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ENUMERATION OF SYMMETRIES
IN
LOCALLY-RESTRICTED TREES

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ABSTRACT

ENUMERATION OF SYMMETRIES IN LOCALLY-RESTRICTED TREES

By

Kathleen A. McKeon

In this thesis, symmetries are enumerated in unlabeled trees with certain restrictions on their degrees. The vertices of a d-tree have degree at most d. The vertices of a (1,d)-tree have degree 1 or d. Trees of these types give rise to significant examples in polymer chemistry. For example, (1,4)-trees represent the alkanes and 4-trees represent the carbon skeletons of alkanes.

A two-variable generating function is used to determine both exact and asymptotic formulas for the number of symmetries in d-trees and (1,d)-trees for d = 3,4. Tables containing the exact and asymptotic number of symmetries are provided for all four types of trees.

To my parents for their love and support, my love and thanks.

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INTRODUCTION

The enumeration of trees is an important problem in graph theory with a distinguished history as well as applications to theoretical chemistry. The first major work in this area was performed by Cayley who determined exact formulas for the number of labeled trees [C89], the number of rooted trees [C57] and the number of free trees [C75,C81]. These results were extended and an asymptotic analysis of the numbers was provided by Pólya [P37] and Otter [O48]. In this thesis, both exact and asymptotic formulas are determined for the number of symmetries in unlabeled trees with certain restrictions on their degrees.

The definitions and notation used in this thesis follow those of Palmer [Pa85] and are given below.

A *graph G* consists of a finite nonempty set V of *vertices* and a set E of *edges* which are unordered pairs of distinct vertices. The cardinality of V is called the *order of G* while the cardinality of E is called the *size of G*. An edge e joining the vertices u and v is denoted by uv and the vertices u and v are said to be *adjacent*. The *degree* of a vertex v is the number of vertices adjacent to v. An *end-vertex* has degree one.

A *walk* in a graph G is a sequence of vertices $w_1, w_2, \ldots, w_m$ such that w_i is adjacent to w_{i+1} for $i = 1$ to $m - 1$. A *path* is a walk in which no vertices are repeated. The *length* of a path is the number of edges used. The *distance* between a pair of vertices u and v is the length of the shortest u - v path. A *cycle* is a walk with at least 3 different vertices that has no repeated vertices except the first and last. A graph is *connnected* if every pair of vertices is joined by a path.

A *tree* is a connected,acyclic graph. A *rooted tree* has one vertex, called the *root*, distinguished from the others. Similarly, an *edge-rooted tree* has one edge, called the *root edge*, distinguished from the others. A *planted tree* is a rooted tree in which the root has degree one. An unrooted tree is also called a *free tree*. In a *d-tree*, all vertices have degree at most d. In a *(1,d)-tree*, the vertices have degree 1 or d.

The *eccentricity* of a vertex *v* is the distance to a vertex farthest from *v*. The *center* of a graph consists of all vertices of minimum eccentricity. The center of a tree contains either one or two vertices.

The *complete graph* of order *n*, denoted K_n, has all possible edges present. The complete graph on two vertices, K_2, consists of two vertices which are joined by an edge.

Two graphs G_1 and G_2 are *isomorphic* if there is a one-to-one function ϕ from the vertex set of G_1 onto the vertex set of G_2 such that for any two vertices u and v of G_1 we have u and v adjacent in G_1 if and only if $\phi(u)$ and $\phi(v)$ are adjacent in G_2. The function ϕ is called an *isomorphism* and is said to *preserve adjacency*. In unlabeled graph enumeration, isomorphic graphs are considered equivalent and are counted as one graph.

An isomorphism from a graph G to itself is an *automorphism* or *symmetry of G*. The set of automorphisms of G forms a permutation group denoted by $\Gamma(G)$ and is called the *automorphism* or *symmetry group of G*. An automorphism of a rooted tree must leave the rooted fixed and an automorphism of an edge-rooted tree must leave the vertices of the root edge fixed.

Cayley's work [C75] was motivated by the problem of enumerating isomers of alkanes, compounds of carbon and hydrogen atoms which have valencies of 4 and 1 respectively. The alkanes have the general formula C_kH_{2k+2} and can be represented by (1,4)-trees. They are the best documented family of chemical compounds and provide a model for much of chemical theory [GoK73].

Generalizing (1,4)-trees, we have (1,d)-trees which give rise to other meaningful examples in polymer chemistry. There is a correspondence between (1,d)-trees and d-trees that also has chemical significance. While 4-trees correspond to the carbon skeletons of alkanes [GoK73], d-trees in general correspond to skeleton polymers, i.e., polymer molecules that have been stripped of their reactive end-groups [GoT76].

The problem addressed in this thesis, the enumeration of symmetries in (1,d)-trees and d-trees for d = 3,4, is also motivated by chemistry. In the study of collections of molecular species, it is almost always the average of some property over an appropriate class of trees that is required. In computing such an average, it is necessary to assign weights to the various trees in the class so as to reflect the (not usually equal) proportions in which they are formed by the chemical process involved. The proper assignment of weights to the trees often involves the orders of their automorphism groups [GoL75]. Consequently, chemists are interested in the orders of the automorphism groups of large trees of various species such as (1,d)-trees and d-trees.

The tool used to do the counting is a two-variable logarithmic generating function, an approach that seems to have originated in the work of Etherington [Et38]. For a given class C of trees, let t(x,y) be the generating function in the two variables x and y such that the coefficient of $y^m x^n$ is the number of trees T in C of order n in which m is the logarithm base 2 of the order of the automorphism group of T. In t(x,2), the coefficent of x^n is the sum of the orders of the automorphism groups of all such trees.

The technique used to do the counting was developed by Pólya in [P37], perfected by Otter [O48] and described as a twenty step algorithm for counting various types of trees by Harary, Robinson and Schwenk [HRS75]. The generating functions t(x,y) and t(x,2) satisfy functional equations from which recurrence relations for their coefficients are determined. By applying an adaption of the twenty-step algorithm and treating t(x,2) as an analytic function, the asymptotic behavior of these coefficients is determined.

CHAPTER I

ENUMERATION OF SYMMETRIES

1.1 Generating Functions

Symmetries are enumerated in four types of trees : d-trees and (1,d)-trees for d = 3,4. Throughout this thesis the type of tree will be specified only when the statement being made does not appy to all four types.

For the planted trees of each type, a two-variable logarithmic generating function is defined as follows:

$$(1.1.1) \qquad T(x,y) = \sum_{n=1}^{\infty} \sum_{m} T_{m,n} y^m x^n.$$

For d-trees, $T_{m,n}$ is the number of planted trees T of order n + 1 in which $m = \log_2|\Gamma(T)|$. Every (1,3)-tree, planted or free, has an even number of vertices and the order of a (1,4)-tree, planted or free, is equal to 2 modulo 3. This is taken into account in the definition of T(x,y) for (1,d)-trees. For (1,3)-trees, $T_{m,n}$ counts planted trees on 2n vertices with 2^m symmetries while for (1,4)-trees $T_{m,n}$ counts planted trees on 3n - 1 vertices with 2^m symmetries.

The values which m may assume in the sum (1.1.1) depend on both d and the type of tree. Since an automorphism of a rooted tree must leave the root fixed, the order of the automorphism group of a planted (1,3)-tree or 3-tree is of the form 2^m where m is an integer. In the case of (1,3)-trees, m ranges from 0 to n - 1. In 3-trees, m ranges from 0 to (n - 1)/2. Similarly, the order of the automorphism group of a planted (1,4)-tree or 4-tree has the form $2^i(3!)^j$. Thus in these two types of trees, m corresponds to an ordered pair of integers (i,j). The ranges of i and j are as follows. For (1,4)-trees, $0 \le i \le n-2$ and $0 \le j \le n-1-i$ while $0 \le i \le (n-1)/2$ and $0 \le j \le (n-1-2i)/3$ for 4-trees.

Note that when y = 1 is substituted in (1.1.1), T(x,1) counts planted trees of the specified type. Substituting y = 2 in (1.1.1) results in a one-variable generating function which counts symmetries in planted trees of the specified type. Define

(1.1.2) $$S_n = \sum_m T_{m,n} 2^m$$

and

(1.1.3) $$T(x,2) = \sum_{n=1}^{\infty} S_n x^n.$$

Then for (1,3)-trees, for example, S_n is the total number of symmetries in all planted (1,3)-trees on 2n vertices.

