m)}{m} \right],
\]

and equating the coefficients, we get the recurrences for \( T_n \) and \( m_n \),

\[
T_n = k \sum_{i=1}^{n-1} \sum_{m \mid i} T_{n-i} m T_m \quad \text{for } n > 1 \text{ and } T_1 = 1.
\]

\[
m_n = k \sum_{i=2}^{n-1} \sum_{m \mid i, m \neq i} m_n-i m T_m \quad \text{for } n > 2 \text{ and } m_1 = 1, m_2 = 0.
\]

Then the value of \( \rho_k \) is obtained by solving numerically the equation

\( m(z) = 1/(ek) \) where \( m(z) \approx \sum_{i \leq 20} m_i z^i \).
Leaves of unlabeled k-trees

We call a black node a *leaf* if only one of its colored neighbor connects with other black nodes. In the sequel we shall weight each black node by $z$ and each leaf by $w$. 
Leaves of unlabeled k-trees

We call a black node a leaf if only one of its colored neighbor 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 unlabeled color-orbits of unlabeled $k$-coding trees, then we have:

Theorem

Let $X_n$ be the random variable associated with the number of leaves of $k$-coding trees, that is $\mathbb{P}(X_n = r) = \frac{[z^n w^r] U(z, w)}{[z^n] U(z, 1)}$. Then there exists positive constants $\mu$ and $\sigma^2$ such that $\mathbb{E}(X_n) = \mu n + O(1)$ and $\mathbb{V}ar(X_n) = \sigma^2 n + O(1)$. Furthermore $X_n$ satisfies a central limit theorem of type $\frac{X_n - \mathbb{E}(X_n)}{\sqrt{\mathbb{V}ar(X_n)}} \rightarrow N(0, 1)$. 
Asymptotic analysis

Leaves of unlabeled k-trees

Sketch of the proof:

- Step 1: By replacing the weight $z$ of each leaf by $zw$, we first obtain the generating function $U(z,w)$.

- Step 2: Study the expansion of $B_{1k}^*(z,w)$ for $|w - 1| \leq \varepsilon$, $|z - \rho_k(w)| < \varepsilon$, $\arg(z - \rho_k(w)) > \phi$ (for some $\phi \in (0,\pi/2)$) and $\varepsilon$, $\varepsilon$ are sufficiently small.

- Step 3: For $m \geq 2$ and $\mu \neq (1^k)$, $C_\mu(z,w)$, $B_{1k}^*(z,w)$, $C_{1k}(z^m,w^m)$ and $B_{1k}^*(z^m,w^m)$ are analytic if $(z,w)$ is close to $(\rho_k,1)$.

- Step 4: Expand $U(z,w)$ locally around $z = \rho_k(w)$ and prove the coefficient for $\left(1 - \frac{z}{\rho_k(w)}\right)^{1/2}$ is zero at $(\rho_k(w),w)$, but the coefficient for $\left(1 - \frac{z}{\rho_k(w)}\right)^{3/2}$ is not zero at $(\rho_k(w),w)$. 
Asymptotic analysis

The degree distribution of unlabeled k-trees

Clearly every black node in the $k$-coding tree has degree $k + 1$. So we concentrate on the degree distribution of colored nodes. Formally the variable $x$ (instead of $z$) takes care of the number of colored nodes. In this way, we have $U(x) = B(x) + C(x) - E(x)$ where

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

$$C(x) = \sum_{\mu \vdash k} \frac{C_\mu(x)}{z_\mu} \quad B_\mu^*(x) = \prod_i C_{\mu_i}(x^i)$$

$$E(x) = \sum_{\mu \vdash k} \frac{B_\mu^*(x) C_\mu(x)}{z_\mu} \quad C_\mu(x) = x \exp \left[ \sum_{m=1}^{\infty} \frac{B_\mu^m(x^m)}{m} \right].$$

