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EFFICIENT DOMINATING SETS IN ORIENTED TREES

by

Quan Yue

**A Dissertation
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Doctor of Philosophy
Department of Mathematics and Statistics**

**Western Michigan University
Kalamazoo, Michigan
June 1995**

EFFICIENT DOMINATING SETS IN ORIENTED TREES

Quan Yue, Ph.D.

Western Michigan University, 1995

An oriented graph \vec{G} is said to have an *efficient dominating set* S if S is a set of vertices of \vec{G} and for each vertex v of \vec{G} , either v is in S and v is adjacent to *no* other vertex in S , or v is not in S but is adjacent from precisely one vertex of S . Not every oriented graph has an efficient dominating set and some oriented graphs may have more than one efficient dominating set. Barkauskas and Host showed that the problem of determining whether an oriented graph has an efficient dominating set is NP-complete.

In Chapter I, we introduce the basic definitions and study the elementary properties of *efficient dominating sets* for an oriented graph in general. Then we discuss the properties of *efficient dominating sets* for a tree T .

In Chapter II, we use combinatorial enumeration techniques to obtain recursive formulas for finding the number of efficient dominating sets among all unlabeled oriented trees (rooted or unrooted) of order p . These formulas are used to generate the number of efficient dominating sets among all unlabeled oriented trees (rooted or unrooted) of order p for each p up to 150. Then we use analysis methods, numerical analysis methods, and the methods of estimation of error to obtain asymptotic formulas for the number of efficient dominating sets in unlabeled oriented trees (rooted or unrooted). In particular, the limit of the p th root of the average number of efficient dominating sets per tree (rooted or unrooted) is determined.

We also define the number of efficient dominating sets in labeled oriented trees. In Chapter III, we obtain analytic formulas for the number of efficient dominating sets among all labeled oriented trees by using the Multivariate Lagrange Formula. Then we use these formulas to determine the number of efficient dominating sets among all labeled oriented trees of order p for each p up to 45. Asymptotic formulas, and the limit of the p th root of the average number of efficient dominating sets per labeled tree are determined as well.

The number of efficient dominating sets for a particular tree T is the number of efficient dominating sets among all orientations of T . The *maximum trees* of order p are the trees which have the maximum number of efficient dominating sets among all trees of order p . In Chapter IV, we modify the algorithm given by Barkauskas and Host to find the maximum trees of order p for each p up to 23. Some interesting properties of maximum trees are given, in particular we show that maximum trees can have arbitrarily large height. The structure of maximum trees is discussed.

We conjectured the maximum trees of order p for each p up to 3300. And we predicted that the limit of the p th root of the number of efficient dominating sets for maximum trees is 1.8525....

We conclude with some open problems in Chapter V for further study.

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**For
My Wife and Son**

ACKNOWLEDGEMENTS

First, I wish to express my gratitude to the many faculty members of Western Michigan University who have contributed so much in many ways to my mathematical education and my academic career.

In particular, I would like to thank Professor Gary Chartrand for serving as second reader on my committee, for his carefully reading this dissertation and for offering many helpful suggestions.

Special thanks to Professor Yousef Alavi, Professor Joseph Buckley and Professor Alfred Boals for serving on my committee and for their support and encouragement.

Above all, I wish to thank Professor Allen Schwenk, my advisor, for his outstanding and stimulating guidance, for his continuous and unselfish help, for the time he has spent with me. It is a great honor to work with him and to be one of his students.

I am also grateful to my friend Reza Rashidi for his assistance in the last month of writing this dissertation.

Finally, I would like to thank my family: my wife Zhou Wang and my son Benjamin Yue for their love, support, and understanding.

Quan Yue

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CHAPTER I

PRELIMINARIES

1.1 Introduction to Efficient Dominating Set

Let $G(V, E)$ be a graph with vertex set V and edge set E . A vertex v is said to dominate itself and its neighbors. A set $S \subseteq V$ is said to be a dominating set of G if for every vertex v of G , v is dominated by at least one member of S . Based on this definition, various concepts can be introduced. Among those include an independent dominating set, in which no two vertices in S are adjacent, a minimum dominating set, in which S has minimum cardinality, and an efficient dominating set, in which every vertex v of G is dominated by exactly one member of S . These definitions and others, as well as a bibliography on dominating sets, can be found in [9].

Barkauskas and Host [1] extended the concept of efficient dominating sets to oriented graphs and made the following definition:

Definition 1 *A vertex v of an oriented graph \vec{G} dominates itself and all vertices adjacent from v . A set S of vertices of \vec{G} is an efficient dominating set for \vec{G} if every vertex of \vec{G} is dominated by exactly one member of S .*

Can a graph G be oriented so that the orientation gives rise to an efficient dominating set? The following proposition answers the question positively.

Proposition 1 *Any graph G can be oriented in such a way so that the oriented graph \vec{G} of G has an efficient dominating set.*

Proof: Take any maximal independent set S of vertices of G . For each vertex v of G not in S , choose a neighbor u of v in S and orient the edge from u to v . For every other neighbor w of v in S , orient the edge from v to w . All other edges of G can be oriented arbitrarily. Then S is an efficient dominating set for oriented graph \vec{G} of G . \square

An oriented graph \vec{G} may have none, one, or more than one dominating set. For example in Figure 1, \vec{G}_1 has no efficient dominating set; \vec{G}_2 has only one efficient dominating set $S = \{1, 3\}$; and \vec{G}_3 has the two efficient dominating sets $S_1 = \{1, 3\}$ and $S_2 = \{2, 4\}$.

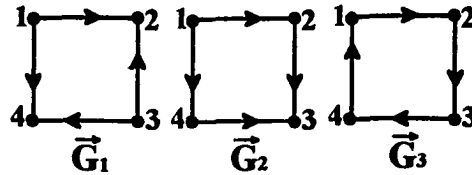


Figure 1. Three Oriented Graphs.

Barkauskas and Host [1] showed that the problem of determining whether an oriented graph has an efficient dominating set is NP-complete.

1.2 Efficient Dominating Sets of Trees

For trees we have the following proposition (also mentioned in [1]):

Proposition 2 *Each orientation of a tree T produces at most one efficient dominating set.*

Proof: Assume \vec{T} is an orientation of tree T and suppose, to the contrary, that \vec{T} has two efficient dominating sets, S_1 and S_2 . Since $S_1 \neq S_2$, we may assume, without loss of generality, that there exists a vertex $v_1 \in S_1 - S_2$. Now, v_1

must be dominated by a unique vertex $w_1 \in S_2 - S_1$. Similarly, since $w_1 \in S_2 - S_1$, w_1 must be dominated by a unique vertex $v_2 \in (S_1 - v_1) - S_2$ and so on. Since \vec{T} is acyclic, this process never repeats a vertex. Thus we have an infinite directed path $v_1 w_1 v_2 w_2 \dots$, contradicting the finite order of \vec{T} . \square

As an immediate consequence, we have the theorem:

Theorem 1 *The number of efficient dominating sets for a tree T is equal to the number of orientations for which T can be efficiently dominated.*

The significance of this theorem is that it allows us to replace the problem of counting the number of efficient dominating sets for a tree T by the problem of counting the number of orientations, each of which has an efficient dominating set of T .

Since each unlabeled tree T of order p has at most 2^{p-1} orientations and each labeled tree of order p has exact 2^{p-1} orientations, from Proposition 1 and Proposition 2 we have the following theorem:

Theorem 2 *The number of efficient dominating sets for an unlabeled or for a labeled tree T of order p lies between 1 and 2^{p-1} .*

For basic terminologies the readers are referred to Chartrand and Lesniak [7]. For related results, see [1], [2], [3], [4], [5], and [6].

CHAPTER II

EFFICIENT DOMINATING SETS IN UNLABELED ORIENTED TREES

We would like to enumerate the number of efficient dominating sets in rooted and in unrooted trees. In order to accomplish this work, we introduce four ordinary generating functions and obtain recursive formulas for the number of efficient dominating sets for rooted trees. Then we find the recursive formulas for the number of efficient dominating sets for unrooted trees. Finally, we use asymptotic analysis and obtain asymptotic formulas.

The notation and terminology follow that in Harary and Palmer [11] (Chapt. 9.5). In particular, $Z(S_n) = Z(S_n; s_1, s_2, \dots, s_n)$ is the cycle index for the symmetric group S_n acting on n objects. This is a polynomial in n variables s_1, s_2, \dots, s_n . For any generating function $g(x)$, $Z(S_n; g(x))$ is a shorthand representation of the substitution $s_1 = g(x), s_2 = g(x^2) \dots$ in $Z(S_n)$.

2.1 Generating Functions

We let

$$A(x) = \sum_{p=1}^{\infty} A_p x^p \tag{1}$$

be the generating function in which A_p is the number of efficient dominating sets among all rooted trees of order p which have the root in the dominating set. (The root is dominated by itself.)

Let

$$C(x) = \sum_{p=1}^{\infty} C_p x^p \quad (2)$$

be the generating function in which C_p is the number of efficient dominating sets among all rooted trees of order p which have the root dominated by one of its children. (The root is dominated from inside.)

We let the third series be

$$B(x) = \sum_{p=1}^{\infty} B_p x^p. \quad (3)$$

In this series $B(x)$, we would like to count sets that are nearly efficient dominating sets. With the exception of the root, every vertex in such a tree will be efficiently dominated by a unique vertex in the dominating set S . But the root is neither in S nor is it dominated by any vertex in S . Such an oriented tree is *not* efficiently dominated, but it can be a branch in a larger efficiently dominated oriented tree provided that the new root is in the efficient dominating set of the larger tree and the new root dominates the root of the branch. Consequently we refer to this case as the root being dominated from outside.

It is not necessary, but for convenience we introduce a fourth series. Let

$$E(x) = \sum_{p=1}^{\infty} E_p x^p \quad (4)$$

be the generating function in which E_p is the number of efficient dominating sets among all rooted trees of order p .

Observe that the number of efficient dominating sets among all rooted trees of order p equals $A_p + C_p$ since for any efficient dominating set S , the root must either be in S or be dominated by one of its children.

Thus we have

$$E(x) = A(x) + C(x). \quad (5)$$

It may seem that $B(x)$ is not involved in counting the number of efficient dominating sets, but we shall soon see that it is needed to calculate $A(x)$ and $C(x)$.

2.2 Functional Relations for the Counting Series

Our object is to find the number of efficient dominating sets among all rooted trees of order p . In the previous section we saw that this number is equal to $A_p + C_p$. We first find the functional relations among $A(x)$, $B(x)$ and $C(x)$ then generate A_p, B_p, C_p for every p up to 150.

Theorem 3 *For the functions introduced in (1), (2) and (3), the following equations hold:*

$$A(x) = x \left[\sum_{n=0}^{\infty} Z(S_n, B(x)) \right] \left[\sum_{n=0}^{\infty} Z(S_n, C(x)) \right] \quad (6)$$

$$B(x) = x \left[\sum_{n=0}^{\infty} Z(S_n, A(x)) \right] \left[\sum_{n=0}^{\infty} Z(S_n, 2C(x)) \right] \quad (7)$$

$$C(x) = A(x)B(x). \quad (8)$$

Proof: First observe by Proposition 2 that if \vec{T} is an oriented tree having an efficient dominating set, then every branch of \vec{T} must be one of type A, type B or type C. On the other hand, any oriented tree \vec{T} that is type A, type B or

type C must have the property that it is built by a root and some (possibly none) oriented branches (of type A , type B or type C). Further, the oriented edges joining the root of \vec{T} with the roots of the branches must be oriented "suitably".

Now we examine the structure of rooted trees of type A , type B and type C .

For rooted trees of type A , any branch of type A is invalid. On the other hand it can have any number of branches of type B if the edge is oriented from the root of the tree to the root of the branch, and it can have any number of branches of type C if the edge is oriented from the root of the branch to the root of the tree. See Figure 2.

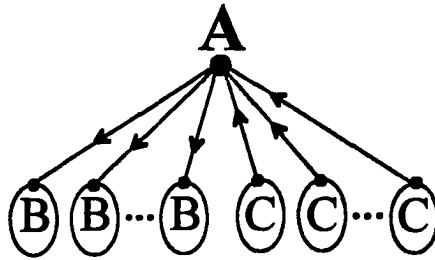


Figure 2. The Structure of a Rooted Tree of Type A .

This allows us to deduce the following equation for $A(x)$:

$$A(x) = x \left[\sum_{n=0}^{\infty} Z(S_n, B(x)) \right] \left[\sum_{n=0}^{\infty} Z(S_n, C(x)) \right]. \quad (9)$$

In this expression, the factor x accounts for the root. Each $Z(S_n, B(x))$ allows for n branches of type B . And similarly, each $Z(S_n, C(x))$ allows n branches of type C . Thus the structure shown in Figure 2 leads us to equation (9).

For rooted trees of type B , any branch of type B is invalid. It can have any number of branches of type A if the edge is oriented from the root of the tree to

the root of the branch, and it can have any number of branches of type C whose edge can be oriented in either direction. See Figure 3.

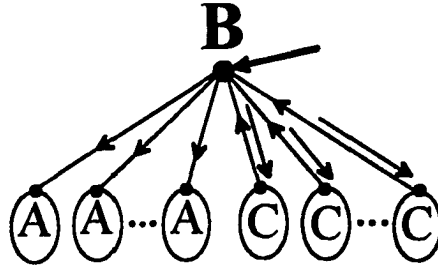


Figure 3. The Structure of a Rooted Tree of Type B.

So

$$B(x) = x \left[\sum_{n=0}^{\infty} Z(S_n, A(x)) \right] \left[\sum_{n=0}^{\infty} Z(S_n, 2C(x)) \right]. \quad (10)$$

For rooted trees of type C , it must have precisely one branch type A and the rest of it must be a rooted tree of type B . Also the edge must be oriented from the root of the branch to the root of the tree of type B . See Figure 4.

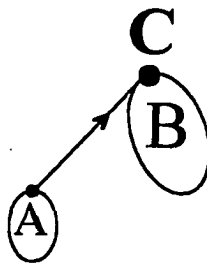


Figure 4. The Structure of a Rooted Tree of Type C.

So

$$C(x) = A(x)B(x). \quad (11)$$

□

2.3 Recurrence Relations and Numerical Values for Rooted Trees

Although the following three equations can be derived from (1), (2) and (3) (see [11]), we would like to use combinatorial arguments to obtain them.

$$A(x) = x \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{B_k + C_k} \quad (12)$$

$$B(x) = x \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{A_k + 2C_k} \quad (13)$$

$$C(x) = A(x)B(x). \quad (14)$$

See Figure 2 again, we examine the following expression:

$$x \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{B_k} \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{C_k}. \quad (15)$$

In this expression, x counts the root. The number 1 represents no branch of order k ; the term x^k represents one branch of order k , x^{2k} represents two branches of order k , and so on. The number B_k represents the number of ways to select a branch of type B of order k , C_k represents the number of ways to select a branch of type C of order k .

Then observe that the product of all these is, by the structure of type A , $A(x)$. That is equation (12). By the same fashion arguments, we can get (13).

And of course (14) is true.

Knowing that $A_1 = 1$, $B_1 = 1$, $C_1 = 0$, theoretically these recurrence relations allow us to compute A_p , B_p , C_p for any particular p . For example, if we want to calculate A_m , B_m , C_m , we only need to know A_p , B_p , C_p for each p up to $m - 1$.

In order to determine A_p , B_p , C_p for each p up to 150 more efficiently we need to modify (12), (13) and (14).

In equation (12) we rewrite the geometric series and then use the binomial theorem with negative exponents to get

$$\begin{aligned}
 A(x) &= x \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{B_k + C_k} \\
 &= x \prod_{k=1}^{\infty} (1 - x^k)^{-B_k - C_k} \\
 &= x \prod_{k=1}^{\infty} \sum_{l=0}^{\infty} \binom{B_k + C_k + l - 1}{l} x^{kl}.
 \end{aligned} \tag{16}$$

Similarly, from (13) we have

$$B(x) = x \prod_{k=1}^{\infty} \sum_{l=0}^{\infty} \binom{A_k + 2C_k + l - 1}{l} x^{kl}. \tag{17}$$

Formally expanding the product of two series in (14) gives

$$C(x) = \sum_{n=2}^{\infty} \left(\sum_{k=1}^{n-1} A_k B_{n-k} \right) x^n. \tag{18}$$

To find out the formulas to calculate A_p , B_p , C_p for each p up to 150, we first introduce some notation. Let $f(x) = \sum_{n=0}^{\infty} f_n x^n$ be any power series, then

$[x^p]f(x) = f_p$. For example $[x^p]e^{-x} = \frac{(-1)^p}{p!}$.

Now suppose we would like to find A_m , B_m , and C_m ($1 \leq m \leq 150$), then

$$A_m = [x^m] \left[x \prod_{k=1}^{m-1} \sum_{l=0}^{\lfloor \frac{m-1}{k} \rfloor} \binom{B_k + C_k + l - 1}{l} x^{kl} \right] \quad (19)$$

$$B_m = [x^m] \left[x \prod_{k=1}^{m-1} \sum_{l=0}^{\lfloor \frac{m-1}{k} \rfloor} \binom{A_k + 2C_k + l - 1}{l} x^{kl} \right] \quad (20)$$

$$C_m = \sum_{k=1}^{m-1} A_k B_{m-k}. \quad (21)$$

With the aid of a computer and *Mathematica*, these three formulas provide A_p , B_p , and C_p for each p up to 150.

2.4 Equations and Numerical Values for Unrooted Trees

Now we are in the position to determine the number of efficient dominating sets among all unrooted trees of order p .

We have seen that

$$E(x) = A(x) + C(x) \quad (22)$$

is the generating function in which E_p is the number of efficient dominating sets among all rooted trees of order p .

We let

$$e(x) = \sum_{p=1}^{\infty} e_p x^p \quad (23)$$

be the generating function in which e_p is the number of efficient dominating sets

among all unrooted trees of order p .

Theorem 4 *The counting series $e(x)$ satisfies*

$$e(x) = A(x) - A(x)C(x) - C^2(x). \quad (24)$$

Proof: We will use the following Theorem (Dissimilarity characteristic theorem for trees) due to Otter [13] and presented in [11].

Theorem 5 *For any tree T of order p*

$$1 = p^* - q^* + s. \quad (25)$$

In the equation p^* is the number of dissimilar vertices of T , or more precisely, the number of equivalence classes of vertices of T under action of the symmetric group of S_p ; q^* is the number of dissimilar edges of T , or more precisely, the number of equivalence classes of edges of T under action of the symmetric group of S_p ; s is the number of symmetric edges of T under action of the symmetric group of S_p .