Similarly, t(x,y) can be defined for free trees. However, we actually only work with t(x,2). Thus, we define

$$t(x,2) = \sum_{n=1}^{\infty} s_n x^n \tag{1.1.4}$$

which counts symmetries in free, i.e., unrooted, trees. For d-trees, s_n is the number of symmetries in all such trees on n vertices. For (1,d)-trees, the relationship between n and the number of vertices is the same as in T(x,y).

1.2 Functional Relations

To obtain formulas for the number of symmetries in these trees, functional relations satisfied by T(x,y), T(x,2) and t(x,2) are now derived.

First observe that rooted and planted trees of a specified type can be formed from planted trees of that type. A rooted tree in which the root has degree k is formed by taking a collection of k planted trees and identifying their roots to form the root of the new tree. Adding a new vertex adjacent to the root of this rooted tree results in a planted tree in which the degree of the vertex adjacent to the root is k + 1. Based on this observation, relations expressing T(x,y) in terms of T(x,y), $T(x^2,y^2)$ and $T(x^3,y^3)$ are derived.

<u>Theorem 1.2.1</u> The generating functions T(x,y) and T(x,2) which count symmetries in planted (1,3)-trees satisfy

$$T(x,y) = x + \frac{1}{2} T(x,y)^2 + (y - \frac{1}{2}) T(x^2,y^2) \tag{1.2.1}$$

and

$$T(x,2) = x + \frac{1}{2} T(x,2)^2 + \frac{3}{2} T(x^2,4). \tag{1.2.2}$$

Proof: The vertex adjacent to the root of a planted (1,3)-tree has degree 1 or 3. The term x counts the symmetries in a planted K_2, the only planted (1,3)-tree in which the vertex adjacent to the root has degree 1.

To count symmetries in those trees in which the vertex adjacent to the root has degree 3, two cases must be considered. Suppose T is the planted (1,3)-tree formed from the planted (1,3)-trees T_1 and T_2 in the manner described above. If $T_1 \neq T_2$, then we have $|\Gamma(T)| = |\Gamma(T_1)|\,|\Gamma(T_2)|$. Then $1/2(T(x,y)^2 - T(x^2,y^2))$ counts symmetries in this case. If $T_1 = T_2$, then we have $|\Gamma(T)| = 2|\Gamma(T_1)|^2$. This case is handled by $yT(x^2,y^2)$ with the factor of y accounting for the additional factor of 2 in the group order. Now (1.2.2) is obtained by substituting $y = 2$ in (1.2.1). //

The same techinique is used to derive the following functional relations which are satisfied by T(x,y) and T(x,2) for d-trees and (1,4)-trees.

Theorem 1.2.2 The generating functions T(x,y) and T(x,2) which count symmetries in planted 3-trees satisfy

(1.2.3) $$T(x,y) = x + \frac{x}{2}\, T(x,y)^2 + x\, T(x,y) + x\,(y - \frac{1}{2})T(x^2,y^2)$$

and

(1.2.4) $$T(x,2) = x + \frac{x}{2}\, T(x,2)^2 + xT(x,2) + \frac{3x}{2}\, T(x^2,4).$$

<u>Theorem 1.2.3</u> The generating functions T(x,y) and T(x,2) which count symmetries in planted (1,4)-trees satisfy

(1.2.5) $$T(x,y) = x + \frac{1}{6x}\, T(x,y)^3 + \frac{1}{x}\,(y - \frac{1}{2})\, T(x^2,y^2)\, T(x,y) + \frac{1}{x}\,(y^{\log_2 3!} - y + \frac{1}{3})\, T(x^3,y^3)$$

and

(1.2.6) $$T(x,2) = x + \frac{1}{6x}\, T(x,2)^3 + \frac{3}{2x}\, T(x^2,4)T(x,2) + \frac{13}{3x}\, T(x^3,8).$$

<u>Theorem 1.2.4</u> The generating functions T(x,y) and T(x,2) which count symmetries in planted 4-trees satisfy

(1.2.7) $$T(x,y) = x + \frac{x}{6}\, T(x,y)^3 + \frac{x}{2}\, T(x,y)^2 + x\,(y - \frac{1}{2})\, T(x^2,y^2) + x\,(1 + (y - \frac{1}{2})\, T(x^2,y^2)\,)\, T(x,y) + x\,(y^{\log_2 3!} - y + \frac{1}{3})\, T(x^3,y^3)$$

and

$$T(x,2) = x + \frac{x}{6}\,T(x,2)^3 + \frac{x}{2}\,T(x,2)^2 + \frac{3x}{2}T(x^2,4) + x\,(1 + \frac{3}{2}T(x^2,4))\;T(x,2) + \frac{13x}{3}T(x^3,8). \tag{1.2.8}$$

Using the following lemma which relates the order of the automorphism group of a free tree to the orders of the automorphism groups of the vertex and edge-rooted versions of the tree, t(x,2) is expressed in terms of T(x,2), $T(x^2,4)$, $T(x^3,8)$ and $T(x^4,16)$.

Lemma 1.2.5 For any tree T,

$$|\Gamma(T)| = \sum_{T_1} |\Gamma(T_1)| \; - \sum_{T_2} |\Gamma(T_2)| + |\Gamma(T_3)| \tag{1.2.9}$$

where the first sum is taken over all different vertex-rooted versions T_1 of T and the second sum is taken over all different edge-rooted versions T_2 of T. If T has a symmetry edge, an edge whose vertices are interchanged by some automorphism of T, then $T_3 = T$. If T does not have a symmetry edge, then T_3 is the empty graph and $|\Gamma(T_3)| = 0$.

Proof: Let $n^*(T)$ be the number of different ways to root T at a vertex, i.e., the number of orbits of the vertices as determined by the automorphism group of T and let $q^*(T)$ be the number of different ways to root T at an edge. Let s(T) be the number of symmetry edges in T. Note that since T is a tree, s(T) is 0 or 1.

Lemma 1.2.5 is a variation of a lemma due to Otter [O48]:

For any tree T,

$$(1.2.10) \qquad 1 = n^*(T) - q^*(T) + s(T) .$$

As in the proof of (1.2.10), the vertex and edge-rooted versions of T can be paired up such that the paired vertex and edge-rooted versions of T have the same automorphism group. Recall that an automorphism of a rooted graph must leave the root fixed while an automorphism of an edge-rooted graph must leave the vertices of the root edge fixed. For each vertex v that is not in the center of T, match the version of T that is rooted at the vertex v with the edge-rooted version that is rooted at the first edge on the path from v to the center of T.

If T has a symmetry edge, the center of T consists of two vertices, u and v. Since the edge uv is a symmetry edge, rooting T at v is equivalent to rooting T at u. Hence if the version of T that is rooted at the vertex v is paired with the version of T that is rooted at the edge uv, then the difference of the two sums in (1.2.9) is 0 and $T_3 = T$. Thus, (1.2.9) holds in this case.

If T does not have a symmetry edge two cases must be considered. If the center of T consist of two vertices u and v, match the version of T that is rooted at the vertex v with the version of T that is rooted at the edge uv. In this case and the case that the center of T consist of just one vertex u, there is one vertex-rooted version of T that cannot be paired with an edge-rooted version. This is the tree that results from rooting T at the vertex u which is in the center of T. Since T does not have a symmetry edge, the vertices in the center of T are all fixed points of the automorphisms of the unrooted tree T. Hence this extra vertex-rooted version of T has the same automorphism group as T and (1.2.9) holds in this case also. //

This lemma can be extended to a statement about the generating functions that count symmetries by multiplying (1.2.9) by x^n and summing over all trees of the appropriate order. Summing the result over all $n \geq 1$ gives $t(x,2)$ on the left side. The first sum on the right side gives the series that counts symmetries in rooted trees and the second sum gives the series that counts symmmetries in edge-rooted trees while $|\Gamma(T_3)|x^n$ sums to the series that counts symmetries in trees with a symmetry edge.

The equations satisfied by $t(x,y)$ can now be stated.