The dominant singularity of $U(x)$ is also $\rho_k$. 
Asymptotic analysis

The degree distribution of unlabeled k-trees

Now we give each colored node of degree $d_i$ with weight $u_i$. Let $u = (u_1, \ldots, u_M)$, $m = (m_1, \ldots, m_M)$ where $m_i \geq 0$ and $d = (d_1, \ldots, d_M)$ where $d_i > 0$, then the coefficient of $x^n u^m$ in the generating function $U^{(d)}(x, u)$ is the number of of unlabeled $k$-trees that there are $m_i$ colored nodes out of $n$ total colored nodes having degree $d_i$. 
Asymptotic analysis

The degree distribution of unlabeled k-trees

**Theorem**

Let $Y_{n,d} = (Y_{n,d_1}, \ldots, Y_{n,d_M})$ be the random vector of the number of colored nodes in an unlabeled k-tree that have degrees $(d_1, \ldots, d_M)$, that is, $\mathbb{P}(Y_{n,d} = m) = \frac{[x^n u^m] U^{(d)}(x,u)}{[x^n] U^{(d)}(x,1)}$. Then there exists an $M$-dimensional vector $\mu$ and an $M \times M$ positive semidefinite matrix $\Sigma$ such that $\mathbb{E}(Y_{n,d}) = \mu n + O(1)$ and $\text{Cov}(Y_{n,d}) = \Sigma n + O(1)$.

Furthermore $Y_{n,d}$ satisfies a central limit theorem of the form

$$\frac{Y_{n,d} - \mathbb{E}(Y_{n,d})}{\sqrt{n}} \rightarrow \mathcal{N}(0,\Sigma).$$
The degree distribution of unlabeled k-trees

Let $C^{(d)}(x,u)$ (resp. $B^{(d)}(x,u)$, $E^{(d)}(x,u)$) be the generating function for color-orbits of $\circ$-rooted (resp. $\bullet$-rooted, $\circ\bullet$-rooted) trees that has each colored node of degree $d_i$ weighted by $u_i$. Let $P^{(d)}(x,u)$ be the generating function for the trees whose root is only connected with the root of a color-orbit of colored node-rooted tree, so that $C^{(d)}(x,1) = P^{(d)}(x,1)$. Here we introduce $P^{(d)}(x,u)$ to distinguish the case that the colored root has degree $d_i$ for some $1 \leq i \leq M$. 
Asymptotic analysis

The degree distribution of unlabeled k-trees

Let $Z(\mathcal{G}_p, B^{*,(d)}_\mu(x,u))$ represent the generating function of a forest consisting of $p$ reduced black-rooted trees counted by $B^{*,(d)}_\mu(x,u)$:

$$Z(\mathcal{G}_p, B^{*,(d)}_\mu(x,u)) = Z(\mathcal{G}_p, B^{*,(d)}_\mu(x,u), B^{*,(d)}_{\mu^2}(x^2,u^2), \ldots, B^{*,(d)}_{\mu^p}(x^p,u^p))$$

$$= \sum_{\lambda \vdash p} \frac{1}{Z_\lambda} B^{*,(d)}_{\mu}(x,u)^{\lambda_1} B^{*,(d)}_{\mu^2}(x^2,u^2)^{\lambda_2} \cdots B^{*,(d)}_{\mu^p}(x^p,u^p)^{\lambda_p}$$

where $\lambda = (1^{\lambda_1} \cdots p^{\lambda_p})$. 
Asymptotic analysis

**The degree distribution of unlabeled k-trees**

The generating function $U(x,u)$ for unlabeled $k$-trees with colored nodes of degree $d$ is given by

$$U^{(d)}(x,u) = B^{(d)}(x,u) + C^{(d)}(x,u) - E^{(d)}(x,u)$$

where

$$B^{(d)}(x,u) = \sum_{\lambda \vdash k+1} \frac{B^{(d)}_{\lambda}(x,u)}{z_{\lambda}}, \quad C^{(d)}(x,u) = \sum_{\mu \vdash k} \frac{C^{(d)}_{\mu}(x,u)}{z_{\mu}}$$

$$E^{(d)}(x,u) = \sum_{\mu \vdash k} \frac{B^{*,(d)}_{\mu}(x,u) P^{(d)}_{\mu}(x,u)}{z_{\mu}}$$

$$B^{(d)}_{\lambda}(x,u) = \prod_{i} P^{(d)}_{\lambda^i}(x^i,u^i), \quad B^{*,(d)}_{\mu}(x,u) = \prod_{i} P^{(d)}_{\mu^i}(x^i,u^i)$$
Asymptotic analysis