To illustrate the Theorem 5, we look the tree T_1 and the tree T_2 both of order 8 in Figure 5.

For tree T_1 , $p^* = 5$, $q^* = 4$ and $s = 0$, so $1 = p^* - q^* + s$. For tree T_2 , $p^* = 4$, $q^* = 4$ and $s = 1$, hence $1 = p^* - q^* + s$.

Observe that each unrooted tree T can give rise to exactly p^* different rooted trees and each unrooted tree T can be “rooted” at an edge in q^* different ways. Also observe that for any unrooted tree T , two end vertices of a symmetric edge (if there is any) must be in the center of T . So s equals 0 or 1.

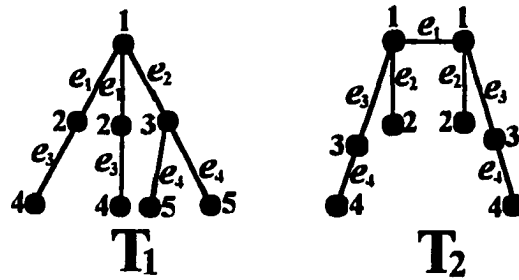


Figure 5. Two Trees of Order 8.

Now we apply Theorem 5 to our problem. First note $s = 0$ since there is no symmetric edge in any oriented tree. Sum (25) over all unrooted oriented trees that have an efficient dominating set and that have exactly p vertices. The result is

$$\sum 1 = \sum p^* - \sum q^* \quad (26)$$

but $\sum 1 = e_p$ and $\sum p^* = E_p$. Furthermore, $\sum q^*$ is the number of efficient dominating sets among all trees that are rooted at an edge and have the order of p . There are nine possible ways to attach two oriented branches to an rooted edge, but only three ways are valid. First, if the receiving branch is type A then the sending branch must be type C . Secondly, if the receiving branch is type B then the sending branch must be type A . Thirdly, if the receiving branch is type C then the sending branch must be type C . See Figure 6.

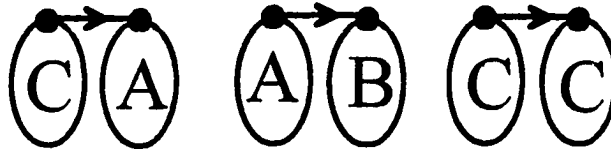


Figure 6. Three Ways to Attach Two Oriented Branches to an Rooted Edge.

Consequently, we have

$$e(x) = E(x) - [A(x)C(x) + B(x)A(x) + C(x)C(x)], \quad (27)$$

or

$$e(x) = E(x) - A(x)B(x) - A(x)C(x) - C^2(x). \quad (28)$$

Recalling that $E(x) = A(x) + C(x)$ and $C(x) = A(x)B(x)$, we get

$$e(x) = A(x) - A(x)C(x) - C^2(x). \quad (29)$$

□

We have A_p, B_p and C_p for every p up to 150 in hand, using (29) we can determine e_p for each p up to 150.

Results of the computations for A_p, B_p, E_p , and e_p for each p up to 20 are reported in Table 1.

2.5 Asymptotic Behavior

In order to determine the asymptotic formulas, we need several lemmas. The first lemma allows us to treat each generating function $A(x), B(x), C(x)$ and $e(x)$ as an analytic function.

Lemma 1 *The power series $A(x)$, $B(x)$ and $C(x)$ all have radius of convergence greater than 0.169.*

Proof: For each rooted tree T of order p ($p \geq 1$), by Theorem 2 the tree T has at most 2^{p-1} efficient dominating sets. As a consequence, each of A_p, B_p , and C_p is bounded above by $2^{p-1}T_p$, where T_p is the number of rooted trees of order p .

Table 1

The Numerical Values of A_p, B_p, E_p and e_p ($1 \leq p \leq 20$)

p	A_p	B_p	E_p	e_p
1	1	1	1	1
2	1	1	2	1
3	3	4	5	2
4	9	11	17	5
5	31	42	58	14
6	112	148	217	42
7	428	583	830	137
8	1683	2287	3303	467
9	6804	9345	13396	1668
10	28055	38597	55501	6163
11	1 17555	1 62473	2 33196	23400
12	4 99119	6 91346	9 92771	90858
13	21 42582	29 75398	42 70258	3 59463
14	92 83573	129 15543	185 35850	14 44592
15	405 46937	565 07803	810 78383	58 83938
16	1783 24751	2488 74733	3570 51942	242 45484
17	7890 41103	11026 26017	15816 77036	1009 24208
18	35100 74658	49105 72241	70433 14680	4238 78271
19	1 56893 34712	2 19714 13534	3 15107 57851	17944 67452
20	7 04285 06010	9 87172 06083	14 15650 84066	76509 56373

Now let r_a, r_b, r_c denote the radius of convergence for $A(x), B(x)$ and $C(x)$ respectively, then

$$r_a = \frac{1}{\lim_{p \rightarrow \infty} \sqrt[p]{A_p}} \geq \frac{1}{\lim_{p \rightarrow \infty} \sqrt[p]{2^{p-1}T_p}} \geq \frac{1}{2 \lim_{p \rightarrow \infty} \sqrt[p]{T_p}} = \frac{0.338...}{2} > 0.169 \quad (30)$$

where 0.338... is well known as the radius of convergence for $T(x) = \sum_{p=1}^{\infty} T_p x^p$.

In the same fashion

$$r_b > 0.169 \text{ and } r_c > 0.169. \quad (31)$$

□

Lemma 2 *The power series $A(x), B(x)$ and $C(x)$ have the same radius of convergence.*

That is $r = r_a = r_b = r_c$.

Proof: Recall that

$$A(x) = x \prod_{k=1}^{\infty} (1 + x^k + x^{2k} + \dots)^{B_k + C_k}. \quad (32)$$

Dividing both sides by x and then taking logarithm on both sides gives us

$$\log\left(\frac{A(x)}{x}\right) = \sum_{k=1}^{\infty} (B_k + C_k) \log(1 + x^k + x^{2k} + \dots)$$

$$\log\left(\frac{A(x)}{x}\right) = \sum_{k=1}^{\infty} (B_k + C_k) \log(1 - x^k)^{-1}$$

$$\begin{aligned}
\log\left(\frac{A(x)}{x}\right) &= \sum_{k=1}^{\infty} (B_k + C_k) \sum_{j=1}^{\infty} \frac{x^{jk}}{j} \\
\log\left(\frac{A(x)}{x}\right) &= \sum_{j=1}^{\infty} \frac{\sum_{k=1}^{\infty} (B_k + C_k) x^{jk}}{j} \\
\log\left(\frac{A(x)}{x}\right) &= \sum_{j=1}^{\infty} \frac{B(x^j) + C(x^j)}{j}.
\end{aligned} \tag{33}$$

Thus for any $x \in [0, r_a)$, we have

$$\begin{aligned}
A(x) &= x \exp\left(\sum_{j=1}^{\infty} \frac{B(x^j) + C(x^j)}{j}\right) \\
&= x \exp\left(B(x) + C(x) + \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j}\right) \\
&\geq x \exp(B(x) + C(x)).
\end{aligned} \tag{34}$$

From this we see that $r_a \leq r_b$ and $r_a \leq r_c$.

By a similar line of reasoning, for any $x \geq 0$, we obtain

$$\begin{aligned}
B(x) &= x \exp\left(\sum_{j=1}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}\right) \\
&= x \exp\left(A(x) + 2C(x) + \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}\right) \\
&\geq x \exp(A(x) + 2C(x)).
\end{aligned} \tag{35}$$

From this we see that $r_b \leq r_a$ and $r_b \leq r_c$.

And of course we have

$$C(x) = A(x)B(x). \tag{36}$$

From this it is easy to see $r_c \leq r_a$ and $r_c \leq r_b$. All these inequalities together imply

$$r = r_a = r_b = r_c. \quad (37)$$

□

Lemma 3 *The limits of $A(x)$, $B(x)$ and $C(x)$ as $x \rightarrow r^-$ exist and are equal to $A(r)$, $B(r)$ and $C(r)$, respectively. Consequently, each of $A(x)$, $B(x)$ and $C(x)$ has the unique singularity at $x = r$ on the circle of convergence.*

Proof: Since $A(x)$ satisfies the functional equation (33), for all x in $(0, r)$ we have

$$\log(A(x)/x) = B(x) + C(x) + \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j} \geq C(x). \quad (38)$$

From this it follows that

$$\frac{C(x)/x}{\log(A(x)/x)} \leq \frac{1}{x}. \quad (39)$$

Note that $C(x) = A(x)B(x)$. Then we have

$$B(x) \frac{(A(x)/x)}{\log(A(x)/x)} \leq \frac{1}{x}. \quad (40)$$

Hence both $A(x)$ and $B(x)$ are bounded above on the interval $(0, r)$. Since both $A(x)$ and $B(x)$ are monotone increasing with respect to x , the left limits at r must exist and we have

$$a = \lim_{x \rightarrow r^-} A(x) = A(r) \quad (41)$$

$$b = \lim_{x \rightarrow r^-} B(x) = B(r) \quad (42)$$

$$ab = \lim_{x \rightarrow r^-} A(x)B(x) = A(r)B(r). \quad (43)$$

□

Lemma 4 *For the series $A(x)$ and $B(x)$, the following equality holds:*

$$a^2b + 2ab^2 + 4ab = 1. \quad (44)$$

Proof: We first define the complex valued functions $F(x, y, z)$ and $G(x, y, z)$, where x, y and z are considered as complex variables:

$$\left. \begin{aligned} F(x, y, z) &= x \exp\left(z + yz + \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j}\right) - y \\ G(x, y, z) &= x \exp\left(y + 2yz + \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}\right) - z \end{aligned} \right\} \quad (45)$$

and consider the equations

$$\left. \begin{aligned} F(x, y, z) &= 0 \\ G(x, y, z) &= 0 \end{aligned} \right\}. \quad (46)$$

We can show that

$$\left. \begin{aligned} y &= A(x) \\ z &= B(x) \end{aligned} \right\} \quad (47)$$

is the unique analytic solution of (46) in the open disk of $|x| < r$.

Note that for fixed y and z , the functions $F(x, y, z)$ and $G(x, y, z)$ have a unique singularity at $x = r$ on the circle of $|x| = r$. The previous lemma implies that $F(r, a, b) = 0$ and $G(r, a, b) = 0$. Furthermore note that $F(x, y, z)$ and $G(x, y, z)$ are both analytic in each variable *separately* in a neighborhood of (r, a, b) .

Now since

$$\left. \begin{aligned} F(r, a, b) &= 0 \\ G(r, a, b) &= 0 \end{aligned} \right\} \quad (48)$$

we know, by the implicit function theorem, that the determinant

$$\begin{vmatrix} F_y & F_z \\ G_y & G_z \end{vmatrix}$$

at the point (r, a, b) must be zero; otherwise, there are the unique solutions $y = y(x)$ and $z = z(x)$ in (45). Both functions of $y(x)$ and $z(x)$ are analytic in a neighborhood of r , especially at $x = r$. Such solutions have to be $y = A(x)$ and $z = B(x)$ but clearly *neither* $A(x)$ *nor* $B(x)$ is analytic at $x = r$.

Now the determinant at the point (r, a, b) is

$$\begin{aligned} \begin{vmatrix} F_y & F_z \\ G_y & G_z \end{vmatrix}_{\substack{x=r \\ y=a \\ z=b}} &= \begin{vmatrix} z(F+y)-1 & (1+y)(F+y) \\ (1+2z)(G+z) & 2y(G+z)-1 \end{vmatrix}_{\substack{x=r \\ y=a \\ z=b}} \\ &= \begin{vmatrix} ab-1 & a^2+a \\ 2b^2+b & 2ab-1 \end{vmatrix} \\ &= -a^2b - 2ab^2 - 4ab + 1. \end{aligned}$$

Letting $-a^2b - 2ab^2 - 4ab + 1 = 0$, we get $a^2b + 2ab^2 + 4ab = 1$. \square

Lemma 5 *Each of the numerical values for r , a and b is bounded above by $r \leq 0.34$, $a \leq 1$ and $b \leq 1$. Consequently,*

$$\sum_{j=1}^{\infty} \frac{B(r^j) + C(r^j)}{j} < 2 \text{ and } \sum_{j=1}^{\infty} \frac{A(r^j) + 2C(r^j)}{j} < 2. \quad (49)$$

Proof: We first show that $r \leq 0.34$. Recall that Proposition 1 guarantees every rooted tree has at least one orientation \vec{T} such that \vec{T} has an efficient dominating set. This gives $E_p \geq T_p$ for each p , where we recall that E_p is the number of efficient dominating sets among all oriented rooted trees of order p and T_p is the number of rooted trees of order p . From $E_p \geq T_p$, we get $r \leq 0.338... < 0.34$, where $0.338...$ is the radius of convergence for $T(x) = \sum_{p=1}^{\infty} T_p x^p$.

To show $a \leq 1$, we assume that $a > 1$. Recall that (35) states

$$B(x) = x \exp(A(x) + 2C(x) + \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}). \quad (50)$$

Letting x approach to r from left on both sides of (50), we get

$$b = r \exp(a + 2ab + \sum_{j=2}^{\infty} \frac{A(r^j) + 2C(r^j)}{j}) \geq r \exp(a).$$

Recalling that $r > 0.169$ and the assumption of $a > 1$, we have $b > 0.169e > 0.45$.

Now since $a > 1$ and $b > 0.45$ we could get $a^2b + 2ab^2 + 4ab \geq 4ab > 1$, contradicting Lemma 4. Thus $a \leq 1$.

By similar arguments, we can show $b \leq 1$.

By $b = r \exp(\sum_{j=1}^{\infty} \frac{A(r^j) + 2C(r^j)}{j})$, $r > 0.169$, and $b \leq 1$, we get

$$\sum_{j=1}^{\infty} \frac{A(r^j) + 2C(r^j)}{j} \leq \log\left(\frac{1}{0.169}\right) < 2. \quad (51)$$

Likewise, we have

$$\sum_{j=1}^{\infty} \frac{B(r^j) + C(r^j)}{j} < 2. \quad (52)$$

Note that (34) and (35) give us

$$a = r \exp\left(\sum_{j=1}^{\infty} \frac{B(r^j) + C(r^j)}{j}\right) \quad (53)$$

and

$$b = r \exp\left(\sum_{j=1}^{\infty} \frac{A(r^j) + 2C(r^j)}{j}\right). \quad (54)$$

We would like to use the truncated series with 150 terms of $\sum_{j=1}^{\infty} \frac{B(r^j) + C(r^j)}{j}$ and $\sum_{j=1}^{\infty} \frac{A(r^j) + 2C(r^j)}{j}$ in (53) and (54) to find numerical values of r , a and b . To ensure accuracy, we need to analyze the errors created by truncating the series after 150 terms. We use $r_t = a / \exp(\sum_{j=1}^{150} \frac{B(r^j) + C(r^j)}{j})$, $a_t = r \exp(\sum_{j=1}^{150} \frac{B(r^j) + C(r^j)}{j})$, and $b_t = r \exp(\sum_{j=1}^{150} \frac{A(r^j) + 2C(r^j)}{j})$ to denote the values given by the truncated series. The next lemma guarantees the accuracy for r , a and b after we excise the “tails” $\delta_1 = \sum_{j=151}^{\infty} \frac{B(r^j) + C(r^j)}{j}$ and $\delta_2 = \sum_{j=151}^{\infty} \frac{A(r^j) + 2C(r^j)}{j}$.

Lemma 6 *The following inequalities hold:*

$$\Delta r = |r - r_t| \leq 10^{-69} \quad (55)$$

$$\Delta a = |a - a_t| \leq 10^{-69} \quad (56)$$

$$\Delta b = |b - b_t| \leq 10^{-69}. \quad (57)$$

Proof: We first estimate the remainders $\delta_1 = \sum_{j=151}^{\infty} \frac{B(r^j) + C(r^j)}{j}$ and $\delta_2 = \sum_{j=151}^{\infty} \frac{A(r^j) + 2C(r^j)}{j}$ and show that

$$\delta_1 \leq 1.06 \times 10^{-70} \text{ and } \delta_2 \leq 1.06 \times 10^{-70}. \quad (58)$$

Observe that

$$\begin{aligned} \delta_1 &= \sum_{j=151}^{\infty} \frac{B(r^j) + C(r^j)}{j} = \sum_{j=151}^{\infty} \frac{\sum_{k=1}^{\infty} (B_k r^{jk} + C_k r^{jk})}{j} \\ &= \sum_{j=151}^{\infty} \frac{r^{150}}{j} \left[\sum_{k=1}^{\infty} B_k r^{jk-150} + C_k r^{jk-150} \right] \\ &= r^{150} \sum_{j=151}^{\infty} \frac{1}{j} \left[\sum_{k=1}^{\infty} B_k r^{jk-150} + C_k r^{jk-150} \right] \\ &= r^{150} \sum_{j=1}^{\infty} \frac{1}{(j+150)} \left[\sum_{k=1}^{\infty} B_k r^{(j+150)k-150} + C_k r^{(j+150)k-150} \right] \\ &= r^{150} \sum_{j=1}^{\infty} \frac{1}{(j+150)} \left[\sum_{k=1}^{\infty} B_k r^{jk+150(k-1)} + C_k r^{jk+150(k-1)} \right]. \end{aligned}$$

Since $r < 1$, we may discard part of the exponents to obtain the bound

$$\begin{aligned}
\delta_1 &\leq r^{150} \sum_{j=1}^{\infty} \frac{1}{(j+150)} \left[\sum_{k=1}^{\infty} B_k r^{jk} + C_k r^{jk} \right] \\
&< r^{150} \sum_{j=1}^{\infty} \frac{(B(r^j) + C(r^j))}{j} \leq (0.34)^{150} \times 2 \quad (\text{by lemma 5}) \\
&\leq 1.06 \times 10^{-70}.
\end{aligned}$$

Similarly, we have $\delta_2 = \sum_{j=151}^{\infty} \frac{A(r^j) + 2C(r^j)}{j} \leq 1.06 \times 10^{-70}$.