<u>Theorem 1.2.6</u> The generating function $t(x,2)$ for symmetries in free (1,3)-trees is given by

$$t(x,2) = \frac{1}{2x} T(x,2)^2 - \frac{1}{3x} T(x,2)^3 + \frac{3}{2x} T(x^2,4) + \frac{13}{3x} T(x^3,8). \tag{1.2.11}$$

<u>Proof</u>: First we determine an expression for the series that counts symmtries in rooted trees. As previously described, this expression can be found by using planted (1,3)-trees to build rooted

(1,3)-trees. The series for rooted (1,3)-trees is equal to

$$(1.2.12)\qquad T(x,2) + \frac{3!}{x} T(x^3,8) + \left[\frac{2}{x} (T(x^2,4)\ T(x,2) - T(x^3,8))\right]$$

$$+ \left[\frac{1}{3!\ x} (T(x,2)^3 - 3\ T(x^2,4)\ T(x,2) + 2\ T(x^3,8))\right].$$

Symmetries in rooted (1,3)-trees in which the root has degree 1, i.e., in planted (1,3)-trees, are counted by T(x,2). To count symmetries in rooted (1,3)-trees in which the root has degree 3, three cases must be considered. Suppose T is the rooted tree formed from the planted (1,3)-trees T_1, T_2 and T_3. The second term of (1.2.12) counts symmetries in the case that all three trees are the same. The case that exactly two of the three trees are the same and the case that all three are different are handled by the first and second bracketed terms of (1.2.12) respectively.

A tree rooted at an edge can be formed by identifying the edges incident to the roots of two planted trees. That edge is the root edge of the edge-rooted tree. When the two trees which are combined are the same, that edge is a symmetry edge. Thus,

$$(1.2.13)\qquad \frac{1}{2x} (T(x,2)^2 + T(x^2,4))$$

counts symmetries in edge-rooted (1,3)-trees and

(1.2.14) $$\frac{2}{x}\, T(x^2,4)$$

counts symmetries in (1,3)-trees that have a symmetry edge. Combining (1.2.12),(1.2.13) and (1.2.14) as in lemma 1.2.5 and using the functional relation (1.2.2) to simplify gives equation (1.2.11).//

The following theorems give the functional equations satisfied by t(x,2) for d-trees and (1,4)-trees.

Theorem 1.2.7 The generating function t(x,2) for symmetries in free 3-trees is given by

(1.2.15) $$t(x,2) = T(x,2) + \frac{x}{6}\, T(x,2)^3 + \frac{3x}{2}\, T(x^2,4)\ T(x,2) + \frac{3}{2} T(x^2,4) + \frac{13x}{3}\, T(x^3,8) - \frac{1}{2}\, T(x,2)^2.$$

Theorem 1.2.8 The generating function t(x,2) for symmetries in free (1,4)-trees is given by

(1.2.16) $$t(x,2) = T(x,2) + \frac{3}{2x}\, T(x^2,4) - \frac{1}{2x}\, T(x,2)^2 + \frac{1}{24\, x^2}\, T(x,2)^4 + \frac{3}{4\, x^2}\, T(x^2,4)\ T(x,2)^2 + \frac{9}{8x^2}\, T(x^2,4)^2 + \frac{71}{4x^2}\, T(x^4,16) + \frac{13}{3x^2}\, T(x^3,8)\ T(x,2).$$

Theorem 1.2.9 The generating function $t(x,2)$ for symmetries in free 4-trees is given by

(1.2.17)
$$t(x,2) = T(x,2) + \frac{3}{2}\,T(x^2,4) - \frac{1}{2}\,T(x,2)^2 + \frac{x}{24}\,T(x,2)^4 + \frac{3x}{4}\,T(x^2,4)\,T(x,2)^2 + \frac{9x}{8}\,T(x^2,4)^2 + \frac{71x}{4}\,T(x^4,16) + \frac{13x}{3}\,T(x^3,8)\,T(x,2).$$

1.3 Recurrence Relations

From the functional equations (1.2.1), (1.2.3), (1.2.5) and (1.2.7), recurrence relations for $T_{m,n}$, the coefficient of $y^m x^n$ in $T(x,y)$, can now be determined. Let B_n, C_n and D_n be the coefficients of x^{2n}, x^{3n} and x^{4n} in $T(x^2,4)$, $T(x^3,8)$ and $T(x^4,16)$ respectively. That is,

(1.3.1)
$$B_n = \sum_m T_{m,n} 2^{2m},$$

(1.3.2)
$$C_n = \sum_m T_{m,n} 2^{3m}$$

and

(1.3.3) $$D_n = \sum_m T_{m,n} 2^{4m}.$$

Then as a consequence of equations (1.2.11),(1.2.15),(1.2.16) and (1.2.17), s_n, the coefficient of x^n in t(x,2), can be expressed in terms of S_n, B_n, C_n and D_n.

Note that throughout this section the subscripts on the variables are always non-negative integers. Otherwise one can assume the value of the variable is zero.

First the formulas for $T_{m,n}$ and s_n will be given for (1,3)-trees. For $n \geq 2$ and $0 \leq m \leq n - 1$, $T_{m,n}$ is expressed in terms of $A_{m,n}$ where $A_{m,n}$ is defined as follows.

(1.3.4) $$A_{m,n} = \begin{cases} 0, \text{ if } m = n - 1 \\ \frac{1}{2}\sum_{k=1}^{n-1}\sum_i T_{i,k}\, T_{m-i,n-k}, \text{ if } m \neq n - 1. \end{cases}$$

Then $T_{0,1} = 1$ and for $n \geq 2$,

(1.3.5) $$T_{m,n} = A_{m,n} + T_{\frac{m-1}{2},\frac{n}{2}} - \frac{1}{2} T_{\frac{m}{2},\frac{n}{2}}.$$

For $n \geq 2$,

(1.3.6)
$$s_n = \frac{1}{2}\sum_{k=1}^{n} S_k S_{n-k+1} - \frac{1}{3}\sum_{i=1}^{n-1}\sum_{j=1}^{n-i} S_i S_j S_{n-i-j+1}$$

$$+ \frac{3}{2} B_{\frac{n+1}{2}} + \frac{13}{3} C_{\frac{n+1}{3}}.$$

Next the equations for $T_{m,n}$ and s_n are given for 3-trees. Here $T_{0,1}$ and $T_{0,2}$ are both equal to 1 and for $n \geq 2$ and $0 \leq m \leq (n-1)/2$,

(1.3.7)
$$T_{m,n+1} = \frac{1}{2}\sum_{k=1}^{n-1}\sum_{i} T_{i,k} T_{m-i,n-k} + T_{m,n}$$

$$+ T_{\frac{m-1}{2},\frac{n}{2}} - \frac{1}{2} T_{\frac{m}{2},\frac{n}{2}}.$$

For free 3-trees, $s_1 = 1$, $s_2 = s_3 = 2$ and for $n \geq 4$,

(1.3.8)
$$s_n = S_n + \frac{1}{6}\sum_{i=1}^{n-3}\sum_{j=1}^{n-i-2} S_i S_j S_{n-i-j-1} - \frac{1}{2}\sum_{k=1}^{n-1} S_k S_{n-k}$$

$$+ \frac{3}{2} B_{\frac{n}{2}} + \frac{13}{3} C_{\frac{n-1}{3}} + \frac{3}{2} D_{n-1}.$$

And now we have the equations for $T_{m,n}$ and s_n for (1,4)-trees. Recall that the group order of a planted (1,4)-tree has the form $2^i(3!)^j$ and in $T_{m,n}$, m corresponds to the ordered pair of integers (i,j). Hence, we write $T_{m,n}$ as $T_{i,j,n}$ where $0 \leq i \leq n - 2$

and $0 \le j \le n - 1 - i$. Then $T_{0,1} = T_{0,0,1} = 1$ and for $n \ge 2$,

(1.3.9)
$$T_{i,j,n} = \frac{1}{6}\sum_{k=1}^{n-1}\sum_{l=1}^{n-k}\sum_{a}\sum_{b}\sum_{c}\sum_{d} T_{a,b,k}T_{c,d,l}T_{i-a-c,j-b-d,n-k-l-1}$$
$$- \frac{1}{2}\sum_{1\le k\le \frac{n}{2}}\sum_{a}\sum_{b} T_{a,b,k}T_{i-2a,j-2b,n-2k+1}$$
$$+ \sum_{1\le k\le \frac{n}{2}}\sum_{a}\sum_{b} T_{a,b,k}T_{i-2a-1,j-2b,n-2k+1}$$
$$+ T_{\frac{i}{3},\frac{j-1}{3},\frac{n+1}{3}} - T_{\frac{i-1}{3},\frac{j}{3},\frac{n+1}{3}} + \frac{1}{3}T_{\frac{i}{3},\frac{j}{3},\frac{n+1}{3}}.$$