The degree distribution of unlabeled k-trees

The generating function $U(x,u)$ for unlabeled $k$-trees with colored nodes of degree $d$ is given by

$$U^{(d)}(x,u) = B^{(d)}(x,u) + C^{(d)}(x,u) - E^{(d)}(x,u)$$

where

$$C^{(d)}_{\mu}(x,u) = x \exp \left[ \sum_{m=1}^{\infty} \frac{B^{*,(d)}_{\mu m}(x^m,u^m)}{m} \right]$$

$$+ \sum_{j=1}^{M} x(u_j - 1) Z(\mathcal{G}_{d_j}, B^{*,(d)}_{\mu}(x,u))$$

$$P^{(d)}_{\mu}(x,u) = x \exp \left[ \sum_{m=1}^{\infty} \frac{B^{*,(d)}_{\mu m}(x^m,u^m)}{m} \right]$$

$$+ \sum_{j=1}^{M} x(u_j - 1) Z(\mathcal{G}_{d_j-1}, B^{*,(d)}_{\mu}(x,u))$$
The degree distribution of unlabeled $k$-trees

The dominant singularity for $B_{1k}^*(x,1)$ is $\rho_k$. As before, for $\mu \neq (1^k)$, $B_\mu^*(x,u)$ and for $m \geq 2$, $B_{1k}^*(x^m,u^m)$ are analytic if $(x,u)$ is close to $(\rho_k,1)$. Next we consider

$$S(x,y,u) = \left( xe^y \exp \left( \sum_{m=2}^{\infty} \frac{B_{1k}^*(d,m,x^m,u^m)}{m} \right) \right)^k$$

$$+ \sum_{j=1}^{M} x(u_j - 1) Z(G_{d_j-1},y,B_{1k}^*(d,x^{d_j-1},u^{d_j-1})), \cdots , B_{1k}^*(d,x^{d_j-1},u^{d_j-1}))^k.$$ 

Since $S(0,y,u) \equiv 0$, $S(x,0,u) \not\equiv 0$ and all coefficients of $S(x,y,1)$ are real and positive, then $y(x,u) = B_{1k}^*(d,x,u)$ is the unique solution of the functional equation $S(x,y,u) = y$. 
The degree distribution of unlabeled k-trees

Furthermore, \((x, y) = (\rho_k, 1/k)\) is the only solution of \(S(x, y, 1) = 0\) and \(S_y(x, y, 1) = 1\) with \(S_x(\rho_k, 1/k, 1) \neq 0, S_{yy}(\rho_k, 1/k, 1) \neq 0\). Consequently, \(B_{1k}^*(d)(x,u)\) can be represented as

\[
B_{1k}^*(d)(x,u) = g(x,u) - h(x,u) \left[ 1 - \frac{x}{\rho_k(u)} \right]^{1/2} \tag{3}
\]

which holds locally around \((x,u) = (\rho_k,1)\) and \(h(\rho_k(u),u) \neq 0\). In view of \(B_{1k}^*(d)(x,u) = P_{1k}^{(d)}(x,u)^k\), \(P_{1k}^{(d)}(x,u)\) also has expansion of square root type, i.e.,

\[
P_{1k}^{(d)}(x,u) = s(x,u) - t(x,u) \left[ 1 - \frac{x}{\rho_k(u)} \right]^{1/2} \tag{4}
\]

where \(t(\rho_k(u),u) \neq 0\).
Asymptotic analysis

The degree distribution of unlabeled k-trees

Based on the equation

\[ C^{(d)}_{\mu}(x,u) - P^{(d)}_{\mu}(x,u) \]

\[ = \sum_{j=1}^{M} x(u_j - 1) \left[ Z(\mathcal{G}_{d_j}, B_{\mu}^{(d)}(x,u)) - Z(\mathcal{G}_{d_j-1}, B_{\mu}^{(d)}(x,u)) \right], \]

we shall next compute the dominant term in the singular expansion of \( U(x,u) \). For simplicity we will omit variables \((x,u)\) and degree \(d\).