Rewriting (53), we find that

$$a = r \exp\left(\sum_{j=1}^{150} \frac{B(r^j) + C(r^j)}{j} + \delta_1\right),$$

which gives $a = a_t e^{\delta_1}$ and

$$r = \frac{a}{\exp\left(\sum_{j=1}^{150} \frac{B(r^j) + C(r^j)}{j} + \delta_1\right)} = \frac{r_t}{e^{\delta_1}}.$$

From this it follows that

$$\begin{aligned}
\Delta r &= |r - r_t| = |r - r e^{\delta_1}| = r(e^{\delta_1} - 1) = r\left[\left(1 + \delta_1 + \frac{\delta_1^2}{2!} + \dots\right) - 1\right] \\
&\leq r \delta_1 e \leq 0.34 \times (1.06 \times 10^{-70}) e \leq 10^{-69}
\end{aligned}$$

and

$$\begin{aligned}
\Delta a &= |a - a_t| = |a_t e^{\delta_1} - a_t| = a_t(e^{\delta_1} - 1) = a_t\left[\left(1 + \delta_1 + \frac{\delta_1^2}{2!} + \dots\right) - 1\right] \\
&\leq a_t \delta_1 e \leq a \delta_1 e \leq 1 \times (1.06 \times 10^{-70}) e \leq 10^{-69}.
\end{aligned}$$

Likewise,

$$b = r \exp\left(\sum_{j=1}^{150} \frac{B(r^j) + C(r^j)}{j} + \delta_2\right)$$

gives $\Delta b = |b - b_i| \leq b_i \delta_2 e \leq b \delta_2 e \leq 1 \times (1.06 \times 10^{-70})e \leq 10^{-69}$. \square

Lemma 7 *The approximation values for r, a and b are as follows:*

$$\left. \begin{aligned} r &= 0.206\ 079\ 634\ 299\ 225\dots \\ a &= 0.405\ 548\ 150\ 115\ 438\dots \\ b &= 0.462\ 567\ 127\ 877\ 550\dots \end{aligned} \right\}. \quad (59)$$

Proof: By the previous lemma, we can use

$$a = r \exp\left(b + ab + \sum_{j=2}^{150} \frac{B(r^j) + C(r^j)}{j}\right) \quad (60)$$

and

$$b = r \exp\left(a + 2ab + \sum_{j=2}^{150} \frac{A(r^j) + 2C(r^j)}{j}\right) \quad (61)$$

to calculate r, a and b with a guaranteed accuracy of 10^{-69} .

Solving $a^2b + 2ab^2 + 4ab = 1$ for a , we obtain

$$a = \frac{1}{\sqrt{b^2(b+2)^2 + b} + b(b+2)}. \quad (62)$$

From (60) and (61), we obtain

$$r = a \exp\left[-(b + ab + \sum_{j=2}^{150} \frac{B(r^j) + C(r^j)}{j})\right] \quad (63)$$

and

$$b = a \exp\left(a + ab - b + \sum_{j=2}^{150} \frac{A(r^j) + C(r^j) - B(r^j)}{j}\right). \quad (64)$$

The following iteration scheme converges:

$$\left. \begin{aligned}
 r_0 &= 0.34 \\
 b_0 &= 1 \\
 a_0 &= \frac{1}{\sqrt{b_0^2(b_0 + 2)^2 + b_0 + b_0(b_0 + 2)}} \\
 r_{i+1} &= \frac{1}{2} \left[r_i + a_i \exp \left[- (b_i + a_i b_i + \sum_{j=2}^{150} \frac{B(r_i^j) + C(r_i^j)}{j}) \right] \right] \\
 b_{i+1} &= \frac{1}{2} \left[b_i + a_i \exp (a_i + a_i b_i - b_i + \right. \\
 &\quad \left. \sum_{j=2}^{150} \frac{A(r_{i+1}^j) + C(r_{i+1}^j) - B(r_{i+1}^j)}{j} \right] \\
 a_{i+1} &= \frac{1}{2} \left[a_i + \frac{1}{\sqrt{b_{i+1}^2(b_{i+1} + 2)^2 + b_{i+1} + b_{i+1}(b_{i+1} + 2)}} \right]
 \end{aligned} \right\} . \quad (65)$$

Using (65), we determine r , a and b up to 69 digits after the decimal point.

The next theorem appears in Harary and Palmer [11].

Theorem 6 *For the function f suppose that the following conditions are satisfied:*

- 1.) $y = f(x)$ is analytic in $|x| < x_0$ and x_0 is the unique singularity on the circle of convergence;
- 2.) If $f(x) = \sum_{n=0}^{\infty} f_n x^n$ is the power expansion of $f(x)$ at the origin, then $y_0 = \sum_{n=0}^{\infty} f_n x_0^n$;
- 3.) There is a function $H(x, y)$ which is analytic in each variable separately in some neighborhood of (x_0, y_0) ;
- 4.) $H(x_0, y_0) = 0$;
- 5.) $H(x, f(x)) = 0$ for $|x| < x_0$;
- 6.) $\frac{\partial H}{\partial y}(x_0, y_0) = 0$;

$$7.) \quad \frac{\partial^2 H}{\partial y^2}(x_0, y_0) \neq 0.$$

Then $f(x)$ can be expanded about x_0 :

$$f(x) = f(x_0) + \sum_{k=1}^{\infty} l_k (x_0 - x)^{k/2}.$$

If $l_1 \neq 0$, then

$$f_n \sim \frac{-l_1(x_0)^{1/2}}{2\sqrt{\pi}} \left[\frac{(x_0)^{-n}}{n^{3/2}} \right].$$

And if $l_1 = 0$ but $l_3 \neq 0$, then

$$f_n \sim \frac{3l_3(x_0)^{3/2}}{4\sqrt{\pi}} \left[\frac{(x_0)^{-n}}{n^{5/2}} \right].$$

Lemma 8 *Each of the functions $A(x)$, $B(x)$, $C(x)$, and $e(x)$ satisfies the conditions in the Theorem 6.*

Proof: We begin by showing that $A(x)$ satisfies the conditions in Theorem 6.

Take $y = A(x)$ and $x_0 = r$; then it is easy to see that the conditions 1.) and 2.) are satisfied, and $y_0 = a$.

Recall that (45) states

$$\left. \begin{aligned} F(x, y, z) &= x \exp\left(z + yz + \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j}\right) - y \\ G(x, y, z) &= x \exp\left(y + 2yz + \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}\right) - z \end{aligned} \right\}$$

and (48) says that

$$\left. \begin{aligned} F(r, a, b) &= 0 \\ G(r, a, b) &= 0 \end{aligned} \right\},$$

where $z = B(x)$.

In $G(x, y, z) = x \exp(y + 2yz + \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}) - z$, observe that

$$G_z(r, a, b) = [2y(G + z)]_{\substack{x=r \\ y=a \\ z=b}} = 2ab - 1 \neq 0. \quad (66)$$

By the implicit function theorem, there is a unique solution $z = z(x, y)$ in some neighborhood of (r, a) with $z(r, a) = b$ and $z_y(r, a) = -\frac{G_y(r, a, b)}{G_z(r, a, b)}$.

Take

$$H(x, y) = F(x, y, z(x, y)) = x \exp(z(x, y) + yz(x, y) + \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j}) - y. \quad (67)$$

Then the function $H(x, y)$ is analytic in each variable separately in some neighborhood of (r, a) ; $H(r, a) = F(r, a, b) = 0$; $H(x, A(x)) = 0$ for $|x| < r$; thus, the conditions of 3.), 4.) and 5.) are satisfied.

To show condition 6.) is satisfied, note that

$$\begin{aligned} \frac{\partial H(x, y)}{\partial y} &= \left[\frac{\partial F(x, y, z)}{\partial y} + \frac{\partial F(x, y, z)}{\partial z} \frac{\partial z(x, y)}{\partial y} \right] \\ &= \{z(x, y)[F(x, y, z(x, y)) + y] - 1\} + (1 + y)[F(x, y, z(x, y)) + y] \left(\frac{-G_y}{G_z} \right). \end{aligned} \quad (68)$$

Since $z(r, a) = b$, $G_y(r, a, z(r, a)) = G_y(r, a, b) = 2b^2 + b$, $G_z(r, a, b) = 2ab - 1$, and $F(r, a, z(r, a)) = 0$, we have

$$\begin{aligned} \frac{\partial H}{\partial y}(r, a) &= [ba - 1] + (1 + a)a \left[\frac{-(2b^2 + b)}{2ab - 1} \right] \\ &= \frac{-a^2b - 2ab^2 - 4ab + 1}{2ab - 1} \\ &= 0 \text{ by Lemma 4.} \end{aligned}$$

So condition 6.) is satisfied.

To show condition 7.) is satisfied, note that

$$\begin{aligned}
\frac{\partial^2 H(x, y)}{\partial y^2} &= \frac{\partial^2 F(x, y, z)}{\partial y^2} + \frac{\partial^2 F(x, y, z)}{\partial y \partial z} \frac{\partial z(x, y)}{\partial y} \\
&+ \left[\frac{\partial^2 F(x, y, z)}{\partial z \partial y} + \frac{\partial^2 F(x, y, z)}{\partial z^2} \frac{\partial z(x, y)}{\partial y} \right] \frac{\partial z(x, y)}{\partial y} \quad (69) \\
&+ \frac{\partial F(x, y, z)}{\partial z} \frac{\partial^2 z(x, y)}{\partial y^2}.
\end{aligned}$$

Then we can show that $\frac{\partial^2 H}{\partial y^2}(r, a) \neq 0$. Therefore, $A(x)$ satisfies all conditions in Theorem 6.

By similar reasoning, $B(x)$, $C(x)$, and $e(x)$ satisfy all conditions in Theorem 6. \square

In view of Theorem 6, we see that in order to obtain the asymptotic formula for f_n , we need the value of l_1 or l_3 (in the case of $l_1 = 0$). Later we shall see that in order to get the value of l_1 or l_3 , the derivative $f'(x)$ is needed. For our problem we need $A'(x)$ and $B'(x)$. The next lemma is developed to find $A'(x)$ and $B'(x)$.

Lemma 9 *The derivatives $A'(x)$ and $B'(x)$ take the following expressions:*

$$A'(x) = \frac{NA(x)}{D(x)} \quad (70)$$

$$B'(x) = \frac{NB(x)}{D(x)} \quad (71)$$

where

$$NA(x) = -A(x)[1 + B(x) - C(x) + xP'(x) - 2xC(x)P'(x) + xB(x)Q'(x) + xC(x)Q'(x)], \quad (72)$$

$$NB(x) = -B(x)[1 + A(x) + C(x) + xQ'(x) + 2xC(x)P'(x) + xA(x)P'(x) - xC(x)Q'(x)], \quad (73)$$

$$P(x) = \sum_{j=2}^{\infty} \frac{B(x^j) + C(x^j)}{j}, \quad (74)$$

$$Q(x) = \sum_{j=2}^{\infty} \frac{A(x^j) + 2C(x^j)}{j}, \quad (75)$$

and

$$D(x) = x[A^2(x)B(x) + 2A(x)B^2(x) + 4A(x)B(x) - 1]. \quad (76)$$

Proof: Observe that (34) and (35) give us

$$A(x) = x \exp(B(x) + C(x) + P(x)) \quad (77)$$

and

$$B(x) = x \exp(A(x) + 2C(x) + Q(x)). \quad (78)$$

Taking derivatives on both sides of (77), we get

$$A'(x) = \frac{A(x)}{x} + A(x)(B'(x) + C'(x) + P'(x)). \quad (79)$$

Recalling that $C(x) = A(x)B(x)$ hence we have that $C'(x) = A(x)B'(x) + A'(x)B(x)$, we have, after substituting in (79) and simplifying,

$$[A(x)B(x) - 1]A'(x) + [A^2(x) + A(x)]B'(x) + \frac{A(x)}{x} + A(x)P'(x) = 0. \quad (80)$$

In the same fashion, when we take derivatives on both sides of (78) and simplify, we get

$$[2B^2(x) + B(x)]A'(x) + [2A(x)B(x) - 1]B'(x) + \frac{B(x)}{x} + B(x)Q'(x) = 0. \quad (81)$$

Solving the system

$$\left. \begin{aligned} [A(x)B(x) - 1]A'(x) + [A^2(x) + A(x)]B'(x) + \frac{A(x)}{x} + A(x)P'(x) &= 0 \\ [2B^2(x) + B(x)]A'(x) + [2A(x)B(x) - 1]B'(x) + \frac{B(x)}{x} + B(x)Q'(x) &= 0 \end{aligned} \right\} \quad (82)$$

for $A'(x)$ and $B'(x)$, we obtain (70) and (71). \square

Before stating the next theorem, we note that we can find $A''(x)$, $B''(x)$, $D'(x)$, $e'(x)$, $e''(x)$, and $e'''(x)$ simply by repeatedly using (70) and (71). Also from (76) and Lemma 4, we see that

$$\lim_{x \rightarrow r^-} D(x) = 0. \quad (83)$$

Theorem 7 *The numbers A_p, B_p, C_p, E_p , and e_p satisfy*

$$A_p = 0.118\ 225\ 232\ 019\ 274 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (84)$$

$$B_p = 0.168\ 498\ 309\ 958\ 195 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (85)$$

$$C_p = 0.123\ 021\ 283\ 918\ 936 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (86)$$

$$E_p = 0.241\ 246\ 515\ 938\ 211 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (87)$$

$$e_p = 0.256\ 881\ 825\ 127\ 051 \frac{r^{-p}}{p^{5/2}} + O\left(\frac{r^{-p}}{p^{7/2}}\right). \quad (88)$$

Proof: We have seen by Lemma 8 that $A(x)$, $B(x)$, $C(x)$, and $e(x)$ all satisfy the conditions in Theorem 6.

To apply Theorem 6 to the function $A(x)$ note that $(x_0, y_0) = (r, a)$, $A(r) = a$, and $f(x) = A(x)$. Thus $A(x)$ can be expanded as

$$A(x) = a - l_1(r - x)^{1/2} + l_2(r - x) + l_3(r - x)^{3/2} + \dots \quad (89)$$

and if $l_1 \neq 0$, then

$$A_p \sim \frac{l_1(r)^{1/2}}{2\sqrt{\pi}} \left[\frac{(r)^{-p}}{p^{3/2}} \right]. \quad (90)$$

So we need the numerical value for l_1 .

Before we go on to find this numerical value for l_1 , we introduce notation designed to suppress terms in the series that do not affect the limit. We define $\omega(\theta)$ as a function of θ with the property that $\lim_{\theta \rightarrow 0^+} \frac{\omega(\theta)}{\theta} = c$ exists; consequently, $\lim_{\theta \rightarrow 0^+} \omega(\theta) = 0$.

After differentiating (89), we have

$$A'(x) = \frac{1}{2}l_1(r - x)^{-1/2} - l_2 + \omega((r - x)^{1/2}). \quad (91)$$

On the other hand, rearranging (89), we have

$$a - A(x) = l_1(r - x)^{1/2} + \omega((r - x)). \quad (92)$$

Hence from (91) and (92) we have

$$A'(x)(a - A(x)) = \frac{1}{2}l_1^2 + \omega((r - x)^{1/2}). \quad (93)$$

Therefore we get

$$\lim_{x \rightarrow r^-} A'(x)(a - A(x)) = \frac{1}{2}l_1^2. \quad (94)$$

Note that $\lim_{x \rightarrow r^-} (a - A(x)) = 0$. At the same time observe by (70) and (83) that $\lim_{x \rightarrow r^-} A'(x) = +\infty$. So by L'Hospital's Rule, we have

$$\lim_{x \rightarrow r^-} A'(x)(a - A(x)) = \lim_{x \rightarrow r^-} \frac{(a - A(x))}{\frac{1}{A'(x)}} = \lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)}. \quad (95)$$

Using (70) we have

$$\begin{aligned} \lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)} &= \lim_{x \rightarrow r^-} \frac{[NA(x)/D(x)]^3}{[D(x)NA'(x) - D'(x)NA(x)]/D^2(x)} \\ &= \lim_{x \rightarrow r^-} \frac{[NA(x)]^3}{[D^2(x)NA'(x) - D(x)D'(x)NA(x)]}. \end{aligned} \quad (96)$$

Observe from (72), (70), (71) and (83) that $\lim_{x \rightarrow r^-} D(x)NA'(x) < +\infty$ together with $\lim_{x \rightarrow r^-} D(x) = 0$, we obtain

$$\lim_{x \rightarrow r^-} D^2(x)NA'(x) = 0. \quad (97)$$

So we have

$$\lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)} = \lim_{x \rightarrow r^-} \frac{[NA(x)]^2}{[-D(x)D'(x)]}. \quad (98)$$

Using (72), (76), (70), and (71) then by computing gives us

$$\begin{aligned} \frac{1}{2}l_1^2 = & [a(1 + b - ab + pr - 2abpr + bqr + abqr)^2]/ \\ & [br(8 + 7a + a^2 + 10b + 6ab - a^2b + 2b^2 + 2ab^2 + 4pr + \\ & 6apr + a^2pr + 2bpr + 4abpr - 2a^2bpr + 4ab^2pr + 4qr + \\ & aqr + 8bqr + 2abqr + a^2bqr + 2b^2qr - 2ab^2qr)], \end{aligned} \quad (99)$$

where

$$p = P'(r) \cong \sum_{j=2}^{150} r^{j-1} [B'(r^j) + C'(r^j)] \quad (100)$$

and

$$q = Q'(r) \cong \sum_{j=2}^{150} r^{j-1} [A'(r^j) + 2C'(r^j)]. \quad (101)$$

Thus l_1 is determined. Finally, we have

$$\frac{l_1(r)^{1/2}}{2\sqrt{\pi}} = 0.118\ 225\ 232\ 019\ 274..., \quad (102)$$

which gives

$$A_p = 0.118\ 225\ 232\ 019\ 274 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (103)$$

By similar arguments we have

$$B_p = 0.168\ 498\ 309\ 958\ 195 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (104)$$

and

$$C_p = 0.123\ 021\ 283\ 918\ 936 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right); \quad (105)$$

consequently we have

$$E_p = A_p + C_p = 0.241\ 246\ 515\ 938\ 211 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (106)$$

Now we apply Theorem 6 to the function $e(x)$. Note that $e(r) = a - a^2b - a^2b^2$, $(x_0, y_0) = (r, a - a^2b - a^2b^2)$ and $f(x) = e(x)$. Thus $e(x)$ can be expanded as

$$e(x) = (a - a^2b - a^2b^2) - m_1(r - x)^{1/2} + m_2(r - x) + m_3(r - x)^{3/2} + \dots \quad (107)$$

By arguments similar to what we employed previously, we get

$$\frac{1}{2}m_1^2 = \lim_{x \rightarrow r^-} e'(x)[(a - a^2b - a^2b^2) - e(x)]. \quad (108)$$

Applications of (70), (71) and $e(x) = A(x) - A(x)C(x) - C^2(x)$ give

$$e'(x) = \frac{A(x)[1 + B(x) + xP'(x) + xB(x)Q'(x)]}{x}. \quad (109)$$

Since all functions appearing in (109) converge as $x \rightarrow r^-$, we know that $e'(x)$ converges to a finite value as $x \rightarrow r^-$. Therefore

$$\frac{1}{2}m_1^2 = \lim_{x \rightarrow r^-} e'(x)[(a - a^2b - a^2b^2) - e(x)] = e'(r) \cdot 0 = 0. \quad (110)$$

As a consequence, $m_1 = 0$,

$$e(x) = (a - a^2b - a^2b^2) + m_2(r - x) + m_3(r - x)^{3/2} + \dots, \quad (111)$$

and

$$e'(x) = -m_2 - \frac{3}{2}m_3(r-x)^{1/2} - 2m_4(r-x) + \omega((r-x)^{3/2}). \quad (112)$$

Thus if $m_3 \neq 0$, then we have

$$e_p \sim \frac{3m_3(r)^{3/2}}{4\sqrt{\pi}} \left[\frac{r^{-p}}{p^{5/2}} \right]. \quad (113)$$

On differentiating (112), however, we have

$$e''(x) = \frac{3}{4}m_3(r-x)^{-1/2} + 2m_4 + \omega((r-x)^{1/2}). \quad (114)$$

On the other hand, from (109) and (112), we have

$$-m_2 = \lim_{x \rightarrow r^-} e'(x) = \frac{a(1+b+rp+rbq)}{r}. \quad (115)$$

Hence from (112) and (114), we have

$$e''(x)(e'(x) + m_2) = -\frac{9}{8}m_3^2 + \omega((r-x)^{1/2}). \quad (116)$$

Therefore we get

$$\lim_{x \rightarrow r^-} [-e''(x)(e'(x) + m_2)] = \frac{9}{8}m_3^2. \quad (117)$$

By (114, $\lim_{x \rightarrow r^-} e''(x) = +\infty$ (or $-\infty$); and by (115), $\lim_{x \rightarrow r^-} (e'(x) + m_2) = 0$.