To write the formula for s_n, we first define

(1.3.10)
$$U_n = \sum_{k=1}^{n-1} S_k S_{n-k} \qquad \text{for } n \ge 2.$$

Then for $n \ge 2$,

(1.3.11)
$$s_n = S_n - \frac{1}{2}U_{n+1} + \frac{3}{4}\sum_{k=2}^{n} U_k B_{\frac{n-k+2}{2}}$$
$$+ \frac{1}{24}\sum_{i=1}^{n-1}\sum_{j=1}^{n-i}\sum_{k=1}^{n-i-j+1} S_i S_j S_k S_{n-i-j-k+2}$$
$$+ \frac{13}{3}\sum_{k=1}^{n-1} S_k C_{\frac{n-k+2}{3}} + \frac{9}{8}\sum_{i=1}^{n/2} B_i B_{\frac{n-2i+2}{2}}$$
$$+ \frac{3}{2}B_{\frac{n+1}{2}} + \frac{71}{4}D_{\frac{n+2}{4}}.$$

Finally, the equations for $T_{m,n}$ and s_n are given for 4-trees. As in planted (1,4)-trees, the group order of a planted 4-tree has the form $2^i(3!)^j$. Thus, $T_{m,n} = T_{i,j,n}$ where $0 \le i \le (n-1)/2$, $0 \le j \le (n-1-2i)/3$. Both $T_{0,0,1}$ and $T_{0,0,2}$ are equal to 1 and for $n \ge 2$,

(1.3.12)
$$T_{i,j,n+1} = \frac{1}{6}\sum_{k=1}^{n-2}\sum_{l=1}^{n-k-1}\sum_{a}\sum_{b}\sum_{c}\sum_{d} T_{a,b,k}T_{c,d,l}T_{i-a-c,j-b-d,n-k-1}$$
$$+ T_{\frac{i-1}{2},\frac{i}{2},\frac{n}{2}} + \frac{1}{3}T_{\frac{i}{3},\frac{i}{3},\frac{n}{3}} + T_{\frac{i}{3},\frac{i-1}{3},\frac{n}{3}}$$
$$+ \sum_{k=1}^{n-2}\sum_{a}\sum_{b} T_{a,b,k}T_{\frac{i-a-1}{2},\frac{i-b}{2},\frac{n-k}{2}} - \frac{1}{2}T_{\frac{i}{2},\frac{i}{2},\frac{n}{2}}$$
$$+ \frac{1}{2}\sum_{k=1}^{n-1}\sum_{a}\sum_{b} T_{a,b,k}\,T_{i-a,j-b,n-k} + T_{i,j,n}$$
$$- \frac{1}{2}\sum_{k=1}^{n-2}\sum_{a}\sum_{b} T_{a,b,k}T_{\frac{i-a}{2},\frac{i-b}{2},\frac{n-k}{2}} - T_{\frac{i-1}{3},\frac{i}{3},\frac{n}{3}}.$$

For $n \ge 5$,

(1.3.13)
$$s_n = S_n + \frac{1}{24}\sum_{i=1}^{n-4}\sum_{j=1}^{n-i-3}\sum_{k=1}^{n-i-j-2} S_iS_jS_kS_{n-i-j-k-1}$$
$$+ \frac{3}{4}\sum_{k=2}^{n-3} U_kB_{\frac{n-k-1}{2}} + \frac{13}{3}\sum_{k=1}^{n-4} S_kC_{\frac{n-k-1}{3}} + \frac{9}{8}\sum_{i=1}^{\frac{n-3}{2}} B_iB_{\frac{n-2i-1}{2}}$$
$$- \frac{1}{2}U_n + \frac{3}{2}B_{\frac{n}{2}} + \frac{71}{4}D_{\frac{n-1}{4}}.$$

1.4 Numerical Results

For each type of tree, values of $T_{m,n}$, S_n and s_n were computed using the CDC Cyber 750 in the Computer Laboratory at Michigan State University. The computation of these numbers was limited by the available accuracy of 14 single precision and 29 double precision floating point digits and by storage restrictions. Another limiting factor was the time required to compute the values using the recurrence relations. For example, in the case of (1,3)-trees, the Fortran programs used to compute S_n for $n \leq 50$ took 52 seconds while an additional 300 seconds were required to compute S_{68}.

The effect of these limiting factors is seen in the maximum value of n for which the numbers could be computed. Due to the difference in the number of possible group orders for the four types of trees, this maximum value of n varies greatly among the different types of trees. For (1,3)-trees, the maximum value of n was 50 while for 3-trees, it was 70. In both these cases, the available accuracy was the most significant limiting factor. For (1,4)-trees, the maximum value of n was 22 while it was 36 for 4-trees. In these two cases, the most significant limiting factor was the storage restriction.

Values of $T_{m,n}$, S_n and s_n appear in the following tables.

Table 1. Coefficients of T(x,y) for Planted (1,3)-trees.

n	m	$T_{m,n}$
4	1	1
	2	0
	3	1
5	1	1
	2	1
	3	1
6	1	1
	2	2
	3	2
	4	1
7	1	1
	2	4
	3	3
	4	3
8	1	1
	2	6
	3	7
	4	7
	5	1
	6	0
	7	1
9	1	1
	2	9
	3	14
	4	14
	5	6
	6	1
	7	1
10	1	1
	2	12
	3	28
	4	28
	5	21
	6	4
	7	3
	8	1

Table 1. (cont'd.).

n	m	$T_{m,n}$
11	1	1
	2	16
	3	50
	4	58
	5	54
	6	17
	7	8
	8	3
12	1	1
	2	20
	3	85
	4	119
	5	126
	6	61
	7	27
	8	9
	9	2
	10	1
13	1	1
	2	25
	3	135
	4	239
	5	273
	6	187
	7	80
	8	32
	9	8
	10	3
14	1	1
	2	30
	3	206
	4	457
	5	580
	6	500
	7	246
	8	112
	9	33
	10	11
	11	3

Table 2. Coefficients of T(x,2) and t(x,2) for (1,3)-trees.

n	S_n	s_n
4	10	8
5	14	56
6	42	24
7	90	168
8	354	240
9	758	608
10	2290	920
11	6002	5680
12	18410	6104
13	51310	18416
14	154106	43008
15	449322	148152
16	1384962	325608
17	4089174	980840
18	12475362	2421096
19	37746786	7336488
20	116037642	19769312
21	355367310	58192608
22	1097869386	164776248
23	3393063162	502085760
24	10546081122	1427051544
25	32810171382	4261678656
26	102465452754	12615722288
27	320522209490	37914214232
28	1005428474218	113567513528
29	3159128678510	343641240328
30	9947763312410	1039134670952
31	31374858270154	3164525151512
32	99133809899138	9638997662848
33	313680433887702	29494412007120
34	994070600867778	90400450050120
35	3154447132624578	278010905513408

Table 3. Coefficients of T(x,y) for Planted 3-trees.

n	m	$T_{m,n}$
4	0	2
	1	1
5	0	3
	1	3
6	0	6
	1	5
7	0	11
	1	11
	3	1
8	0	22
	1	22
	2	1
	3	1
9	0	43
	1	48
	2	4
	3	3
10	0	88
	1	101
	2	13
	3	5
11	0	179
	1	221
	2	37
	3	13
	4	1
12	0	372
	1	480
	2	103
	3	25
	4	3

Table 4. Coefficients of T(x,2) and t(x,2) for 3-trees.