\[ U(x,u) = -\frac{kP_{1k}^{k+1}}{(k+1)!} + \frac{P_{1k}}{k!} \]

\[ + \frac{1}{k!} \sum_{j=1}^{M} x(u_j - 1) \left[ Z(\mathcal{G}_{d_j}, B_{1k}^{(d)}) - Z(\mathcal{G}_{d_j-1}, B_{1k}^{(d)}) \right] + M_1, \]
Asymptotic analysis

The degree distribution of unlabeled k-trees

where $M_1$ is an analytic function around $(x,u) = (\rho_k,1)$. It is now convenient to write $U(x,u) = f(x,u) + h_1(x,u) \left[ 1 - \frac{x}{\rho_k(u)} \right]^{1/2}$. Then by substituting $P_{1k}, B_{1k}^*$ with its representation in eq. (4) and eq. (3), we obtain

$$h_1(x,u) = \frac{s^k t}{(k-1)!} - \frac{t}{k!} + \frac{h}{k!} \sum_{j=1}^{M} x(u_j - 1)$$

$$\times \left[ Z'(\mathcal{G}_{d_j-1},g,X_2,\cdots,X_{d_j-1}) - Z'(\mathcal{G}_{d_j},g,X_2,\cdots,X_{d_j}) \right]$$

where $X_i$ are analytic functions around $(x,u) = (\rho_k,1)$ and $Z'$ is the derivative w.r.t. the first variable of $Z(\mathcal{G}_k,x_1,\cdots,x_k)$, namely $Z'(\mathcal{G}_k,x_1,\cdots,x_k) = Z(\mathcal{G}_{k-1},x_1,\cdots,x_{k-1})$. 
Asymptotic analysis

The degree distribution of unlabeled k-trees

Furthermore, by replacing $s, t$ by $g = s^k$ and $h = ks^{k-1}t$, we can further simplify $h_1(x,u)$, that is

$$h_1(x,u) = \frac{h}{k!} g - \frac{1}{k} + \frac{h}{k!} \sum_{j=1}^M x(u_j - 1)$$

$$\times \left[ Z'(S_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) - Z'(S_{d_j}, g, X_2, \cdots, X_{d_j}) \right].$$

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

$$g(\rho_k(u),u) = \frac{1}{k} + g(\rho_k(u),u) \frac{k-1}{k} \sum_{j=1}^M x(u_j - 1)$$

$$\times \left[ Z(S_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) - Z'(S_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) \right]$$
Asymptotic analysis

The degree distribution of unlabeled k-trees

and consequently \( h(ρ_k(u), u) \equiv 0 \) and \( U(x, u) \) has a local expansion around \((x, u) = (ρ_k, 1)\) of the form

\[
U(x, u) = w(x, u) + r(x, u) \left[ 1 - \frac{x}{ρ_k(u)} \right]^{3/2}.
\] (5)

where \( r(ρ_k(u), u) \neq 0 \) since \( r(ρ_k, 1) = r \neq 0 \) and \( w, r \) are analytic function around \((x, u) = (ρ_k, 1)\). Thus a central limit theorem follows. More precisely by setting \( A(u) = \log ρ_k(1) - \log ρ_k(u) \), \( μ = (A_{u_j}(1))_{1 ≤ j ≤ M} \) and \( Σ = (A_{u_i u_j}(1) + δ_{i,j} A_{u_j}(1))_{1 ≤ j ≤ M} \) then

\[
E(Y_{n,d}) = μ n + O(1) \text{ and } Cov(Y_{n,d}) = Σ n + O(1).
\]
Thanks for your attention!