Then using L'Hospital's Rule, we have

$$\frac{9}{8}m_3^2 = \lim_{x \rightarrow r^-} [-e''(x)(e'(x) + m_2)] = \lim_{x \rightarrow r^-} \frac{[e''(x)]^3}{e'''(x)}. \quad (118)$$

Again, using (70) and (71) repeatedly, we can find $e''(x)$ and $e'''(x)$. Then by computing, we get

$$\begin{aligned} \frac{9}{8}m_3^2 = & [a(1 + 3b + b^2 + 2pr + 2bpr - 2abpr + 4bqr \\ & + 2abqr + 2b^2qr + p^2r^2 - 2abp^2r^2 + 2bpqr^2 \\ & + 2abpqr^2 + bq^2r^2 + b^2q^2r^2)^2]/ \\ & [br^3(8 + 7a + a^2 + 10b + 6ab - a^2b + 2b^2 \\ & + 2ab^2 + 4pr + 6apr + a^2pr + 2bpr + 4abpr \\ & - 2a^2bpr + 4ab^2pr + 4qr + aqr + 8bqr + 2abqr \\ & + a^2bqr + 2b^2qr - 2ab^2qr)]. \end{aligned} \quad (119)$$

So the numerical value for m_3 is determined. Finally, we have

$$\frac{3m_3(r)^{3/2}}{4\sqrt{\pi}} = 0.256\ 881\ 825\ 127\ 051..., \quad (120)$$

which gives

$$e_p = 0.256\ 881\ 825\ 127\ 051 \frac{r^{-p}}{p^{5/2}} + O\left(\frac{r^{-p}}{p^{7/2}}\right). \quad (121)$$

□

Table 2 compares E_p and e_p with the values given by (87) and (88) without the *big-O* terms denoted by \tilde{E}_p and \tilde{e}_p .

We have seen that $E_p = A_p + C_p$. One interesting question to ask is what is the percentage of contribution of A_p (or C_p) to E_p ? As a consequence of Theorem 7, we have the next corollary which states that the contribution of A_p is close to but not quite one half for large p .

Corollary 1 *For A_p, C_p and E_p we have*

Table 2

The Numerical Values of E_p , e_p and Approximations ($1 \leq p \leq 20$)

p	E_p	\tilde{E}_p	e_p	\tilde{e}_p
1	1	1	1	1
2	2	2	1	1
3	5	5	2	2
4	17	17	5	4
5	58	58	14	12
6	217	214	42	38
7	830	825	137	126
8	3303	3278	467	436
9	13396	13329	1668	1577
10	55501	55222	6163	5880
11	2 33196	2 32266	23400	22484
12	9 92771	9 89164	90858	87773
13	42 70258	42 56867	3 59463	3 48674
14	185 35850	184 83233	14 44592	14 05796
15	810 78383	808 71973	58 83938	57 40888
16	3570 51942	3562 21293	242 45484	237 06761
17	15816 77036	15783 06674	1009 24208	988 58678
18	70433 14680	70294 43464	4238 78271	4158 34737
19	3 15107 57851	3 14531 55614	17944 67452	17627 18453
20	14 15650 84066	14 13235 55961	76590 56373	75241 40369

$$\lim_{p \rightarrow \infty} \frac{A_p}{E_p} = 0.490\ 059\ 852\ 510\ 180\dots \quad (122)$$

and

$$\lim_{p \rightarrow \infty} \frac{C_p}{E_p} = 0.509\ 940\ 147\ 489\ 820\dots \quad (123)$$

We recall that the number of efficient dominating sets for a particular tree T (rooted or unrooted) is the number of orientations of T which can give rise to an efficient dominating set. From Theorem 7 we have the following corollary which determines the average number of efficient dominating sets per tree among all trees (rooted or unrooted) of order p .

Corollary 2 *Let \overline{E}_p be the average number of efficient dominating sets per tree among all rooted trees of order p , and let \overline{e}_p be the average number of efficient dominating sets per tree among all unrooted trees of order p . Then*

$$\overline{E}_p = 0.548\ 382\ 241\ 124\ 567 \left(\frac{\eta}{r}\right)^p + O\left(\frac{\left(\frac{\eta}{r}\right)^p}{p}\right) \quad (124)$$

and

$$\overline{e}_p = 0.480\ 198\ 176\ 010\ 462 \left(\frac{\eta}{r}\right)^p + O\left(\frac{\left(\frac{\eta}{r}\right)^p}{p}\right). \quad (125)$$

In particular, we have

$$\lim_{p \rightarrow \infty} \frac{\overline{E}_p}{\overline{e}_p} = 1.141\ 991\ 512\ 088\ 998\dots \quad (126)$$

and

$$\lim_{p \rightarrow \infty} \sqrt[p]{E_p} = \lim_{p \rightarrow \infty} \sqrt[p]{e_p} = \frac{\eta}{r} = 1.641\ 704\ 470\ 457\ 124\dots, \quad (127)$$

where $\eta = 0.338\ 321\ 856\ 899\ 208\dots$ is the radius of convergence of the counting series $T(x) = \sum_{p=1}^{\infty} T_p x^p$ for rooted trees.

Proof: By using techniques similar to that used to find A_p, B_p , and C_p , we are able to determine the number of rooted trees of order p for each p up to 150. Then we determine η with 65 digits accuracy, and consequently we get

$$T_p = 0.439\ 924\ 012\ 571\ 025 \frac{\eta^{-p}}{p^{3/2}} + O\left(\frac{\eta^{-p}}{p^{5/2}}\right) \quad (128)$$

and

$$t_p = 0.534\ 949\ 606\ 142\ 307 \frac{\eta^{-p}}{p^{5/2}} + O\left(\frac{\eta^{-p}}{p^{7/2}}\right), \quad (129)$$

where t_p is the number of unrooted trees of order p . We notice that the last two digits of the coefficients in the asymptotic formulas of T_p and t_p in Harary and Palmer [11] (p213 and p214) are incorrect.

Using (87), (88), (128), and (129), we have

$$\overline{E}_p = \frac{E_p}{T_p} = 0.548\ 382\ 241\ 124\ 567 \left(\frac{\eta}{r}\right)^p + O\left(\frac{\left(\frac{\eta}{r}\right)^p}{p}\right), \quad (130)$$

and

$$\overline{e}_p = \frac{e_p}{t_p} = 0.480\ 198\ 176\ 010\ 462 \left(\frac{\eta}{r}\right)^p + O\left(\frac{\left(\frac{\eta}{r}\right)^p}{p}\right); \quad (131)$$

consequently, we have

$$\lim_{p \rightarrow \infty} \frac{\overline{E}_p}{\overline{e}_p} = 1.141\ 991\ 512\ 008\ 998\dots \quad (132)$$

and

$$\lim_{p \rightarrow \infty} \sqrt[p]{E_p} = \lim_{p \rightarrow \infty} \sqrt[p]{\bar{e}_p} = \frac{\eta}{r} = 1.641\ 704\ 470\ 457\ 124.... \quad (133)$$

□

The limit given in (126) says that, on the average, a rooted tree can give rise to about 14% more efficient dominating sets than an unrooted tree for large p .

We conclude with Tables 3 and 4. Table 3 compares \bar{E}_p and \bar{e}_p with the approximate values $\widetilde{\bar{E}}_p$ and $\widetilde{\bar{e}}_p$ given by ignoring the *big-O* terms in (130) and (131) ($1 \leq p \leq 30$). Table 4 gives values for $\frac{A_p}{E_p}$, $\frac{\bar{E}_p}{\bar{e}_p}$, $\sqrt[p]{E_p}$ and $\sqrt[p]{\bar{e}_p}$.

Table 3

The Numerical Values of \bar{E}_p , $\tilde{\bar{E}}_p$, \bar{e}_p and $\tilde{\bar{e}}_p$ ($1 \leq p \leq 30$)

p	\bar{E}_p	$\tilde{\bar{E}}_p$	\bar{e}_p	$\tilde{\bar{e}}_p$
1	1	1	1	1
2	2	1	1	1
3	3	2	2	2
4	4	4	3	3
5	6	7	5	6
6	11	11	7	9
7	17	18	12	15
8	29	29	20	25
9	47	48	35	42
10	77	78	58	68
11	127	128	100	112
12	208	210	165	184
13	342	345	276	302
14	562	567	457	496
15	923	930	760	814
16	1517	1527	1255	1337
17	2491	2507	2075	2195
19	4092	4115	3422	3604
19	6721	6756	5644	5916
20	11037	11091	9296	9712
21	18125	18209	15309	15945
22	29764	29893	25195	26176
23	48875	49076	41459	42974
24	80255	80568	68197	70550
25	1 31781	1 32269	1 12159	1 15823
26	2 16382	2 17147	1 84421	1 90147
27	3 55291	3 56490	3 03200	3 12166
28	5 83367	5 85252	4 98407	5 12484
29	9 57843	9 60811	8 19207	8 41347
30	15 72686	15 77367	13 46350	13 81242

Table 4

The Numerical Values of A_p/E_p , \bar{E}_p/\bar{e}_p , $\sqrt[p]{\bar{E}_p}$ and $\sqrt[p]{\bar{e}_p}$

p	A_p/E_p	\bar{E}_p/\bar{e}_p	$\sqrt[p]{\bar{E}_p}$	$\sqrt[p]{\bar{e}_p}$
1	1.00000	1.00000	1.00000	1.00000
2	0.50000	2.00000	1.41421	1.00000
3	0.60000	1.50000	1.44225	1.25992
4	0.52941	1.33333	1.41421	1.31607
5	0.53448	1.20000	1.43097	1.37973
6	0.51613	1.57143	1.49130	1.38309
7	0.51566	1.41667	1.49892	1.42616
8	0.50954	1.45000	1.52335	1.45422
9	0.50791	1.34286	1.53387	1.48444
10	0.50549	1.32759	1.54401	1.50087
14	0.50084	1.22976	1.57185	1.54880
18	0.49836	1.19579	1.58731	1.57162
22	0.49680	1.18135	1.59716	1.58511
26	0.49574	1.17330	1.60399	1.59416
30	0.49497	1.16811	1.60900	1.60068
34	0.49438	1.16443	1.61283	1.60562
38	0.49392	1.16167	1.61586	1.60950
42	0.49355	1.15952	1.61831	1.61262
46	0.49324	1.15779	1.62034	1.61519
50	0.49298	1.15638	1.62204	1.61734
60	0.49249	1.15375	1.62531	1.62144
70	0.49214	1.15194	1.62765	1.62436
80	0.49188	1.15061	1.62940	1.62655
90	0.49168	1.14959	1.63077	1.62824
100	0.49151	1.14879	1.63186	1.62960
110	0.49138	1.14814	1.63275	1.63070
120	0.49127	1.14761	1.63350	1.63162
130	0.49118	1.14716	1.63413	1.63240
140	0.49110	1.14678	1.63467	1.63307
150	0.49103	1.14645	1.63514	1.63365

CHAPTER III

EFFICIENT DOMINATING SETS IN LABELED ORIENTED TREES

For labeled trees, the problem of finding the number of efficient dominating sets among all rooted trees of order p and the problem of finding the number of efficient dominating sets among all unrooted trees of order p are equivalent. This is because each labeled unrooted tree can be rooted in exactly p ways; consequently, if the number of efficient dominating sets among all labeled rooted trees of order p is divided by p , the result is precisely the number of efficient dominating sets among all labeled unrooted trees of the same order p .

The tool used to do the counting is three interrelated exponential generating functions, and the technique used to derive the exact formulas is based on the Multivariate Lagrange Inversion Formula.

3.1 Generating Functions

In order to enumerate efficient dominating sets in labeled rooted trees we introduce four exponential generating functions. The definitions of these four exponential generating functions are similar to those of four ordinary generating functions in Chapter II.

We let

$$A(x) = \sum_{p=1}^{\infty} A_p x^p / p! \tag{1}$$

be the exponential generating function in which A_p is the number of efficient dominating sets among all labeled rooted trees of order p which have the root in

the dominating set. (The root is dominated by itself.)

Let

$$C(x) = \sum_{p=1}^{\infty} C_p x^p / p! \quad (2)$$

be the exponential generating function in which C_p is the number of efficient dominating sets among all labeled rooted trees of order p which have the root dominated by one of its children. (The root is dominated from inside.)

We let the third series be

$$B(x) = \sum_{p=1}^{\infty} B_p x^p / p!. \quad (3)$$

In this series, B_p counts sets of which the root is dominated from outside.

We refer to this case as the root being “dominated from outside”.

For convenience we introduce a fourth series.

Let

$$E(x) = \sum_{p=1}^{\infty} E_p x^p / p! \quad (4)$$

be the exponential generating function in which E_p is the number of efficient dominating sets among all labeled rooted trees of order p and we have

$$E(x) = A(x) + C(x). \quad (5)$$

3.2 Functional Relations for the Counting Series

Our object is to find an analytic formula for the number of efficient dominating sets among all labeled rooted trees of order p . In the previous section we

saw that this number is equal to $A_p + B_p$. We first find the functional relations among $A(x)$, $B(x)$ and $C(x)$ and then use the Multivariate Lagrange's Inversion Formula to find the analytic formulas for A_p , B_p and C_p . Based on the definitions of four exponential generating functions, we have the following theorem:

Theorem 8 *For the functions introduced in (1), (2) and (3), the following equations hold:*

$$A(x) = x \exp[B(x) + C(x)] \quad (6)$$

$$B(x) = x \exp[A(x) + 2C(x)] \quad (7)$$

$$C(x) = A(x)B(x). \quad (8)$$

Proof: The idea to prove this theorem is similar to that we used to prove Theorem 3 in Chapter II.

By the similar arguments in the proof of Theorem 3, we obtain the following structure of labeled rooted trees of type A , type B and type C .

For labeled rooted trees of type A , any branch of type A is invalid. On the other hand it can have any number of branches of type B if the edge is oriented from the root of the tree to the root of the branch, and it can have any number of branches of type C if the edge is oriented from the root of the branch to the root of the tree. See Figure 7.

This allows us to deduce the following equation for $A(x)$:

$$A(x) = x \left[\sum_{n=0}^{\infty} \frac{B^n(x)}{n!} \right] \left[\sum_{n=0}^{\infty} \frac{C^n(x)}{n!} \right]. \quad (9)$$

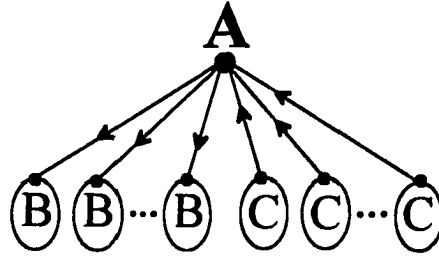


Figure 7. The Structure of Labeled Rooted Tree of Type A.

In this expression, the factor x accounts for the root. Each $\frac{B^n(x)}{n!}$ allows for n branches of type B . And similarly, each $\frac{C^n(x)}{n!}$ allows n branches of type C . Thus the structure shown in Figure 7 leads us to equation (9), which immediately gives (6).

For labeled rooted trees of type B , any branch of type B is invalid. It can have any number of branches of type A if the edge is oriented from the root of the tree to the root of the branch, and it can have any number of branches of type C whose edge can be oriented in either direction. See Figure 8.

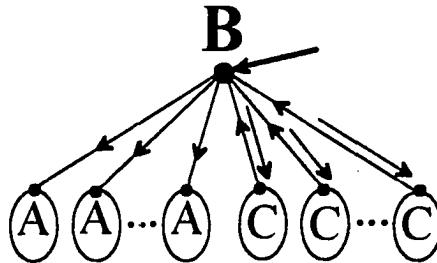


Figure 8. The Structure of Labeled Rooted Tree of Type B.

So we get

$$B(x) = x \left[\sum_{n=0}^{\infty} \frac{A^n(x)}{n!} \right] \left[\sum_{n=0}^{\infty} \frac{(2C(x))^n}{n!} \right], \quad (10)$$

which yields (7).

For labeled rooted trees of type C , it must have precisely one branch type A , and the rest of it must be a labeled rooted tree of type B . Also the edge must be oriented from the root of the branch to the root of the tree of type B . See Figure 9.

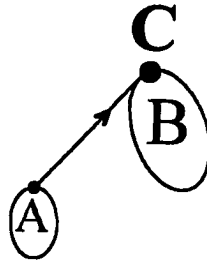


Figure 9. The Structure of Labeled Rooted Tree of Type C .