n	S_n	s_n
4	4	8
5	9	4
6	16	14
7	41	21
8	78	35
9	179	49
10	382	158
11	889	191
12	1992	425
13	4648	828
14	10749	1864
15	25462	3659
16	59891	8324
17	142793	17344
18	340761	39601
19	819533	87407
20	1975109	199984
21	4784055	453361
22	11617982	1053816
23	28316757	2426228
24	69185852	5672389
25	169516558	13270695
26	416268547	31277150
27	1024543728	73874375
28	2526631078	175419550
29	6242969248	417535487
30	15452300967	997758788
31	38310417739	2390172398
32	95126958081	5743235470
33	236548880263	13832781125
34	589014148511	33401381861
35	1468545756633	80825852570

Table 5. Coefficients of T(x,y) for Planted (1,4)-trees.

n	i	j	$T_{i,j,n}$
4	2	1	1
	1	2	1
5	3	1	1
	1	2	1
	2	2	1
	0	4	1
6	4	1	1
	2	2	2
	3	2	2
	1	3	1
	2	3	1
	1	4	1
7	5	1	1
	3	2	4
	4	2	2
	1	3	1
	2	3	3
	3	3	3
	2	4	2
	0	5	1
8	6	1	1
	4	2	6
	5	2	3
	2	3	4
	3	3	8
	4	3	4
	1	4	1
	2	4	3
	3	4	5
	1	5	3
	1	6	1

Table 5 (cont'd.).

n	i	j	$T_{i,j,n}$
9	7	1	1
	5	2	9
	6	2	3
	3	3	11
	4	3	15
	5	3	7
	1	4	1
	2	4	7
	3	4	12
	4	4	8
	2	5	8
	3	5	2
	0	6	1
	1	6	2
	2	6	2
10	8	1	1
	6	2	12
	7	2	4
	4	3	24
	5	3	26
	6	3	10
	2	4	6
	3	4	26
	4	4	32
	5	4	12
	1	5	1
	2	5	7
	3	5	23
	4	5	6
	1	6	6
	2	6	6
	3	6	5
	1	7	3
	1	8	1

Table 6. Coefficients of T(x,2) and t(x,2) for (1,4)-trees.

n	S_n	s_n
4	96	144
5	1560	1584
6	4848	32544
7	28848	30528
8	248352	188928
9	1446240	4030848
10	12905664	12029184
11	99071040	66104064
12	649236480	524719872
13	4924099200	2364433920
14	49007023872	28794737664
15	304778309376	194617138176
16	2301818168832	962354727936
17	18389782387200	6901447938048
18	138110895596544	112061234884608
19	1094304243348480	366020989931520
20	8691945066848256	2592919032274944
21	68039592521668608	19913392024584192
22	541189487303208960	140498248288886784

Table 7. Coefficients of T(x,y) for Planted 4-trees.

n	i	j	$T_{i,j,n}$
4	0	0	2
	1	0	1
	0	1	1
5	0	0	3
	1	0	4
	0	1	1
6	0	0	6
	1	0	8
	2	0	1
	0	1	2
7	0	0	12
	1	0	18
	2	0	2
	3	0	1
	0	1	5
	1	1	1
8	0	0	25
	1	0	40
	2	0	9
	3	0	2
	0	1	10
	1	1	3
9	0	0	52
	1	0	94
	2	0	26
	3	0	6
	0	1	22
	1	1	10
	1	2	1

Table 7 (cont'd.).

n	i	j	$T_{i,j,n}$
10	0	0	113
	1	0	214
	2	0	79
	3	0	14
	4	0	1
	0	1	51
	1	1	30
	2	1	1
	3	1	1
	0	2	1
	1	2	2
11	0	0	245
	1	0	504
	2	0	219
	3	0	45
	4	0	5
	0	1	116
	1	1	87
	2	1	6
	3	1	2
	0	2	4
	1	2	5
12	0	0	542
	1	0	1180
	2	0	612
	3	0	127
	4	0	22
	0	1	270
	1	1	243
	2	1	28
	3	1	5
	0	2	15
	1	2	11
	2	2	2

Table 8. Coefficients of T(x,2) and t(x,2) for 4-trees.

n	S_n	s_n
4	10	8
5	17	28
6	38	20
7	106	43
8	253	143
9	716	249
10	1903	546
11	5053	1223
12	13786	2703
13	39293	8107
14	107641	18085
15	302807	44013
16	860099	114919
17	2450684	327712
18	7038472	800937
19	20316895	2146066
20	58849665	5827711
21	171217429	15923828
22	499926666	43886143
23	1464276207	121888966
24	4301706250	340209504
25	12671810107	955859391
26	37419912977	2700771322
27	110759884262	7652412896
28	328525197554	21784431688
29	976350258323	62248194140
30	2906960957827	178463482459

CHAPTER II

ASYMPTOTIC BEHAVIOR

2.1 Asymptotic Analysis

An adaptation of the twenty-step algorithm [HRS75] is used to study the behavior of the coefficients of $T(x,2)$ and $t(x,2)$ for large values of n. In the asymptotic analysis, the generating functions $T(x,2)$ and $t(x,2)$ are regarded as power series in the complex variable x. For each type of tree, let ρ be the radius of convergence of $T(x,2)$.

Observe that in a planted d-tree or (1,d)-tree, the maximum possible group order for each n is $((d-1)!)^{\alpha(n-1)}$ where α is 1 for (1,d)-trees and $(d-1)^{-1}$ for d-trees. This maximum group order is attained by a planted (1,d)-tree in which every end-vertex except the root is at the same level in the tree. While such trees do not exist for all values of n, they do exist for infinitely many values of n. This observation leads to the following lemmas concerning ρ.

Lemma 2.1.1 For all four types of trees, the radius of convergence ρ of $T(x,2)$ satisfies $0 < \rho < 1$.

Proof: Note that as previously stated, $T(x,1)$ is the series that counts the planted trees of the specified type. It follows from the above observation that the coefficients of $T(x,2)$ are bounded above by the coefficients of $T(((d-1)!)^{\alpha}x,1)$, which has a positive radius of convergence [P37], [O48]. Hence $\rho > 0$.

The upper bound on ρ is obtained by considering the behavior of $T(x,2)$ as x approaches ρ from below. As in step 4 of the twenty-step algorithm, the functional equation for $T(x,2)$ and the monotonicity of $T(x,2)$ show that $T(\rho,2) < \infty$. This together with the fact that $S_n \geq 1$ for infinitely many n shows that $\rho < 1$. //

Lemma 2.1.2 $T(x^k,2^k)$ has radius of convergence $\sigma_k > \rho$ for all $k \geq 2$.

Proof: Let $M = \log_2((d-1)!)^{\alpha}$. By the earlier observation, for infinitely many n, $S_n \geq 2^{M(n-1)}$. Thus, $\rho < 2^{-M}$.

For $k = 2$, $T(x^2,2^2) \leq T(2^M x^2,2)$ which converges when $x \leq (\rho 2^{-M})^{1/2}$. This shows $\sigma_2 \geq (\rho 2^{-M})^{1/2}$. Hence since $\rho < 2^{-M}$, we may conclude that $\sigma_2 > \rho$. The result is then shown for $k \geq 3$ by induction on k. //

As a result of the functional relations for $t(x,2)$ and lemma 2.1.2, we can conclude that ρ is also the radius of convergence of $t(x,2)$ and that $t(\rho,2)$ is finite.

In step 5 of the twenty-step algorithm a new function $F(x,y)$ is defined by replacing each occurrence of $T(x,2)$ in its functional relation by the variable y. The appropriate definitions of F for each type of tree are as follows.

For (1,3)-trees,

(2.1.1) $$F(x,y) = x + \frac{1}{2} y^2 + \frac{3}{2} T(x^2,4) - y.$$

For 3-trees,

(2.1.2) $$F(x,y) = x + \frac{1}{2} xy^2 + xy + \frac{3x}{2} T(x^2,4) - y.$$

For (1,4)-trees,

(2.1.3) $$F(x,y) = x + \frac{1}{6x} y^3 + \frac{3}{2x} T(x^2,4)\, y + \frac{13}{3x} T(x^3,8) - y.$$

For 4-trees,

(2.1.4) $$F(x,y) = x + \frac{1}{6} xy^3 + \frac{1}{2} xy^2 + xy(1 + \frac{3}{2} T(x^2,4)) + \frac{3x}{2} T(x^2,4) + \frac{13x}{3} T(x^3,8) - y.$$

<u>Lemma 2.1.3</u> $F(x,y)$ satisfies the following conditions:

(i) $F(x,y)$ is analytic for all y and for all x in a neighborhood of $x = 0$ which contains $x = \rho$.

(ii) $F(x,T(x,2)) = 0$ for all x with $|x| \leq \rho$.

(iii) The first partial derivative of F with respect to y, $F_y(x,y)$ satisfies $F_y(\rho,T(\rho,2)) = 0$ and if $|x| \leq \rho$ but $x \neq \rho$, then $F_y(x,T(x,2)) \neq 0$.

(iv) $F_{yy}(\rho,T(\rho,2)) \neq 0$.

(v) $x = \rho$ is the unique singularity of $T(x,2)$ on its circle of convergence.

Proof: Part (i) is a consequence of lemma 2.1.2 since $T(x^k,2^k)$ is analytic at $x = \rho$ for $k \geq 2$. That $F(x,T(x,2)) = 0$ for $|x| < \rho$ follows directly from the definition of F and the functional equation for $T(x,2)$. That $F_y(x,T(x,2)) \neq 0$ if $|x| \leq \rho$ but $x \neq \rho$ can be shown by combining the techniques of Otter [O48] and step 10 of the twenty-step algorithm [HRS75]. The justification of the remaining statements of this lemma is described in steps 6 through 13 of the twenty-step algorithm. //

As a consequence of lemma 2.1.3, $x = \rho$ is a branch point of order 2 of $T(x,2)$ and therefore, as in step 14 of the twenty-step algorithm, $T(x,2)$ and $t(x,2)$ both have expansions in $(\rho - x)^{1/2}$ near $x = 0$.

(2.1.5) $$T(x,2) = T(\rho,2) - b_1(\rho - x)^{\frac{1}{2}} + b_2(\rho - x) + b_3(\rho - x)^{\frac{3}{2}} + \ldots.$$

(2.1.6) $$t(x,2) = t(\rho,2) + a_1(\rho - x)^{\frac{1}{2}} + a_2(\rho - x) + a_3(\rho - x)^{\frac{3}{2}} + \ldots.$$

2.2 Asymptotic formulas

The asymptotic formulas for the coefficients of $T(x,2)$ and $t(x,2)$ are found by evaluating the contribution of $(\rho - x)^{k/2}$ in the above expansions (2.1.5) and (2.1.6). Note that by the binomial theorem and the definition of the gamma function, if $s \neq 0, -1, -2, \ldots$ then the coefficient of x^n in $(1 - x)^{-s}$ is

$$\frac{\Gamma(s + n)}{\Gamma(s)\,\Gamma(n + 1)}. \tag{2.2.1}$$

From Stirling's formula, this latter expression is equal to

$$\frac{n^{s-1}}{\Gamma(s)}\left(1 + \frac{s(s-1)}{2n} + O(1/n^2)\right). \tag{2.2.2}$$

Lemma 2.1.3 allows the application of Pólya's lemma, step 17 of the twenty-step algorithm, which uses the above observations to give the asymptotic formulas for the coefficients of $T(x,2)$ and $t(x,2)$.

Theorem 2.2.1 The asymptotic behavior of the number of symmetries in planted d or (1,d)-trees is given by

$$S_n \sim \frac{b_1}{2}\left(\frac{\rho}{\pi}\right)^{\frac{1}{2}} n^{\frac{-3}{2}} \rho^{-n}. \tag{2.2.3}$$

Theorem 2.2.2 The asymptotic behavior of the number of symmetries in free d or (1,d)-trees is given by

$$s_n \sim \frac{3a_3}{4}\left(\frac{\rho^3}{\pi}\right)^{\frac{1}{2}} n^{\frac{-5}{2}} \rho^{-n}. \tag{2.2.4}$$

Formula (2.2.3) accounts for the contribution of $-b_1(\rho - x)^{1/2}$ to the coefficient of x^n. For the free trees, it will be shown that $a_1 = 0$. Thus formula (2.2.4) accounts for the contribution of $a_3(\rho - x)^{3/2}$ to the coefficient of x^n. As can be seen by (2.2.2), in both cases the relative error in the asymptotic approximation is O(1/n). Note that for planted trees, the asymptotic number of symmetries is of the form $cn^{-3/2}\rho^{-n}$ where c is a constant. For free trees, the asymptotic number of symmetries has the form $cn^{-5/2}\rho^{-n}$.

Formulas (2.2.3) and (2.2.4) can be refined by taking into account the contribution of additional terms of the expansions (2.1.5) and (2.1.6). When the contribution of one additional term is added,

(2.2.5) $$S_n \sim \sqrt{\frac{\rho}{\pi}}\, n^{\frac{-3}{2}} \rho^{-n} \left(\frac{b_1}{2} + \frac{12b_3\rho + 3b_1}{16n}\right)$$

and

(2.2.6) $$s_n \sim \sqrt{\frac{\rho^3}{\pi}}\, n^{\frac{-5}{2}} \rho^{-n} \left(\frac{3a_3}{4} + \frac{45a_3 - 60a_5\rho}{32n}\right).$$

2.3 Numerical Analysis

Evaluation of these asymptotic formulas requires computation of ρ, b_1, b_3, a_3 and a_5. The relations $F(\rho, T(\rho,2)) = 0$ and $F_y(\rho, T(\rho,2)) = 0$ combine to provide equations from which ρ and $T(\rho,2)$ can be computed. The corresponding equations for the four types of trees are as follows.

For (1,3)-trees,

(2.3.1) $$\rho = \frac{1}{2}(1 - 3\, T(\rho^2,4)).$$

For 3-trees,

(2.3.2) $$\rho\, (T(\rho,2) + 1) = 1.$$

For (1,4)-trees,

(2.3.3) $$\rho = \frac{1}{2}(T(\rho,2)^2 + 3\, T(\rho^2,4)).$$

For 4-trees,

(2.3.4) $$\rho(\frac{1}{2}\, T(\rho,2)^2 + T(\rho,2) + \frac{3}{2}\, T(\rho^2,4) + 1) = 1.$$

The following method is used to obtain equations for the b_i's and the a_i's. Using both the functional relation for $T(x,2)$ and its expansion in $(\rho - x)^{1/2}$ to evaluate $T_x(x,2)(T(\rho,2) - T(x,2))$ provides the means for determining the b_i's. To illustrate, from equation (1.2.2) for (1,3)-trees, after a bit of work, we have

(2.3.5) $$T_x(x,2)\ (T(\rho,2) - T(x,2)) = 1 + 3xT_x(x^2,4).$$

When the expansion (2.1.5) is used to substitute for $T(x,2)$

and $T_x(x,2)$ and the Taylor series expansion about $x = \rho$ is used to substitute for $3xT_x(x^2,4)$ in (2.3.5), coefficients of $(\rho - x)^{-1/2}$, $(\rho - x)^0$, $(\rho - x)^{1/2}$,... can be compared to express the b_i's in terms of $T(\rho^k,2^k)$ and $T_x(\rho^k,2^k)$ for various values of k. In a similar manner, $t_x(x,2)$ is evaluated to obtain expressions for the a_i's in terms of the b_i's and to show $a_1 = 0$. The equations for b_1 and a_3 are given below. Since the equations for b_3 and a_5 are much more complicated, they are omitted.

In the expansions of T(x,2) and t(x,2) for (1,3)-trees,

(2.3.6) $$b_1 = \sqrt{2(1 + 3\rho T_x(\rho^2,4))}$$

and

(2.3.7) $$a_3 = \frac{b_1^3}{3\rho}.$$

In the expansions of T(x,2) and t(x,2) for 3-trees,

(2.3.8) $$b_1 = \frac{1}{\rho}\sqrt{2(T(\rho,2) + 3\rho^3 T_x(\rho^2,4))}$$

and

(2.3.9) $$a_3 = \frac{b_1^3 \rho}{3}.$$

In the expansions of T(x,2) and t(x,2) for (1,4)-trees,

$$b_1 = \sqrt{\frac{T(\rho,2)(6\rho T_x(\rho^2,4) - 2) + 4\rho + 26\rho^2 T_x(\rho^3,8)}{T(\rho,2)}} \tag{2.3.10}$$

and

$$a_3 = \frac{b_1^3 T(\rho,2)}{3\rho^2}. \tag{2.3.11}$$

In the expansions of T(x,2) and t(x,2) for 4-trees,

$$b_1 = \frac{1}{\rho}\sqrt{\frac{2\,(T(\rho,2) + 3\rho^3 T_x(\rho^2,4)(1 + T(\rho,2)) + 13\rho^4 T_x(\rho^3,8))}{1 + T(\rho,2)}} \tag{2.3.12}$$

and

$$a_3 = \frac{b_1^3 \rho\,(T(\rho,2) + 1)}{3}. \tag{2.3.13}$$

The numerical methods necessary to actually compute values of ρ, $T(\rho^k,2^k)$ and $T_x(\rho^k,2^k)$ for various k depend on d. First we will deal with the case that $d = 3$.