Thus we have

$$C(x) = A(x)B(x). \quad (11)$$

□

3.3 Analytic Formulas for Labeled Rooted Trees

We have seen from the previous section that the four exponential generating functions satisfy the following equations:

$$A(x) = x \exp[B(x) + C(x)] \quad (12)$$

$$B(x) = x \exp[A(x) + 2C(x)] \quad (13)$$

$$C(x) = A(x)B(x) \quad (14)$$

and

$$E(x) = A(x) + C(x). \quad (15)$$

We first find analytic formulas for the coefficients of A_p and B_p ; then using (14) we can find the coefficients of C_p . Finally, we are able to find E_p , which, we recall, is the number of efficient dominating sets among all labeled rooted trees of order p . The technique we use is based on the “Multivariate Lagrange Inversion Formula”.

Letting $u = A(x)$, $v = B(x)$, from (12), (13) and (14) we have

$$\left. \begin{aligned} u &= xe^{v+uv} \\ v &= xe^{u+2uv} \end{aligned} \right\}. \quad (16)$$

Some notation is needed prior to stating the next theorem.

Let $R[(u, v)] = \{\sum_{i,j} c_{ij}u^i v^j \mid c_{ij} \in \mathbf{R}, i \geq 0, j \geq 0\}$ be the collection of all double power series with real coefficients; let $R[(u, v)]_1 = \{f \in R[(u, v)] \mid f(0, 0) \neq 0\}$ be the subset of $R[(u, v)]$ with the property that each member of $R[(u, v)]_1$ has nonzero value at the point $(0, 0)$.

Another notation is also very standard. Let $f(u, v) = \sum_{i,j} c_{ij}u^i v^j$ be any double power series, then $[u^i v^j]f(u, v)$ extracts the coefficient of $u^i v^j$ so that $[u^i v^j]f(u, v) = c_{ij}$, for example, $[u^i v^j]e^{2u-v} = \frac{2^i (-1)^j}{i! j!}$. The following theorem appears in Goulden and Jackson [8] :

Theorem 9 (Multivariate Lagrange) Let $\phi_1(u, v), \phi_2(u, v) \in R[(u, v)]_1$, and suppose

$$\left. \begin{aligned} u &= t_1 \phi_1(u, v) \\ v &= t_2 \phi_2(u, v) \end{aligned} \right\}. \quad (17)$$

Then

$$\left. \begin{aligned} u(t_1, t_2) &= \sum_{i,j} t_1^i t_2^j [u^i v^j] \{u \phi_1^i(u, v) \phi_2^j(u, v) \Delta\} \\ v(t_1, t_2) &= \sum_{i,j} t_1^i t_2^j [u^i v^j] \{v \phi_1^i(u, v) \phi_2^j(u, v) \Delta\} \end{aligned} \right\}, \quad (18)$$

where

$$\Delta = \begin{vmatrix} 1 - \frac{u}{\phi_1(u, v)} \frac{\partial \phi_1(u, v)}{\partial u} & \frac{-v}{\phi_1(u, v)} \frac{\partial \phi_1(u, v)}{\partial v} \\ \frac{-u}{\phi_2(u, v)} \frac{\partial \phi_2(u, v)}{\partial u} & 1 - \frac{v}{\phi_2(u, v)} \frac{\partial \phi_2(u, v)}{\partial v} \end{vmatrix}. \quad (19)$$

For our problem we have

$$\left. \begin{aligned} u &= t_1 \phi_1(u, v) \\ v &= t_2 \phi_2(u, v) \end{aligned} \right\}, \quad (20)$$

where

$$\left. \begin{aligned} t_1 &= t_2 = x \\ \phi_1(u, v) &= e^{v+uv} \\ \phi_2(u, v) &= e^{u+2uv} \end{aligned} \right\}. \quad (21)$$

So the conditions in Theorem 9 are satisfied, $u(t_1, t_2) = u(x) = A(x)$, and $v(t_1, t_2) = v(x) = B(x)$.

Note that

$$\begin{aligned}
\Delta &= \begin{vmatrix} 1 - \frac{u}{\phi_1(u,v)} \frac{\partial \phi_1(u,v)}{\partial u} & \frac{-v}{\phi_1(u,v)} \frac{\partial \phi_1(u,v)}{\partial v} \\ \frac{-u}{\phi_2(u,v)} \frac{\partial \phi_2(u,v)}{\partial u} & 1 - \frac{v}{\phi_2(u,v)} \frac{\partial \phi_2(u,v)}{\partial v} \end{vmatrix} \\
&= \begin{vmatrix} 1 - uv & -v(1+u) \\ -u(1+2v) & 1 - 2uv \end{vmatrix} \\
&= 1 - 4uv - u^2v - 2uv^2,
\end{aligned} \tag{22}$$

which gives

$$A(x) = \sum_{i,j} x^i x^j [u^i v^j] \{u(e^{v+uv})^i (e^{u+2uv})^j (1 - 4uv - u^2v - 2uv^2)\}. \tag{23}$$

Making the substitution $p = i + j$, we find that

$$A(x) = \sum_{p=0}^{\infty} x^p \sum_{i=0}^p [u^i v^{p-i}] \{u(e^{v+uv})^i (e^{u+2uv})^{p-i} (1 - 4uv - u^2v - 2uv^2)\}. \tag{24}$$

That is,

$$A(x) = \sum_{p=0}^{\infty} x^p \sum_{i=0}^p [u^i v^{p-i}] \{(e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2)\}. \tag{25}$$

Similarly, we have

$$B(x) = \sum_{p=0}^{\infty} x^p \sum_{i=0}^p [u^i v^{p-i}] \{(e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3)\}. \tag{26}$$

Thus we have following formulas for the coefficients A_p and B_p :

$$A_p/p! = \sum_{i=0}^p [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2) \} \quad (27)$$

and

$$B_p/p! = \sum_{i=0}^p [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3) \}. \quad (28)$$

Because of the factor of $u - 4u^2v - u^3v - 2u^2v^2$ in (27), we see that

$$A_0 = \sum_{i=0}^{p=0} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2) \} = 0. \quad (29)$$

Similarly, we have

$$B_0 = \sum_{i=0}^{p=0} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3) \} = 0. \quad (30)$$

So $A_0 = 0$ and $B_0 = 0$. Observe that

$$A_1/1! = \sum_{i=0}^{p=1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2) \} = 1 \quad (31)$$

and

$$B_1/1! = \sum_{i=0}^{p=1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3) \} = 1, \quad (32)$$

so $A_1 = 1$ and $B_1 = 1$.

Observe that for $p \geq 2$, and $i = 0$ or $i = p$,

$$[u^0 v^{p-0}] \{ (e^{v+uv})^0 (e^{u+2uv})^{p-0} (u - 4u^2v - u^3v - 2u^2v^2) \} = 0 \quad (33)$$

and

$$[u^p v^{p-p}] \{ (e^{v+uv})^p (e^{u+2uv})^{p-p} (u - 4u^2v - u^3v - 2u^2v^2) \} = 0. \quad (34)$$

So for $p \geq 2$, we have

$$A_p/p! = \sum_{i=1}^{p-1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2) \}. \quad (35)$$

Likewise, for $p \geq 2$ we have

$$B_p/p! = \sum_{i=1}^{p-1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3) \}. \quad (36)$$

Putting all these observations together we have

$$A(x) = x + \sum_{p=2}^{\infty} A_p x^p / p! \quad (37)$$

and

$$B(x) = x + \sum_{p=2}^{\infty} B_p x^p / p!, \quad (38)$$

where

$$A_p/p! = \sum_{i=1}^{p-1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (u - 4u^2v - u^3v - 2u^2v^2) \} \quad (39)$$

and

$$B_p/p! = \sum_{i=1}^{p-1} [u^i v^{p-i}] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} (v - 4uv^2 - u^2v^2 - 2uv^3) \}. \quad (40)$$

Note that if $F(u, v) = \sum_{m,n} F_{mn} u^m v^n$ is any double power series, then we have

$$[u^m v^n] \{ F(u, v) u^i v^j \} = [u^{m-i} v^{n-j}] F(u, v). \quad (41)$$

Form this observation we see that, essentially, we need to find a formula for

$$[u^m v^n] \{ (e^{v+uv})^i (e^{u+2uv})^{p-i} \}. \quad (42)$$

To find a formula for (42), we use the tool based on Taylor expansion in two variables. Suppose that the function $F(u, v)$ can be expanded as a double power series at the origin $(0, 0)$:

$$F(u, v) = \sum_{m,n} F_{mn} u^m v^n. \quad (43)$$

Then we know that the coefficient F_{mn} can be determined as follows:

$$F_{mn} = [u^m v^n] F(u, v) = \frac{1}{m!n!} F_{u^m v^n}(0, 0). \quad (44)$$

For our problem we have

$$F(u, v) = (e^{v+uv})^i (e^{u+2uv})^{p-i} = e^{f(u,v)}, \quad (45)$$

where

$$\begin{aligned} f(u, v) &= (v + uv)i + (u + 2uv)(p - i) \\ &= (p - i)u + iv + uv(2p - i). \end{aligned} \quad (46)$$

We first find $F_{u^m v^n}(0, 0)$. Taking the derivative with respect to v we have

$$F_{v^n} = e^{f(u,v)} \{i + u(2p - i)\}^n. \quad (47)$$

Then taking the m th derivative with respect to u and using binomial formula for

derivatives give us

$$\begin{aligned}
 F_{u^m v^n} &= \sum_{k=0}^m \binom{m}{k} \{e^{f(u,v)}\}_{u^{m-k}} \{(i+u(2p-i))^n\}_{u^k} \\
 &= \sum_{k=0}^{\min\{m,n\}} \binom{m}{k} \{e^{f(u,v)}\} \{(p-i)+v(2p-i)\}^{m-k} \times \\
 &\quad n(n-1)\dots(n-k+1) \{(i+u(2p-i))^{n-k} (2p-i)^k\}.
 \end{aligned} \tag{48}$$

Evaluating $F_{u^m v^n}$ at the point $(0,0)$ gives

$$\begin{aligned}
 F_{u^m v^n}(0,0) &= \sum_{k=0}^{\min\{m,n\}} \binom{m}{k} e^0 (p-i)^{m-k} \frac{n!}{(n-k)!} i^{n-k} (2p-i)^k \\
 &= \sum_{k=0}^{\min\{m,n\}} m!n! \frac{(2p-i)^k (p-i)^{m-k} i^{n-k}}{k!(m-k)!(n-k)!}.
 \end{aligned} \tag{49}$$

Thus we obtain

$$[u^m v^n]F(u,v) = \frac{1}{m!n!} F_{u^m v^n}(0,0) = \sum_{k=0}^{\min\{m,n\}} \frac{(2p-i)^k (p-i)^{m-k} i^{n-k}}{k!(m-k)!(n-k)!}. \tag{50}$$

Now from (39), (41) and (45) we have

$$\begin{aligned}
 A_p/p! &= \sum_{i=1}^{p-1} [u^{i-1} v^{p-i}]F(u,v) - 4 \sum_{i=1}^{p-1} [u^{i-2} v^{p-i-1}]F(u,v) \\
 &\quad - \sum_{i=1}^{p-1} [u^{i-3} v^{p-i-1}]F(u,v) - 2 \sum_{i=1}^{p-1} [u^{i-2} v^{p-i-2}]F(u,v)
 \end{aligned} \tag{51}$$

Discarding the terms with the value of zero we have

$$\begin{aligned}
 A_p/p! &= \sum_{i=1}^{p-1} [u^{i-1}v^{p-i}]F(u, v) - 4 \sum_{i=2}^{p-1} [u^{i-2}v^{p-i-1}]F(u, v) \\
 &\quad - \sum_{i=3}^{p-1} [u^{i-3}v^{p-i-1}]F(u, v) - 2 \sum_{i=2}^{p-1} [u^{i-2}v^{p-i-2}]F(u, v).
 \end{aligned} \tag{52}$$

Finally, using (50) and discarding the terms with the value of zero we have

$$\begin{aligned}
 A_p/p! &= \sum_{i=1}^{p-1} \sum_{k=0}^{\min\{i-1, p-i\}} \frac{(2p-i)^k (p-i)^{i-1-k} i^{p-i-k}}{k!(i-1-k)!(p-i-k)!} \\
 &\quad - 4 \sum_{i=2}^{p-1} \sum_{k=0}^{\min\{i-2, p-i-1\}} \frac{(2p-i)^k (p-i)^{i-2-k} i^{p-i-1-k}}{k!(i-2-k)!(p-i-1-k)!} \\
 &\quad - \sum_{i=3}^{p-1} \sum_{k=0}^{\min\{i-3, p-i-1\}} \frac{(2p-i)^k (p-i)^{i-3-k} i^{p-i-1-k}}{k!(i-3-k)!(p-i-1-k)!} \\
 &\quad - 2 \sum_{i=2}^{p-2} \sum_{k=0}^{\min\{i-2, p-i-2\}} \frac{(2p-i)^k (p-i)^{i-2-k} i^{p-i-2-k}}{k!(i-2-k)!(p-i-2-k)!}.
 \end{aligned} \tag{53}$$

Similarly, we have

$$\begin{aligned}
B_p/p! &= \sum_{i=1}^{p-1} \sum_{k=0}^{\min\{i, p-i-1\}} \frac{(2p-i)^k (p-i)^{i-k} i^{p-i-1-k}}{k!(i-k)!(p-i-1-k)!} \\
&\quad - 4 \sum_{i=1}^{p-2} \sum_{k=0}^{\min\{i-1, p-i-2\}} \frac{(2p-i)^k (p-i)^{i-1-k} i^{p-i-2-k}}{k!(i-1-k)!(p-i-2-k)!} \\
&\quad - \sum_{i=2}^{p-2} \sum_{k=0}^{\min\{i-2, p-i-2\}} \frac{(2p-i)^k (p-i)^{i-2-k} i^{p-i-2-k}}{k!(i-2-k)!(p-i-2-k)!} \\
&\quad - 2 \sum_{i=1}^{p-3} \sum_{k=0}^{\min\{i-1, p-i-3\}} \frac{(2p-i)^k (p-i)^{i-1-k} i^{p-i-3-k}}{k!(i-1-k)!(p-i-3-k)!}.
\end{aligned} \tag{54}$$

Formulas (53) and (54) allow us to compute A_p and B_p ; then using (14) we can determine C_p . Finally, we can determine the number of efficient dominating sets among all labeled rooted trees of order p , which is $E_p = A_p + C_p$. We use (53) and (54) to determine E_p for each p up to 45. Results of the computations for A_p , B_p , and E_p for each p up to 30 are reported in Tables 5, 6, and 7.

3.4 Asymptotic Analysis

Although formulas (53) and (54) permit us to determine the number of efficient dominating sets among all labeled rooted trees of order p for each p , they do not tell us the asymptotic behavior of the number of efficient dominating sets. In particular, they cannot tell us whether the p th root of the average number of efficient dominating sets per labeled rooted tree has a limit, in other words does $\lim_{p \rightarrow \infty} \sqrt[p]{\frac{E_p}{pp^{p-2}}}$ exist? And if it exists, what is the limit?

Table 5
The Numerical Values of A_p ($1 \leq p \leq 30$)

p	A_p
1	1
2	2
3	15
4	184
5	3025
6	65016
7	16 90759
8	520 76480
9	18474 67521
10	7 42757 60800
11	333 60397 40671
12	16557 64670 11968
13	8 99897 92688 90065
14	531 54835 71151 92704
15	33905 40418 13137 97175
16	23 22693 14681 67927 13216
17	1700 77818 38345 84011 52641
18	1 32565 44053 30551 73350 73280
19	109 58364 83612 18672 57433 06991
20	9575 83929 85744 36499 24125 44000
21	8 81973 32093 58057 70892 92154 61201
22	853 96499 76565 09336 86558 13349 35552
23	86715 71947 61985 46413 47804 74353 53575
24	92 14879 45372 00863 49618 24968 17601 08544
25	10227 23091 60612 89110 67156 22779 66441 70625
26	11 83360 18654 66379 19441 55786 57636 73821 42976
27	1425 09259 93483 48960 04543 61062 81678 00042 91039
28	1 78348 22932 01662 10710 33624 65147 02973 36517 42720
29	231 61990 30183 02434 85692 58406 88566 44290 29799 45041
30	31173 83324 96609 85192 17163 02189 81667 34014 28992 00000

Table 6

The Numerical Values of B_p ($1 \leq p \leq 30$)

p	B_p
1	1
2	2
3	21
4	232
5	4105
6	87336
7	23 06269
8	712 64768
9	25416 96273
10	10 25246 15200
11	461 86252 08901
12	22978 39234 22208
13	12 51422 42191 48249
14	740 47562 48589 29792
15	47303 46916 11296 45325
16	32 44806 19350 94643 75296
17	2378 75321 55213 89915 93761
18	1 85600 92590 51475 81262 23872
19	153 65534 62054 13972 86733 60373
20	13430 34598 07609 97858 17477 12000
21	12 37916 23615 90349 22212 13608 49321
22	1199 42059 50809 01260 32423 31057 95072
23	1 21870 60548 40403 76459 61498 26520 41661
24	129 57996 25489 71351 30995 71775 33996 72832
25	14389 09221 75559 48257 17727 94368 34066 80625
26	16 65719 35340 58136 88317 37594 89282 07089 90976
27	2006 88218 27298 23109 75165 78436 64177 74824 23589
28	2 51262 43552 27165 33396 86170 97822 26640 76196 57728
29	326 43905 90231 86902 76870 97191 10420 31310 79338 97593
30	43951 39799 04190 54381 09758 19094 95401 27900 80512 00000

Table 7

The Numerical Values of E_p ($1 \leq p \leq 30$)

p	E_p
1	1
2	4
3	27
4	352
5	5825
6	1 26576
7	33 13723
8	1025 78176
9	36536 53473
10	14 73515 92000
11	663 53182 81691
12	33003 32303 55456
13	17 96963 58654 93793
14	1063 06989 80225 06752
15	67900 18964 88223 06875
16	46 56970 92536 07545 89696
17	3413 56938 30917 65759 21217
18	2 66311 88192 89294 09738 35264
19	220 32456 32737 66238 19285 44923
20	19267 04366 72894 29029 01657 60000
21	17 75759 02142 45706 84327 43476 26241
22	1720 41209 17698 20911 79727 43549 29664
23	1 74795 81919 29745 60163 46101 78109 55067
24	185 84184 58175 96037 64102 88083 80273 13152
25	20635 49228 67235 04411 01747 45646 45413 90625
26	23 88696 51407 05492 17156 45527 75427 88544 75776
27	2877 79884 59348 05625 56047 36559 45333 09034 88603
28	3 60285 72290 66541 12755 34425 62717 99104 40206 99136
29	468 06254 69035 67027 68320 17988 67917 85790 61064 82273
30	63017 03575 44228 46319 17768 56061 94786 70985 72800 00000

In order to find the asymptotic formulas, we first prove several lemmas. The first lemma allows us to treat each generating function $A(x)$, $B(x)$, $C(x)$ and $E(x)$ as an analytic function. Some of these lemmas are parallel to those in Chapter II.