Note that the functional equations (1.2.1) and (1.2.3) are actually quadratics in T(x,y) which can be extended to quadratics in $T(x^k,2^k)$ for $k \geq 1$. Thus, applying the quadratic formula and the mononicity of $T(x^k,2^k)$ results in the following equations for $T(x^k,2^k)$ when $|x| \leq \rho$.

For (1,3)-trees,

$$T(x^k,2^k) = 1 - \sqrt{1 - (2^{k+1} - 1)T(x^{2k},2^{2k}) - 2x^k}. \tag{2.3.14}$$

For 3-trees,

$$(2.3.15) \qquad T(x^k,2^k) = \frac{1 - x^k - \sqrt{1 - 2x^k - x^{2k}(1 + (2^{k+1} - 1)T(x^{2k},2^{2k}))}}{x^k}.$$

In each of the above equations, $T(x^k,2^k)$ is expressed in terms of $T(x^{2k},2^{2k})$. Thus for $|x| \le \rho$, if $T(x^{16},2^{16})$ is estimated by a partial sum, then equation (2.3.14) or (2.3.15) can be used repeatedly to determine $T(x^8,2^8)$, $T(x^4,2^4)$, $T(x^2,2^2)$ and $T(x,2)$.

Similarly, from equations (1.2.1) and (1.2.3) $T_x(x^k,2^k)$ can be expressed in terms of $T(x^k,2^k)$, $T(x^{2k},2^{2k})$ and $T_x(x^{2k},2^{2k})$. Again by starting with a partial sum for $T_x(x^k,2^k)$ for $k \ge 16$, $T_x(x^k,2^k)$ can then be calculated for $k < 16$ and $|x| < \rho$.

Note that ρ is actually significantly less than 2^{-M} where $M = ((d - 1)!)^{\alpha}$. Calculation of successive terms of $T(x^{16},2^{16})$ and $T_x(x^{16},2^{16})$ indicate that their nth terms are less than 10^{-27} when $x \le \rho$ and n is about 20. The exact value of n for which this is true depends on d and the type of tree. To estimate the error in the partial sum approximation of $T(x^{16},2^{16})$ note that the twenty-step algorithm can be applied to determine the asymptotic behavior of the coefficients of $T(x^{16},2^{16})$. The coefficient of x^{16n} is asymptotic to $C(\sigma_{16})^{-16n}\, n^{-3/2}$ where C is a constant and σ_{16} is the radius of convergence of $T(x^{16},2^{16})$. Thus if we disregard the factor of $n^{-3/2}$ then $T(x^{16},2^{16})$ behaves like the geometric series $\sum Cr^n$ where $r = (x/\sigma_{16})^{16}$. If $x \le \rho$, then $r < 1$ and by comparing σ_{16} with the radius of $T(x^{16},1)$, it can be seen that r is in fact closer to 0 than to 1. This provides a bound on the error in the partial sum approximation.

Equations (2.3.1) and (2.3.2) provide the means for calculating ρ. For (1,3)-trees, ρ is the unique solution of

(2.3.16) $$g(x) = x + \frac{1}{2}(3\ T(x^2,4) - 1) = 0.$$

While for 3-trees, ρ is the unique solution of

(2.3.17) $$g(x) = x(T(x,2) + 1) - 1 = 0.$$

The following iterative method can then be used to compute ρ. Given initial lower and upper bounds for ρ, $l_n < \rho < h_n$, then

(2.3.18) $$l_{n+1} = l_n - l_n \frac{g(l_n)}{g'(l_n)}$$

and

(2.3.19) $$h_{n+1} = l_n - \frac{g(l_n)}{g'(l_n)}.$$

Note that (2.3.19) is just Newton's Method applied to g and l_n. Since g is increasing and concave up for $|x| < \rho$,each iteration produces a new upper bound h_{n+1} such that $\rho < h_{n+1} < h_n$. Formula (2.3.18) is a modification of Newton's Method : the line with slope $g'(l_n)/l_n$ is used rather than the tangent line to estimate g(x). For these particular functions, each iteration of (2.3.18) provides a new lower bound l_{n+1} such that $l_n < l_{n+1} < \rho$. Note that since T(x,2) is not defined for $x < \rho$, the lower bound is modified each time to give a new lower bound and a new upper bound for ρ.

When $d = 4$ the functional equations (1.2.5) and (1.2.7) are cubics in $T(x,y)$. Hence a numerical method is required to compute $T(x^k,2^k)$ for $|x| < \rho$. For (1,4)-trees, the cubic with root $T(x^k,2^k)$ is

(2.3.20)
$$G_k(z) = \frac{1}{6}z^3 + ((2^k - \frac{1}{2})T(x^{2k},2^{2k}) - x^k)\, z + (6^k - 2^k + \frac{1}{3})\, T(x^{3k},2^{3k}) + x^{2k}.$$

For 4-trees, the cubic with root $T(x^k,2^k)$ is

(2.3.21)
$$G_k(z) = \frac{x^k}{6} z^3 + \frac{x^k}{2} z^2 + (x^k(1 + (2^k - \frac{1}{2})T(x^{2k},2^{2k})) - 1)\, z + x^k(1 + (2^k - \frac{1}{2})T(x^{2k},2^{2k}) + (6^k - 2^k + \frac{1}{3})T(x^{3k},2^{3k})).$$

If $0 < x < \rho$ and $z < T(x^k,2^k)$, then G_k is decreasing and concave up. Therefore application of Newton's method to the function G_k starting with z_0, a partial sum of $T(x^k,2^k)$, produces z_1 such that $z_0 < z_1 < T(x^k,2^k)$. Consequently, $T(x^k,2^k)$ can be estimated by a partial sum for $k \geq 16$ and Newton's method can then be applied to G_k to calculate $T(x^k,2^k)$ for $k < 16$. As with 3 and (1,3)-trees, the functional relations (1.2.5) and (1.2.7) supply equations for $T_x(x^k,2^k)$ in terms of $T(x^k,2^k)$, $T(x^{2k},2^{2k})$, $T(x^{3k},2^{3k})$, $T_x(x^{2k},2^{2k})$ and $T_x(x^{3k},2^{3k})$.

Here the functions with unique root $x = \rho$ are

(2.3.22) $$g(x) = T(x,2)^2 + 3T(x^2,4) - 2x \quad \text{for } (1,4)\text{-trees}$$

and

(2.3.23) $$g(x) = x(\frac{1}{2}T(x,2)^2 + T(x,2) + \frac{3}{2}T(x^2,4) + 1) - 1 \text{ for 4-trees.}$$

In these two cases $g(x)$ is increasing and concave up. However, the modified Newton's method which worked when $d = 3$ does not provide a new lower bound for ρ. Instead the bisection method is used to determine bounds for ρ. Given $l_n < \rho < h_n$, let $x_n = (l_n + h_n) / 2$. The following criteria was used to determine the relationship between ρ and x_n. First estimate $T(x_n{}^k,2^k)$ for $k > 1$ as described earlier. When $k = 1$ and Newton's method is applied to G_1 with initial guess z_0, a partial sum of $T(x_n,2)$, an estimate z_m such that $G_1'(z_m) > 0$ indicates $x_n > \rho$.

2.4 Numerical Results

In the computations, $T(x^k,2^k)$ was calculated to at least 20 digits and ρ to at least 12 digits. The computed values of ρ, b_1, b_3, a_3 and a_5 appear in the following table.

Table 9. Radii and Constants.