Lemma 10 *The power series $A(x)$, $B(x)$ and $C(x)$ all have radius of convergence greater than $1/(2e)$.*

Proof: Recall that Theorem 2 says that the number of efficient dominating sets for a labeled tree T of order p is bounded above by 2^{p-1} . As a consequence, the number of efficient dominating sets among all labeled rooted trees of order p is bounded above by $2^{p-1}(pp^{p-2})$, where pp^{p-2} is the number of labeled rooted trees of order p . So each of A_p , B_p , and C_p is bounded above by $2^{p-1}(pp^{p-2})$.

Now let r_a , r_b , r_c denote the radius of convergence for each of the series $A(x)$, $B(x)$ and $C(x)$, respectively. Then by Stirling's Formula we obtain

$$r_a = \frac{1}{\lim_{p \rightarrow \infty} \sqrt[p]{A_p/p!}} \geq \frac{1}{\lim_{p \rightarrow \infty} \sqrt[p]{(2^{p-1}pp^{p-2})/p!}} > \frac{1}{2 \lim_{p \rightarrow \infty} \sqrt[p]{p^p/p!}} = \frac{1}{2e}. \quad (55)$$

In the same fashion we get

$$r_b > 1/(2e) \text{ and } r_c > 1/(2e). \quad (56)$$

□

Lemma 11 *The power series $A(x)$, $B(x)$ and $C(x)$ have the same radius of convergence.*

That is $r = r_a = r_b = r_c$.

Proof: From

$$A(x) = x \exp[B(x) + C(x)], \quad (57)$$

it follows that $r_a \leq r_b$ and $r_a \leq r_c$, and from

$$B(x) = x \exp[A(x) + 2C(x)], \quad (58)$$

we have $r_b \leq r_a$ and $r_b \leq r_c$. Further, from

$$C(x) = A(x)B(x), \quad (59)$$

it is easy to see that $r_c \leq r_a$ and $r_c \leq r_b$.

All these inequalities together imply

$$r = r_a = r_b = r_c. \quad (60)$$

□

Lemma 12 *The limits of $A(x)$, $B(x)$ and $C(x)$ as $x \rightarrow r^-$ exist and are equal to $A(r)$, $B(r)$ and $C(r)$, respectively. Consequently, $A(x)$, $B(x)$ and $C(x)$ each has a unique singularity at $x = r$ on the circle of convergence.*

Proof: Since $A(x)$ satisfies the functional equation (57), it follows that for all x in $(0, r)$,

$$\log(A(x)/x) = B(x) + C(x) \geq C(x). \quad (61)$$

From this it follows that

$$\frac{C(x)/x}{\log(A(x)/x)} \leq \frac{1}{x}. \quad (62)$$

Note that $C(x) = A(x)B(x)$; so we have

$$B(x) \frac{(A(x)/x)}{\log(A(x)/x)} \leq \frac{1}{x}. \quad (63)$$

Hence $A(x)$ and $B(x)$ are both bounded above on the interval $(0, r)$. Since $A(x)$ and $B(x)$ are both monotone increasing with respect to x , the left limits at r must exist and we have

$$a = \lim_{x \rightarrow r^-} A(x) = A(r) \quad (64)$$

$$b = \lim_{x \rightarrow r^-} B(x) = B(r) \quad (65)$$

$$c = \lim_{x \rightarrow r^-} C(x) = \lim_{x \rightarrow r^-} A(x)B(x) = A(r)B(r) = ab. \quad (66)$$

□

Lemma 13 *For the series $A(x)$ and $B(x)$, the following equality holds:*

$$a^2b + 2ab^2 + 4ab = 1. \quad (67)$$

Proof: We first define the complex valued functions $F(x, y, z)$ and $G(x, y, z)$, where x, y and z are considered as a complex variables:

$$\left. \begin{aligned} F(x, y, z) &= x \exp(z + yz) - y \\ G(x, y, z) &= x \exp(y + 2yz) - z \end{aligned} \right\}. \quad (68)$$

Then by similar arguments in the proof of Lemma 4 we can show that the deter-

minant

$$\begin{vmatrix} F_y & F_z \\ G_y & G_z \end{vmatrix}$$

at the point (r, a, b) must be zero. Hence we have

$$\begin{aligned} \begin{vmatrix} F_y & F_z \\ G_y & G_z \end{vmatrix}_{\substack{x=r \\ y=a \\ z=b}} &= \begin{vmatrix} z(F+y)-1 & (1+y)(F+y) \\ (1+2z)(G+z) & 2y(G+z)-1 \end{vmatrix}_{\substack{x=r \\ y=a \\ z=b}} \\ &= \begin{vmatrix} ab-1 & a^2+a \\ 2b^2+b & 2ab-1 \end{vmatrix} \\ &= -a^2b - 2ab^2 - 4ab + 1. \end{aligned}$$

Letting $-a^2b - 2ab^2 - 4ab + 1 = 0$, we get $a^2b + 2ab^2 + 4ab = 1$. \square

Lemma 14 *Approximation values for r, a and b are:*

$$\left. \begin{aligned} r &= 0.211\,786\,319\,502\,999\dots \\ a &= 0.405\,691\,735\,408\,684\dots \\ b &= 0.462\,417\,002\,919\,618\dots \end{aligned} \right\}. \quad (69)$$

Proof: Taking the limit as $x \rightarrow r^-$ on both sides of (57), (58), and noting that $c = ab$ give us

$$a = r \exp[b + ab] \quad (70)$$

and

$$b = r \exp[a + 2ab]. \quad (71)$$

Solving $a^2b + 2ab^2 + 4ab = 1$ for a , we get

$$a = a(b) = \frac{1}{\sqrt{b^2(b+2)^2 + b + b(b+2)}}, \quad (72)$$

where $a(b)$ is the function of b defined by (72).

From (70) and (71) we get

$$r = a \exp[-(b + ab)] \quad (73)$$

and

$$b = a(b) \exp[a(b) + a(b)b - b]. \quad (74)$$

Newton's Method is used to find the root of (74) with 80 digits; this root is the value of b . Substituting b back to (72) we get the value for a ; and substituting a and b back to (73) we get the value for r . \square

Lemma 15 *The functions $A(x)$, $B(x)$ and $C(x)$ all satisfy the conditions in Theorem 6 of Chapter II.*

Proof: We start to show $A(x)$ satisfies the conditions in Theorem 6. Recall that (68) states that

$$\left. \begin{aligned} F(x, y, z) &= x \exp[z + yz] - y \\ G(x, y, z) &= x \exp[y + 2yz] - z \end{aligned} \right\}.$$

In the equation $G(x, y, z) = x \exp[y + 2yz] - z$, observe that $G_z(r, a, b) = 2ab - 1 \neq 0$. By the implicit function theorem, there is a unique solution $z = z(x, y)$

in some neighborhood of (r, a) with $z(r, a) = b$ and $z_y(r, a) = -\frac{G_y(r, a, b)}{G_z(r, a, b)}$.

Taking

$$H(x, y) = F(x, y, z(x, y)) = x \exp[z(x, y) + yz(x, y)] - y, \quad (75)$$

we can show that $A(x)$ satisfies all conditions in Theorem 6.

By similar reasoning, $B(x)$ and $C(x)$ also satisfy all conditions in Theorem 6. \square

To obtain the asymptotic formula for f_n in Theorem 6 we need the value of l_1 ; in order to get the value of l_1 the derivative $f'(x)$ is needed. For our problem we need $A'(x)$ and $B'(x)$. The next lemma is developed to find $A'(x)$ and $B'(x)$.

Lemma 16 *The derivatives $A'(x)$ and $B'(x)$ give us the following expressions:*

$$A'(x) = \frac{NA(x)}{D(x)} \quad (76)$$

$$B'(x) = \frac{NB(x)}{D(x)} \quad (77)$$

where

$$NA(x) = -A(x)[1 + B(x) - A(x)B(x)], \quad (78)$$

$$NB(x) = -B(x)[1 + A(x) + A(x)B(x)] \quad (79)$$

and

$$D(x) = x[A^2(x)B(x) + 2A(x)B^2(x) + 4A(x)B(x) - 1]. \quad (80)$$

Proof: Recalling that (57) and (58) give us

$$A(x) = x \exp[B(x) + C(x)] \quad (81)$$

and

$$B(x) = x \exp[A(x) + 2C(x)]. \quad (82)$$

Taking derivatives on both sides of (81), we get

$$A'(x) = \frac{A(x)}{x} + A(x)[B'(x) + C'(x)], \quad (83)$$

and recalling $C(x) = A(x)B(x)$ hence $C'(x) = A(x)B'(x) + A'(x)B(x)$, by substituting in (83) and simplifying, we have

$$[A(x)B(x) - 1]A'(x) + [A^2(x) + A(x)]B'(x) + \frac{A(x)}{x} = 0. \quad (84)$$

In the same fashion taking derivatives on both sides of (82) and then simplifying, we get

$$[2B^2(x) + B(x)]A'(x) + [2A(x)B(x) - 1]B'(x) + \frac{B(x)}{x} = 0.$$

Solving this system

$$\left. \begin{aligned} [A(x)B(x) - 1]A'(x) + [A^2(x) + A(x)]B'(x) + \frac{A(x)}{x} &= 0 \\ [2B^2(x) + B(x)]A'(x) + [2A(x)B(x) - 1]B'(x) + \frac{B(x)}{x} &= 0 \end{aligned} \right\} \quad (85)$$

for $A'(x)$ and $B'(x)$ gives (76) and (77). \square

Note that we can find $A''(x)$, $B''(x)$ and $D'(x)$ by using (76) and (77). Also

from (80) and Lemma 13 we see that

$$\lim_{x \rightarrow r^-} D(x) = 0. \quad (86)$$

Theorem 10 *The numbers A_p, B_p, C_p and E_p , satisfy*

$$A_p/p! = 0.114\,598\,043\,314\,091 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (87)$$

$$B_p/p! = 0.163\,253\,135\,017\,791 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (88)$$

$$C_p/p! = 0.119\,222\,531\,386\,030 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (89)$$

$$E_p/p! = 0.233\,820\,574\,700\,121 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (90)$$

Proof: We have seen by Lemma 15 that $A(x), B(x)$ and $C(x)$ all satisfy the conditions in Theorem 6.

To apply Theorem 6 to the function $A(x)$ note that $(x_0, y_0) = (r, a)$, $A(r) = a$, and $f(x) = A(x)$. Thus $A(x)$ can be expanded as

$$A(x) = a - l_1(r - x)^{1/2} + l_2(r - x) + l_3(r - x)^{3/2} + \dots \quad (91)$$

and if $l_1 \neq 0$, then

$$A_p/p! \sim \frac{l_1(r)^{1/2}}{2\sqrt{\pi}} \left[\frac{(r)^{-p}}{p^{3/2}} \right]. \quad (92)$$

So we need the numerical value for l_1 . Recall that $\omega(\theta)$ is a function with the property that $\lim_{\theta \rightarrow 0^+} \frac{\omega(\theta)}{\theta} = c$ exists.

On differentiating (91), we have

$$A'(x) = \frac{1}{2}l_1(r-x)^{-1/2} - l_2 + \omega((r-x)^{1/2}). \quad (93)$$

On the other hand rearranging (91) we have

$$a - A(x) = l_1(r-x)^{1/2} + \omega((r-x)). \quad (94)$$

From (93) and (94) we have

$$A'(x)(a - A(x)) = \frac{1}{2}l_1^2 + \omega((r-x)^{1/2}). \quad (95)$$

Therefore we get

$$\lim_{x \rightarrow r^-} A'(x)(a - A(x)) = \frac{1}{2}l_1^2. \quad (96)$$

Note that $\lim_{x \rightarrow r^-} (a - A(x)) = 0$. At the same time observe from (76) and (86) that $\lim_{x \rightarrow r^-} A'(x) = +\infty$. So by L'Hospital's Rule we have

$$\lim_{x \rightarrow r^-} A'(x)(a - A(x)) = \lim_{x \rightarrow r^-} \frac{(a - A(x))}{\frac{1}{A'(x)}} = \lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)}. \quad (97)$$

Using (76) we have

$$\begin{aligned} \lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)} &= \lim_{x \rightarrow r^-} \frac{[NA(x)/D(x)]^3}{[D(x)NA'(x) - D'(x)NA(x)]/D^2(x)} \\ &= \lim_{x \rightarrow r^-} \frac{[NA(x)]^3}{[D^2(x)NA'(x) - D(x)D'(x)NA(x)]}. \end{aligned} \quad (98)$$

Observe from (78), (76), (77) and (86) that

$$\lim_{x \rightarrow r^-} D^2(x) N A'(x) = 0. \quad (99)$$

So we have

$$\lim_{x \rightarrow r^-} \frac{[A'(x)]^3}{A''(x)} = \lim_{x \rightarrow r^-} \frac{[N A(x)]^2}{[-D(x) D'(x)]}. \quad (100)$$

Using (78), (80), (76), (77) and by computing, we have

$$\begin{aligned} \frac{1}{2} l_1^2 &= [a(1+b-ab)^2]/ \\ &\quad [br(8+7a+a^2+10b+6ab-a^2b+2b^2+2ab^2)]. \end{aligned} \quad (101)$$

Thus l_1 is determined. Finally, we have

$$\frac{l_1(r)^{1/2}}{2\sqrt{\pi}} = 0.114\ 598\ 043\ 314\ 091\dots, \quad (102)$$

which gives

$$A_p/p! = 0.114\ 598\ 043\ 314\ 091 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (103)$$

By similar arguments we have

$$B_p/p! = 0.163\ 253\ 135\ 017\ 791 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right) \quad (104)$$

and

$$C_p/p! = 0.119\ 222\ 531\ 386\ 030 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (105)$$

Consequently we have

$$E_p/p! = A_p/p! + C_p/p! = 0.233\ 820\ 574\ 700\ 121 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right). \quad (106)$$

□

So, the number of efficient dominating sets among all labeled rooted oriented trees, which is E_p , satisfies the following equation:

$$E_p = p![0.233\ 820\ 574\ 700\ 121 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right)], \quad (107)$$

and the number of efficient dominating sets among all labeled unrooted oriented trees, which is E_p/p , satisfies the equation

$$E_p/p = (p-1)![0.233\ 820\ 574\ 700\ 121 \frac{r^{-p}}{p^{3/2}} + O\left(\frac{r^{-p}}{p^{5/2}}\right)]. \quad (108)$$

Table 8 compares E_p with the values given by (107) without the error terms denoted by \tilde{E}_p .

As a consequence of the above theorem we have the next corollary which states the percentage of contribution of A_p to E_p in this version.

Corollary 3 *For A_p, C_p and E_p we have*

$$\lim_{p \rightarrow \infty} \frac{A_p}{E_p} = 0.490\ 111\ 032\ 620\ 054... \quad (109)$$

and

$$\lim_{p \rightarrow \infty} \frac{C_p}{E_p} = 0.509\ 888\ 967\ 379\ 946.... \quad (110)$$

Table 8

The Numerical Values of E_p and Approximations ($1 \leq p \leq 20$)

p	E_p	\tilde{E}_p
1	1	1
2	4	4
3	27	28
4	352	349
5	5825	5890
6	1 26576	1 26941
7	33 13723	33 29514
8	1025 78176	1029 40208
9	36536 53473	36660 70940
10	14 73515 92000	14 77973 76635
11	663 53182 81691	665 38419 35629
12	33003 32303 55456	33088 18775 60932
13	17 96963 58654 93793	18 01255 29827 06998
14	1063 06989 80225 06752	1065 43848 20339 51208
15	67900 18964 88223 06875	68041 97322 08841 02670
16	46 56970 92536 07545 89696	46 66119 89644 78480 41452
17	3413 56938 30917 65759 21217	4319 90076 25730 46271 86618
18	2 66311 88192 89294 09738 35264	2 66779 66966 46703 86671 63197
19	220 32456 32737 66238 19285 44923	220 69209 86342 56224 57994 93452
20	19267 04366 72894 29029 01657 60000	19297 64376 43587 22098 68331 83774

We notice that these two ratios are very close to the ratios of Corollary 1 in Chapter II.

From Theorem 10 we have the following corollary which determines the average number of efficient dominating sets per labeled tree (rooted or unrooted) among all labeled trees (rooted or unrooted) of order p .

Corollary 4 *Let \overline{E}_p be the average number of efficient dominating sets per tree among all labeled rooted trees of order p and let \overline{e}_p be the average number of efficient dominating sets per tree among all labeled unrooted trees of order p . Then*

$$\overline{E}_p = \overline{e}_p = \frac{p![0.233\ 820\ 574\ 700\ 121 \frac{r^{-p}}{p^{3/2}} + O(\frac{r^{-p}}{p^{5/2}})]}{pp^{p-2}}; \quad (111)$$

in particular we have

$$\lim_{p \rightarrow \infty} \sqrt[p]{\overline{E}_p} = \lim_{p \rightarrow \infty} \sqrt[p]{\overline{e}_p} = \frac{1}{er} = 1.737\ 031\ 183\ 292\ 427.... \quad (112)$$

Proof: Since there are pp^{p-2} labeled rooted trees of order p and there are p^{p-2} labeled unrooted trees of order p , using (107) and (108) we quickly get (111). From (111) and using Stirling's Formula again we have

$$\lim_{p \rightarrow \infty} \sqrt[p]{\overline{E}_p} = \lim_{p \rightarrow \infty} \sqrt[p]{\overline{e}_p} = \lim_{p \rightarrow \infty} \sqrt[p]{\frac{p!}{p^p r^p}} = \frac{1}{er} = 1.737\ 031\ 183\ 292\ 427....$$

Note in Corollary 2 that the p th root of the average number of efficient dominating sets per tree among all unlabeled rooted trees of order p is 1.641 704..., which is smaller than 1.737 031.... \square

We conclude with Table 9 which gives values for $\frac{A_p}{E_p}$, $\frac{C_p}{E_p}$ and $\sqrt[p]{\overline{E}_p}$ ($1 \leq p \leq 45$).

Table 9

The Numerical Values of A_p/E_p , C_p/E_p and $\sqrt[3]{E_p}$

p	A_p/E_p	C_p/E_p	$\sqrt[3]{E_p}$
1	1.0	0	1.
2	0.5	0.5	1.414 213 562
3	0.555 555 555 6	0.444 444 444 4	1.442 249 570
4	0.522 727 272 7	0.477 272 727 3	1.531 407 157
5	0.519 313 304 7	0.480 686 695 3	1.562 727 240
6	0.513 651 877 1	0.486 348 122 9	1.591 961 348
7	0.510 229 430 8	0.489 770 569 2	1.611 031 361
8	0.507 676 018 7	0.492 323 981 3	1.626 215 638
9	0.505 649 354 7	0.494 350 645 3	1.637 984 160
10	0.504 071 654 7	0.495 928 345 3	1.647 538 163
11	0.502 770 115 8	0.497 229 884 2	1.655 400 849
12	0.501 696 349 9	0.498 303 650 1	1.661 997 363
13	0.500 788 070 3	0.499 211 929 7	1.667 607 244
14	0.500 012 612 6	0.499 987 387 4	1.672 437 170
15	0.499 341 818 6	0.500 658 181 4	1.676 638 974
16	0.498 756 205 3	0.501 243 794 7	1.680 327 700
17	0.498 240 402 6	0.501 759 597 4	1.683 591 882
18	0.487 782 673 4	0.502 217 326 6	1.686 500 806
19	0.497 373 723 3	0.502 626 276 7	1.689 109 462
20	0.497 006 155 4	0.502 993 844 6	1.691 462 050
22	0.496 372 352 7	0.503 627 647 3	1.695 536 329
24	0.495 845 239 4	0.504 154 760 6	1.698 941 948
26	0.495 399 972 2	0.504 600 027 8	1.701 831 013
28	0.495 018 864 1	0.504 981 135 9	1.704 312 750
30	0.494 688 981 7	0.505 311 018 3	1.706 467 623
33	0.494 269 684 6	0.505 730 315 4	1.709 215 611
36	0.493 920 744 5	0.506 079 255 5	1.711 510 246
39	0.493 625 824 7	0.506 374 175 3	1.713 455 162
42	0.493 373 282 6	0.506 626 717 4	1.715 124 643
45	0.493 154 597 0	0.506 845 403 0	1.716 573 328

CHAPTER IV

TREES WITH THE MAXIMUM NUMBER OF EFFICIENT DOMINATING SETS

4.1 Introduction

In Chapter III we obtained analytic formulas for counting the number of efficient dominating sets among all labeled (rooted or unrooted) trees of order p .

The number of efficient dominating sets for a particular labeled tree T (rooted or unrooted) is the number efficient dominating sets among all orientations of T , denoted by $e(T)$. We know that there are pp^{p-2} labeled rooted trees of order p and that there are p^{p-2} labeled unrooted trees of order p . One natural question we may ask is which labeled tree (rooted or unrooted) has the maximum or minimum number of $e(T)$ among all pp^{p-2} labeled rooted trees or among all p^{p-2} labeled unrooted trees of order p .

A *maximum tree* of order p is a tree having the largest possible value of $e(T)$ among all labeled oriented trees of order p . Similarly, we can define a *minimum tree* of order p . We shall see that minimum trees of order p are unique and in fact are the star $K_{1,p-1}$. So we will focus on the problem of finding maximum trees.

Note that each unlabeled unrooted tree T of order p gives rise to exactly $p!/|Aut(T)|$ labeled trees of order p and $pp!/|Aut(T)|$ labeled rooted trees of order p , where $|Aut(T)|$ is the order of the automorphism group of T . Furthermore, each such tree has the same value of $e(T)$. In other words, the number $e(T)$ is invariant under labeling and rooting. Thus we only need to search the tree which has maximum value of $e(T)$ among all unlabeled trees of order p .

4.2 Minimum Trees

The problem of finding minimum trees of order p is quite easy because we have the following theorem which asserts that the unique minimum tree of order p is the star $K_{1,p-1}$.

Theorem 11 *The minimum tree of order p is the star $K_{1,p-1}$.*

Proof: Let $K_{1,p-1}$ be rooted at the vertex with degree of $p-1$. Label the root 1 and all children from left to right $2, 3, \dots, p-1$.

We claim that $e(K_{1,p-1}) = p$.

If the root is in an efficient dominating set, then each child must be dominated by the root. So there is only one corresponding orientation. If the root is not in an efficient dominating set, then the root must be dominated by exactly one of its children and every other child must be in the dominating set. We can choose one child from $\{2, 3, \dots, p-1\}$ to dominate the root, so there are precisely $p-1$ such orientations. Consequently, there are $1 + (p-1)$ efficient dominating sets, so $e(K_{1,p-1}) = p$.

Now, we show that if a tree T of order p is not a star $K_{1,p-1}$, then $e(T) > p$. We prove this statement by induction.

The statement is true for $p \leq 3$ since there is only one tree isomorphic to $K_{1,p-1}$ of order p for $p \leq 3$. When $p = 4$, there are two trees, namely, P_4 and $K_{1,3}$, and $e(P_4) = 6 > 4$. So the statement is true for $p \leq 4$.

Assume that the statement is true for p , where $p \geq 4$.

Let T be a tree of order $p+1$ which is not the star $K_{1,p}$. Root T at an end vertex v such that $T_1 = T - v$ is not a star $K_{1,p-1}$, and let v_1 be the unique neighbor of v . By the induction hypothesis, $e(T_1) > p$.

For each orientation of T_1 with an efficient dominating set S_1 , orient the edge vv_1 from v_1 to v . We will now show that the resulting orientation of T gives an efficient dominating set.

Consider the efficient dominating set S_1 for T_1 . If v_1 is in S_1 then S_1 is the efficient dominating set for T as well. If v_1 is dominated by one of its children, then $S_1 \cup \{v\}$ is the efficient dominating set for T . We can obtain at least one more orientation of T with an efficient dominating set. Orient every edge downward from the root v and then select vertices with even distance from the root (including the root). These vertices form an efficient dominating set.

So we have $e(T) \geq e(T_1) + 1 > p + 1$.

Therefore, the minimum tree of order p is the star $K_{1,p-1}$. \square

4.3 Finding the Maximum Trees

Unlike minimum trees, the task of finding maximum trees is much more complicated. We start with the algorithm given by Barkauskas and Host [1].

We use $T \oplus u$ to denote the rooted tree formed by joining the root of T to a new vertex u which then becomes the new root.

For any vertex v of T we define the triple (a, b, c) as follows:

a is the number of efficient dominating sets of T with v in the dominating set (v dominates itself);

b is the number of efficient dominating sets of $T \oplus u$, where v is the root of T and u is in the dominating set. (v is dominated from outside);

c is the number of efficient dominating sets of T with v in the dominated by one of its children (v is dominated from inside).

Observe that for every vertex v , $e(T) = a(v) + c(v)$. That is, $a + c$ is an invariant for all vertices of T .

Theorem 12 (*Barkauskas and Host*) *Let T_1 and T_2 be two trees with triples (a_1, b_1, c_1) and (a_2, b_2, c_2) at the respective roots v_1 and v_2 . If T is formed from T_1 and T_2 by adding the edge v_1v_2 and rooting T at $v = v_1$, the triple (a, b, c) for T at v is given by:*

$$\begin{aligned} a &= a_1(b_2 + c_2) \\ b &= b_1(a_2 + 2c_2) \\ c &= c_1(a_2 + 2c_2) + b_1a_2. \end{aligned}$$

To find the number of efficient dominating sets for a tree T , we may repeatedly use Theorem 12.

The implementation of the algorithm given by Barkauskas and Host is described as follows:

- 1.) Draw the tree as a rooted tree, with the root at the top. Number the root 1.
- 2.) Proceed down to the next level and number all vertices at distance 1 from the root 2, 3, ... sequentially from left to right.
- 3.) Go to the next level and continue numbering sequentially from left to right at each level as we proceed down the tree.
- 4.) For each leaf set $a = 1, b = 1$, and $c = 0$ initially.
- 5.) From the leaves use Theorem 12 to update the triple for the parent of vertex i for each vertex. When vertex 2 has been processed, the triple for vertex 1 (the root) (a_1, b_1, c_1) is obtained, and $e(T) = a_1 + c_1$.

Theoretically, we can use this algorithm to find the maximum trees and the corresponding number of efficient dominating sets for each order of p .

In view of the algorithm given by Barkauskas and Host, we see that in order to find the maximum trees of order p , we need to list all unlabeled trees

of order p , find the number of efficient dominating sets for each, and then finally select the maximum trees. The larger the value of p , the harder the work will be. For example, when $p = 13$, there are 1301 unlabeled trees have to be listed and searched.

We would like to modify the algorithm and use it to find the maximum trees of order p for each p up to 23.

In order to find the maximum trees of order p ($p \geq 2$), we will search among all unlabeled rooted trees. But we do not list all such trees. Instead we shall use the following code scheme introduced by Beyer and Hedetniemi [10] and developed by Kubicka [12] to generate all rooted trees of order p .

The algorithm (code scheme) uses the “level sequence code” to identify each rooted tree. Each vertex is labeled with its level, and the branches are arranged in lexicographically decreasing order. The labels are converted to a sequence by means of a postorder traversal. For example, the rooted tree shown in Figure 10 has the level sequence code $[0, 1, 2, 3, 2, 3, 2, 1, 2, 2, 1, 2, 1, 2, 1]$.

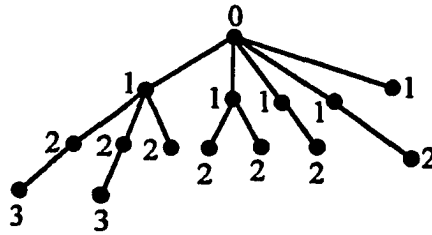


Figure 10. A Rooted Tree With Its Level Sequence Code.

We arrange the codes for all the rooted trees in reverse lexicographic order. Thus the path rooted at one end gives the first and largest code, $[0, 1, 2, \dots, p-1]$; the center rooted star gives the last and smallest code, $[0, 1, 1, \dots, 1]$.

To generate all codes for rooted trees of order p , we do following:

1.) Make an initial array of dimension p : (The code for the path)

$$v_1 = [v_1(1), v_1(2), v_1(3), \dots, v_1(p)] = [0, 1, 2, \dots, p-2, p-1].$$

The code v_{i+1} for the tree that follows v_i can be computed as follows:

2.) Case a) If the last entry of v_i has $v_i(p) > 1$, then we reduce it by 1.

Thus

$$v_{i+1} = [v_i(1), v_i(2), v_i(3), \dots, v_i(p-1), v_i(p) - 1].$$

Go to 2.)

Case b) If the last entry of v_i has $v_i(p) = 1$, then from the last entry, search backward to find the first entry $v_i(k)$ such that $v_i(k) > 1$; if there is no such entry, then stop. (We have reached the last code, namely the star.) From the k entry, search backward to find the first entry, say $v_i(k-l)$ with $v_i(k-l) = v_i(k) - 1$. We reduce $v_i(k)$ by 1, and let the entries from $v_i(k-l)$ to the new $v_i(k)$ form a block that repeat as many times as needed, with the possibility of a partial block at the end. Then v_{i+1} is made of as follows:

$$v_{i+1} = [v_i(1), v_i(2), v_i(3), \dots, \underbrace{v_i(k-l), \dots, v_i(k) - 1}_{\text{block}}, \underbrace{v_i(k-l), \dots, v_i(k) - 1}_{\text{block}}, \dots].$$

Go to 2.)

To see how 2.b) works, we see an example below. Suppose we have following code for a rooted tree of order 24 :

$$[0, 1, 2, 3, 4, 5, 2, 3, 4, 3, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]$$

Then the code for the next tree shall be

$$[0, 1, 2, 3, 4, 5, \underbrace{2, 3, 4, 3, 2}_{\text{block}}, \underbrace{2, 3, 4, 3, 2}_{\text{block}}, \underbrace{2, 3, 4, 3, 2}_{\text{block}}, \underbrace{2, 3, 4}_{\text{partial block}}].$$

To see how the algorithm works, we generate all codes for rooted trees of order p for $p = 5$. We obtain the following codes:

[0, 1, 2, 3, 4]
 [0, 1, 2, 3, 3]
 [0, 1, 2, 3, 2]
 [0, 1, 2, 3, 1]
 [0, 1, 2, 2, 2]
 [0, 1, 2, 2, 1]
 [0, 1, 2, 1, 2]
 [0, 1, 2, 1, 1]
 [0, 1, 1, 1, 1]

The correspondence between codes and rooted trees are illustrated as in Figure 11.

With this code scheme, we write a program to search the maximum trees and determine the corresponding number of efficient dominating sets of order p for each p up to 23, see Figure 17. We include the programs written in C in Appendix A.

The algorithm introduced above is basically an exhaustive search algorithm, that is, it searches all rooted trees. We shall see that it is not necessary to search all rooted trees. Some trees with certain structures cannot possibly be maximum trees. In the next section, we discuss the possibilities of improving the

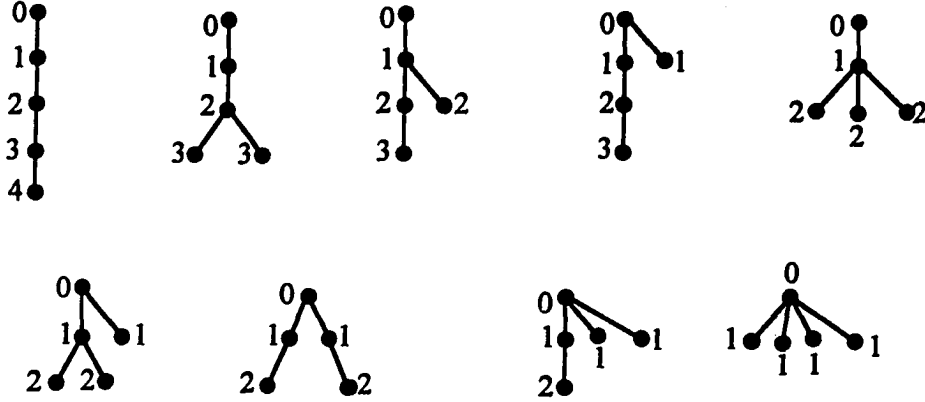


Figure 11. All Rooted Trees of Order 5 and Corresponding Codes.

algorithm.

4.4 Possible Improvements for the Algorithm

It is clear that any rooted tree T with root degree at least 2 can be built from two smaller rooted trees. So if we know the number of efficient dominating sets for each smaller rooted tree, we may find the number of efficient dominating sets for tree T .

Theorem 13 Let T_1 and T_2 be two trees with triples (a_1, b_1, c_1) and (a_2, b_2, c_2) at the respective roots v_1 and v_2 . If T is formed from T_1 and T_2 by identifying v_1 and v_2 , say $v = v_1 = v_2$, then the triple (a, b, c) for T at v is given by:

$$a = a_1 a_2$$

$$b = b_1 b_2$$

$$c = b_1 c_2 + c_1 b_2.$$

Proof: Recall that a_i ($i = 1, 2$) counts the number of efficient dominating sets for which v_i is in an efficient dominating set of T_i . Now suppose S_i ($i = 1, 2$) is an efficient dominating set of T_i for which v_i ($i = 1, 2$) is in S_i . Then observe

that $S = S_1 \cup S_2 - \{v_1, v_2\} \cup \{v\}$ is an efficient dominating set of T for which v is in S . This gives us $a \geq a_1 a_2$.

Conversely, if S is an efficient dominating set for which v is in S , then $S_1 = S - V(T_2) \cup \{v_1\}$ is an efficient dominating set of T_1 for which v_1 is in S_1 ; while $S_2 = S - V(T_1) \cup \{v_2\}$ is an efficient dominating set of T_2 for which v_2 is in S_2 . This gives us $a \leq a_1 a_2$. Thus $a = a_1 a_2$.

Similarly, we can show $b = b_1 b_2$.

To show that $c = b_1 c_2 + c_1 b_2$, we recall that c_i ($i = 1, 2$) counts the number of efficient dominating sets of T_i for which v_i is dominated by one of its children. Suppose that S_1 is an efficient dominating set of T_1 for which v_1 is dominated from outside, and that S_2 is an efficient dominating set of T_2 for which v_2 is dominated by one of its children. Then observe that $S = S_1 \cup S_2 - \{v_1, v_2\} \cup \{v\}$ is an efficient dominating set of T for which v is dominated by one of its children. In other words, every such S_1 and S_2 can contribute 1 to c . The number of such sets S_1 and S_2 is $b_1 c_2$. By symmetry we have $c \geq b_1 c_2 + c_1 b_2$.

Conversely, suppose that S is an efficient dominating set of T for which v is dominated by one of its children, say v is dominated by its child w . If w is one vertex of T_1 , counted by $c_1 b_2$; if w is one vertex of T_2 , counted by $b_1 c_2$. So $c \leq b_1 c_2 + c_1 b_2$. Thus $c = b_1 c_2 + c_1 b_2$. \square

By induction we get the following theorem:

Theorem 14 *Let T_i ($1 \leq i \leq n$) be n trees with triples (a_i, b_i, c_i) ($1 \leq i \leq n$) at the respective roots v_i ($1 \leq i \leq n$). If T is formed from T_i ($1 \leq i \leq n$) by identifying v_i ($1 \leq i \leq n$) as a single vertex v , then the triple (a, b, c) for T at v is given by:*

$$a = \prod_{i=1}^n a_i$$

$$b = \prod_{i=1}^n b_i$$

$$c = (\prod_{i=1}^n b_i)(\sum_{i=1}^n \frac{a_i}{b_i}).$$

We recall that a *branch at a vertex u* of a tree T is a maximal subtree containing u as an end-vertex. So the number of branches at u is the degree of u . We say a rooted tree is a *planted tree* if it has only one branch at the root.

Note that any rooted tree can be constructed by merging a finite number planted trees at the root. In particular, a maximum tree is constructed by merging a finite number planted trees.

Let T_1 with the triple (a_1, b_1, c_1) and T_2 with the triple (a_2, b_2, c_2) be two rooted trees of the same size q with roots v_1 and v_2 . If $a_1 \leq a_2, b_1 \leq b_2$, and $c_1 \leq c_2$, and among these three inequalities, at least one is strict, then by Theorem 13, it is clear that T_1 will never appear in a maximum tree as a proper subtree. We say that T_1 is dominated by T_2 and denote this by $T_2 \Rightarrow T_1$. The *potential planted trees* are planted trees not dominated by any other planted tree.

The *weight at a vertex u* of T is the maximum number of edges in any branch at u . So the weight at each end-vertex of T is the size of T .