	Type of Tree			
	(1,3)	3	(1,4)	4
ρ	.301398653	.384173339	.116663460	.319078317
b_1	2.403442218	5.076889680	1.544582575	3.844874351
a_3	15.354599582	16.757111017	37.009971072	13.381537712
b_3	3.588139413		14.591292087	
a_5	-17.824935398		-341.927657398	

Formulas (2.2.3) and (2.2.4) were used to determine the asymptotic number of symmetries in planted and free d-trees while the refinements (2.2.5) and (2.2.6) gave significantly better results for the asymptotic number of symmetries in planted and free (1,d)-trees. The exact number of symmetries is compared to the asymptotic number in Tables 10 - 17.

Table 10. Number of Symmetries in Planted (1,3)-trees.

Vertices	Exact	Asymptotic		Relative Error
48	10546081122	104637	E05	-.007808
52	102465452754	101826	E06	-.006241
56	1005428474218	100021	E07	-.005186
60	9947763312410	990417	E07	-.004383
64	99133809899138	987582	E08	-.003788
68	994070600867778	990798	E09	-.003292
72	10023140394172682	999410	E10	-.002897
76	101556839584864874	101296	E12	-.002571
80	1033496930259584098	103112	E13	-.002299
84	10558761198762257586	105369	E14	-.002068
88	108257452313403277290	108055	E15	-.001871
92	1113533377484472278586	111164	E16	-.001701
96	11487547694267472245250	114697	E17	-.001554
100	118829269415696976059298	118660	E18	-.001425

Table 11. Number of Symmetries in Free (1,3)-trees.

Vertices	Exact	Asymptotic		Relative Error
48	1427051544	134470	E04	-.057708
52	12615722288	120224	E05	-.047033
56	113567513528	109211	E06	-.038356
60	1039134670952	100573	E07	-.032148
64	9638997662848	937220	E07	-.027679
68	90400450050120	882491	E08	-.023798
72	856418820307400	838609	E09	-.020796
76	8184345855878800	803432	E10	-.018331
80	78821355356607416	775368	E11	-.016297
84	764368300213840728	753216	E12	-.014590
88	7458653276030440720	736061	E13	-.013145
92	73191173128569457416	723197	E14	-.011907
96	721899672085668985128	714074	E15	-.010840
100	7153568644231221969760	708266	E16	-.009912

Table 12. Number of Symmetries in Planted 3-trees.

Vertices	Exact	Asymptotic		Relative Error
15	10749	11109	E00	.033511
20	819533	839670	E00	.024572
25	69185852	706783	E02	.021572
30	6242969248	635872	E04	.018542
35	589014148511	598567	E06	.016218
40	57398241292347	582234	E08	.014377
45	5732097451950746	580603	E10	.012899
50	583553860753045319	590376	E12	.011690
55	60336483976084984447	609812	E14	.010685
60	6318602632078649428839	638076	E16	.009837
65	668812989635611814991086	674907	E18	.009112

Table 13. Number of Symmetries in Free 3-trees.

Vertices	Exact	Asymptotic		Relative Error
15	3659	3306	E00	-.096398
20	199984	192467	E00	-.037587
25	13270695	131658	E02	-.007908
30	997758788	997370	E03	-.000389
35	80825852570	810687	E05	.003005
40	6907362937687	693805	E07	.004443
45	614475723485527	617618	E09	.005114
50	56409655488848540	567140	E11	.005395
55	5311321843821516910	534038	E13	.005471
60	510635048525607184087	513411	E15	.005435
65	49958747518253245317394	502254	E17	.005338

Table 14. Number of Symmetries in Planted (1,4)-trees.

Vertices	Exact	Asymptotic	Relative Error
32	99071040	886729 E02	-.104957
35	649236480	658419 E03	.014143
38	4924099200	494957 E04	.005172
41	49007023872	375966 E05	-.232832
44	304778309376	288131 E06	-.054621
47	2301818168832	222519 E07	-.033291
50	18389782387200	173004 E08	-.059241
53	138110895596544	135302 E09	-.020335
56	1094304243348480	106372 E10	-.027947
59	8691945066848256	840194 E10	-.033365
62	68039592521668608	666426 E11	-.020531
65	541189487303208960	.530604 E12	-.019560

Table 15. Number of Symmetries in Free (1,4)-trees.

Vertices	Exact	Asymptotic	Relative Error
32	66104064	403949 E02	-.388920
35	524719872	271748 E03	-.482109
38	2364433920	186644 E04	-.210619
41	28794737664	130459 E05	-.546935
44	194617138176	925649 E05	-.524374
47	962354727936	665358 E06	-.308615
50	6901447938048	483710 E07	-.299118
53	112061234884608	355181 E08	-.683047
56	366020989931520	263123 E09	-.281125
59	2592919032274944	196473 E10	-.242271
62	19913392024584192	147751 E11	-.258030
65	140498248288886784	111827 E12	-.204070

Table 16. Number of Symmetries in Planted 4-trees.

Vertices	Exact	Asymptotic		Relative Error
14	39293	36783	E00	-.063881
16	302807	291494	E00	-.037361
18	2450684	237300	E01	-.031697
20	20316895	197264	E02	-.029066
22	171217429	166745	E03	-.026119
24	1464276207	142888	E04	-.024172
26	12671810107	123846	E05	-.022662
28	110759884262	108381	E06	-.021478
30	976350258323	956329	E06	-.020506
32	8669904767404	849899	E07	-.019714
34	77481380765038	760054	E08	-.019050
36	696342460242332	683469	E09	-.018488

Table 17. Number of Symmetries in Free 4-trees.

Vertices	Exact	Asymptotic		Relative Error
14	18085	12273	E00	-.321363
16	114919	86334	E00	-.248741
18	800937	631693	E00	-.211308
20	5827711	476779	E01	-.181875
22	43886143	369013	E02	-.159159
24	340209504	291592	E03	-.142906
26	2700771322	234464	E04	-.131865
28	21784431688	191346	E05	-.121640
30	178463482459	158167	E06	-.113728
32	1480989441806	132206	E07	-.107315
34	12424948660563	111592	E08	-.101872
36	105244459584049	950122	E08	-.097224

The limited range of numbers for which the exact values could be computed for (1,4)-trees is not large enough to exhibit the nice decline in the relative error found in the other types of trees. In fact, for free (1,4)-trees there are large jumps in the relative error at various points in Table 15. The explanation of this can be found by comparing the ratio of consecutive coefficients, s_{n+1}/s_n for both the exact and asymptotic numbers. The ratio of the asymptotic values is steadily approaching ρ^{-1} while the ratio of the exact values jumps around as the relative error does. This is caused by the free (1,4)-trees that have a factor of 4! in their group order. Examples of such (1,4)-trees are those in which the number of vertices is of the form $5 + 6(3^i - 1)$. The existence of these trees is not reflected in the asymptotic formula (2.2.4) or its refinement (2.2.6). A similar phenomenon occurs in the case of (1,3)-trees; however, the jumps are much smaller and their effect is only seen when the number of vertices is less than 40.

CONCLUSION

The results presented in this thesis can be combined with formulas for the asymptotic number of trees of the specified type to give an asymptotic formula for the expected group order of these trees. The relevant formulas for the number of these trees appear in [O48] and [BaKP81]. Since the number of such trees is asymptotic to $C\beta^{-n}n^{-5/2}$ where β is the radius of convergence of the series that counts the trees and C is a constant, the expected group order is asymptotic to $A(\beta/\rho)^n$ where A is a constant. In other words, the expected group order is asymptotic to an exponential function of the ratio of the two radii.

Generally when the twenty-step algorithm is applied, the planted trees simply provide a means for getting at the results for the free trees. But removing the root from a planted (1,3)-tree of order 2n produces a binary tree of order 2n - 1. Since these trees have the same automorphism group, Table 10 provides values for the number of symmetries in binary trees. Thus the results for planted trees are also of interest.

Note that this application of the twenty-step algorithm is independent of the value of d. Thus the solution of this problem is theoretically possible for larger values of d. However, it becomes unmanagable since the functional relations for the generating functions become more complex and the number of possible group orders increases greatly as d increases.

The success of the techinique used here relies heavily on the degree restrictions of these trees. Significant modifications would be required to apply this method to the problem of estimating the group order of an arbitrary tree of large order. This is due to the fact that for each n, there is a tree on n vertices which has (n - 1)! symmetries. Thus the series that counts symmetries in trees does not converge.

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