A vertex v is a *centroid vertex* of a tree T if v has minimum weight, and the *centroid* of T consists of all centroid vertices. The weights at each vertex of the tree in Figure 12 are indicated and the vertices circled are centroid vertices.

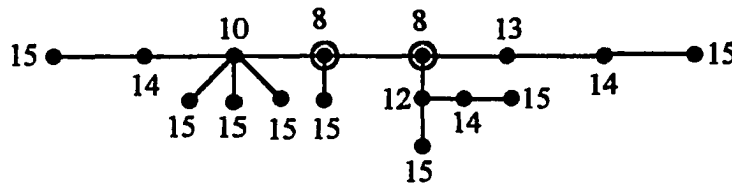


Figure 12. The Weights at the Vertices and the Centroid Vertices of a Tree.

Next, we show the following theorem:

Theorem 15 *Every tree T of size q can be rooted at a vertex such that T is built from branches, each having the size no larger than $\left\lceil \frac{q}{2} \right\rceil$.*

Proof: It is enough to show that any centroid vertex of T has weight no larger than $\left\lceil \frac{q}{2} \right\rceil$.

Let T be tree of size q and let $w(v)$ denote the weight of v .

Assume v is a centroid vertex of T . Then we show the weight $w(v) \leq \left\lceil \frac{q}{2} \right\rceil$. Suppose, to the contrary, that $w(v) \geq \left\lceil \frac{q}{2} \right\rceil + 1$. Then v has a branch B with more than $\left\lceil \frac{q}{2} \right\rceil$ edges. Let u be the unique neighbor of v in B , then we have

$$w(u) \leq \max\{q - \text{size of } B + 1, \text{size of } B - 1\} \leq \left\lceil \frac{q}{2} \right\rceil < w(v),$$

contradicting the assumption that v is a centroid vertex. \square

By Theorem 15 we see that to find all maximum trees of size q for each q , we can first find all potential planted trees of size at most $\left\lceil \frac{q}{2} \right\rceil$. Then we use these trees to construct all potential trees and search among these trees, and finally select the maximum trees.

We determined all potential planted trees of size q for each q up to 22. There are only 382 potential planted trees of size q for $0 \leq q \leq 22$. This is a very small number compared with the total number of planted trees of size q for $0 \leq q \leq 22$ which is 55 469 207. So we could write a program and use these results to find the maximum trees of size q for each q up to 44.

4.5 Some Properties of Maximum Trees

In this section we intend to discuss some properties regarding the number of efficient dominating sets of trees.

Let T_q^* denote a maximum tree of size q . It is clear that $e(T_q^*) < e(T_{q+1}^*)$,

so $\lim_{q \rightarrow \infty} e(T_q^*) = \infty$. To measure the rate of increase of $e(T_q^*)$, we consider the sequence $\{e^{1/q}(T_q^*)\}$. By examining the data in Figure 17, we see that $e^{1/q}(T_q^*)$ has an irregular behavior; in particular, it is not monotone. Nevertheless, we have the next theorem which says that this sequence is bounded both below and above.

Theorem 16 *The q th root $e^{1/q}(T_q^*)$ is bounded between 1 and 2.*

From Theorem 2 we can easily prove the above theorem. In fact, we will show later that the lower bound can be increased to 1.852509; Barkauskas, Bange, and Clark showed the upper bound can be reduced to 1.9332. They also showed the following theorem:

Theorem 17 *(Barkauskas, Bange, and Clark) The limit $\lim_{q \rightarrow \infty} e^{1/q}(T_q^*)$ exists.*

Note that the problem of finding maximum trees T_q^* of size q is the same problem as that of finding maximum $(a + c)$ -trees of size q . We can define a maximum a -tree T_q^a of size q , a maximum b -tree T_q^b of size q , and a maximum c -tree T_q^c of size q . Similarly, that is the tree with the maximum value of a , maximum value of b , and maximum value of c , respectively, among all trees and all rootings of size q . We denote the a value of T_q^a by $a(T_q^a)$, the b value of T_q^b by $b(T_q^b)$, and the c value of T_q^c by $c(T_q^c)$. We have following proposition:

Proposition 3 *The following inequalities hold:*

- 1.) $e(T_q^*) < a(T_{q+2}^a) < e(T_{q+2}^*)$
- 2.) $e(T_q^*) < b(T_{q+1}^b) < e(T_{q+2}^*)$
- 3.) $e(T_q^*) < c(T_{q+2}^c) < e(T_{q+2}^*)$.

Proof: Let T_q^* be the maximum tree of size q and rooted at v with the triple of (a, b, c) .

To show that $e(T_q^*) < a(T_{q+2}^a)$, attach a path $u_0u_1u_2$ to T_q^* by identifying v and u_0 and denote the new tree by T' . Root T' at u_2 then by using Theorem 12 we get the triple of T' : $(2a + 2c, 2a + b + c, b + c)$. Note the size of T' is $q + 2$, so we have $a(T_{q+2}^a) \geq a(T') = 2a + 2c = 2(a + c) = 2e(T_q^*) > e(T_q^*)$.

To show $a(T_{q+2}^a) < e(T_{q+2}^*)$ just note that $e(T_{q+2}^*) \geq a(T_{q+2}^a) + c(T_{q+2}^a) > a(T_{q+2}^a)$.

To show $e(T_q^*) < b(T_{q+1}^b)$, attach a path v_0v_1 to T_q^* by identifying v and v_0 and denote the new tree by T'' . Root T'' at v_1 ; then by using Theorem 12 we get the triple of T'' : $(b + c, a + 2c, a)$. Note the size of T'' is $q + 1$, so we have $b(T_{q+1}^b) \geq b(T'') = a + 2c > a + c = e(T_q^*)$.

To show $b(T_{q+1}^b) < e(T_{q+2}^*)$, let T_{q+1}^b be rooted at r with the triple of (x, y, z) , attach a path v_0v_1 to T_{q+1}^b by identifying r and v_0 and denote the new tree by T''' . Root T''' at v_1 ; then by using Theorem 12 we get the triple of T''' : $(y + z, x + 2z, x)$. Note the size of T''' is $q + 2$, so we have $e(T_{q+2}^*) \geq e(T''') = x + y + z > y = b(T_{q+1}^b)$.

To show that $e(T_q^*) < c(T_{q+2}^c)$, attach a path $u_0u_1u_2$ to T_q^* by identifying v and u_0 and denote the new tree by T'''' . Root T'''' at u_1 then by using Theorem 12 we get the triple of T'''' : $(b + c, a + 2c, 2a + 2c)$. Note the size of T'''' is $q + 2$, so we have $c(T_{q+2}^c) \geq c(T'') = 2a + 2c = 2(a + c) = 2e(T_q^*) > e(T_q^*)$.

To show $c(T_{q+2}^c) < e(T_{q+2}^*)$, just note that $e(T_{q+2}^*) \geq a(T_{q+2}^c) + c(T_{q+2}^c) > c(T_{q+2}^c)$.

Since the limit of the q th root of $e(T_q^*)$ exists, as an immediate consequence, we have following theorem:

Theorem 18 *The limit of the q th roots of $a(T_q^a), b(T_q^b), c(T_q^c)$ and $e(T_q^*)$ all exist*

as q goes to infinity; furthermore, they all have the same limit. That is:

$$s = \lim_{q \rightarrow \infty} a^{1/q}(T_q^a) = \lim_{q \rightarrow \infty} b^{1/q}(T_q^b) = \lim_{q \rightarrow \infty} c^{1/q}(T_q^c) = \lim_{q \rightarrow \infty} e^{1/q}(T_q^*)$$

Now we are ready to state the following theorem:

Theorem 19 *The number $\lim_{q \rightarrow \infty} e^{1/q}(T_q^*)$ is bounded below by s_0 , where $s_0 = 1.85\ 250\ 901\dots$*

Proof: Suppose we have a tree T rooted at v of size q with the triple (a, b, c) in which $b \geq a$. We follow the process described below to get a rooted tree T' , having size $nq + 1$.

Merge n copies of T by identifying all the roots, and let the resulting tree be \bar{T} rooted at the merged root v . Then we consider the tree $\bar{T} \oplus u$. Note that the rooted tree $\bar{T} \oplus u$ has the size $nq + 1$, and by Theorems 14 and 12, $\bar{T} \oplus u$ has the triple $(b^n + ncb^{n-1}, a^n + 2ncb^{n-1}, a^n)$ at the root u . See Figure 13.

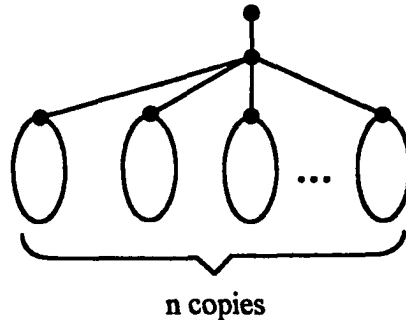


Figure 13. Merging n Copies of a Planted Trees to Get a New Planted Tree.

Let $f(n) = (a^n + 2ncb^{n-1})^{1/(nq+1)}$. Observe that $f(n) > b^{1/q}$ if n is large enough. This is because

$$(a^n + 2ncb^{n-1})^{1/(nq+1)} > b^{1/q} \Leftrightarrow (a^n + 2ncb^{n-1})^q > b^{nq+1}$$

$$\Leftrightarrow b^{nq}[(\frac{a}{b})^n + \frac{2nc}{b}]^q > b^{nq+1} \Leftrightarrow [(\frac{a}{b})^n + \frac{2nc}{b}]^q > b.$$

On the other hand since $\lim_{n \rightarrow \infty} f(n) = b^{1/q}$, we see that $f(n)$ has the maximum value for fixed a, b, c , and q . Assume $f(n)$ has the maximum $f(m)$ as $n = m$, then we obtain a rooted tree T' of size $mq + 1$.

Next, we treat the procedure above as a processor, called a *PB*-processor.

We obtain:

$$\text{Input: } T = T_1 = \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, (a, b, c) = (1, 1, 1), q = 1;$$

(Note T_1 is the best b -tree of height 1.)

$$\text{Output: } m = 1, (mq + 1) = 2, (a, b, c) = (2, 3, 1),$$

$$T' = T_2 = \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, f(m) = \sqrt{3} = 1.732.$$

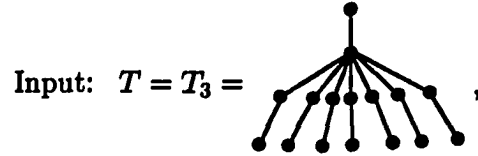
(Note T_2 is the best b -tree of height 2.)

$$\text{Input: } T = T_2 = \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, (a, b, c) = (2, 3, 1), q = 2;$$

$$\text{Output: } m = 7, (mq + 1) = 15, (a, b, c) = (7290, 10334, 128),$$

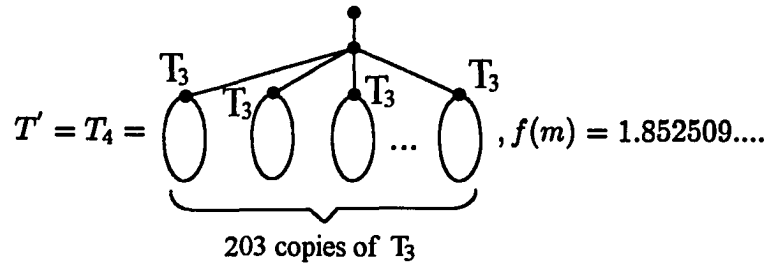
$$T' = T_3 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \quad / \quad \backslash \\ \bullet \quad \bullet \quad \bullet \quad \bullet \\ / \quad \backslash \quad / \quad \backslash \quad / \quad \backslash \\ \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \end{array}, f(m) = 1.8519....$$

(Note T_3 is the best b -tree of height 3.)



$$(a, b, c) = (7290, 10334, 128), q = 15.$$

Output: $m = 203, (mq + 1) = 3046.$

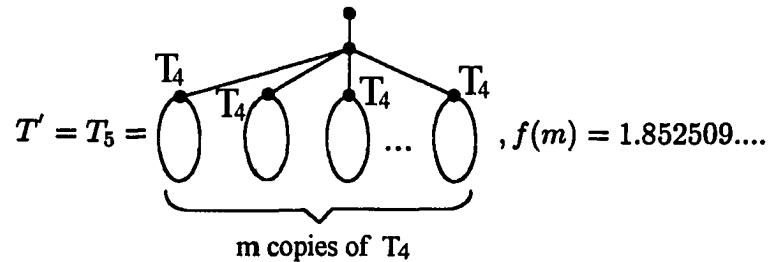


(The tree T_4 is the suspected “best” b -tree of height 4.)

Input: $T = T_4, q = 3046.$

Output: $m = 73\ 333\ 249\ 055\ 790\ 776\ 849\ 088\ 160\ 446\ 381,$

$(mq + 1) = 223\ 373\ 076\ 623\ 938\ 706\ 282\ 322\ 536\ 719\ 676\ 527,$



(The tree T_5 is the suspected “best” b -tree of height 5.)

The tree T_5 has the size about 2×10^{35} , so it is a huge tree!

By using this PB -processor, we get the bounded (by 2) monotone increasing

sequence $\{b^{1/q(T_h)}(T_h)\}$ and hence it has a limit, say s_0 . Then we obtain the desired result. \square

4.6 Further Discussion of Maximum Trees

In the previous section we obtained a lower bound s_0 for s . In this section, we discuss the limit of $\lim_{q \rightarrow \infty} e^{1/q}(T_q^*)$ and the structure of maximum trees.

First we state the following conjecture:

Conjecture 1 *The limit $\lim_{q \rightarrow \infty} b^{1/q}(T_q^b)$ is equal to its lower bound s_0 .*

We have following reasons:

- 1.) The data we have so far indicates $b^{1/q}(T_q^b) < 1.852509$.
- 2.) The data we have so far indicates that $b(T_q^b) > a(T_q^a)$ and $b(T_q^b) > c(T_q^c)$ if $q > 1$; so b is more important in the structure of maximum b -trees (also in the structure of maximum trees).

3.) We note that, by the data, the maximum b -tree is unique, and all maximum b -trees are planted trees. Furthermore, every branch of height h in a maximum b -tree of height $h + 1$ is again a maximum b -tree. That is every branch of a maximum b -tree is again a maximum b -tree. See Figure 18.

4.) If 3.) is correct, every tree T_h obtained by the processor PB above can be thought as the “best” b -tree of height h since it is built by the “best” b -tree of height $(h - 1)$ and in the “best” combination. By observation of data we see that T_1, T_2 and T_3 are the “best” b -trees of height 1, 2 and 3 respectively in the sense that there exists no other tree of height 1, or 2 or 3 has the larger value of qth root of b . It is conceivable to believe that every member of $\{T_h\}$ is indeed a maximum b -tree. (The data we have so far tells us that T_1, T_2 and T_3 are maximum b -trees; see Figure 18.) So, $\lim_{q \rightarrow \infty} b^{1/q}(T_q^b) = s_0$.

If our conjecture is correct, then we get the basic picture of the structure of maximum b -trees from the analysis above.

We now would like to discuss the structure of maximum trees. The basic idea is that maximum trees of height h are built from maximum b -trees of height $\leq h$.

Suppose we have a maximum b -tree T of size q rooted at v with the triple (a, b, c) . (So $b > a$ if $q > 1$.) We follow the process described below to get a rooted tree T'' of size mq .

Merge n copies of T by identifying all the roots to form a new root. Let the resulting tree be \bar{T} rooted at v . Then we consider the tree \bar{T} . Note that the rooted tree \bar{T} has size nq , and by Theorem 14 we note \bar{T} has the triple (a^n, b^n, ncb^{n-1}) at v . See Figure 14.

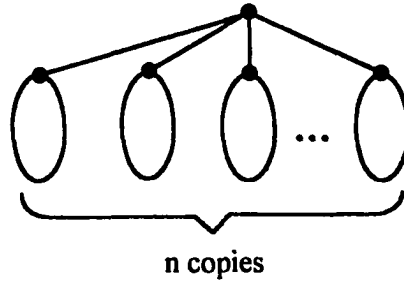


Figure 14. Merging n Copies of a Planted Trees to Get a New Tree.

Let $g(n) = (a^n + ncb^{n-1})^{1/(nq)} = e^{1/(nq)}(\bar{T})$. Observe that $g(n) > b^{1/q}$ if n is large enough. This is because

$$(a^n + ncb^{n-1})^{1/(nq)} > b^{1/q} \Leftrightarrow (a^n + ncb^{n-1}) > b^n$$

On the other hand since $\lim_{n \rightarrow \infty} g(n) = b^{1/q}$, we see that $g(n)$ has a maximum value for fixed a, b, c , and q . Assume $g(n)$ attains its maximum $g(m)$ at

$n = m$. Then we obtain a rooted tree T'' of size mq .

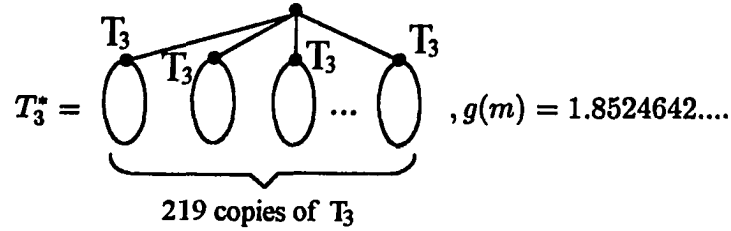
Next, we treat the process above as a processor, called the *PE*-processor, and observe what we get:

Input: $T = T_1 = \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, (a, b, c) = (1, 1, 1), q = 1$
 (Note T_1 is the best maximum b -tree of height 1.)
 Output: $m = 1, (mq) = 1, (a, b, c) = (1, 1, 1),$
 $T'' = T_1^* = \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, g(m) = 2$
 (Note T_1^* is the best tree of height 1.)

Input: $T = T_2 = \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, (a, b, c) = (2, 3, 1), q = 2.$
 (Note T_2 is the best maximum b -tree of height 2.)
 Output: $m = 7, (mq) = 14, (a, b, c) = (128, 2187, 5103),$
 $T_2^* = \begin{array}{c} \bullet \\ / \backslash / \backslash / \backslash / \backslash \\ \bullet \bullet \bullet \bullet \bullet \bullet \bullet \end{array}, g(m) = 1.84337....$
 (Note T_2^* is the best tree of height 2.)

Input: $T = T_3 = \begin{array}{c} \bullet \\ / \backslash / \backslash / \backslash / \backslash / \backslash \\ \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \end{array},$
 $(a, b, c) = (7290, 10334, 128), q = 15.$
 (Note T_3 is the best maximum b -tree of height 3.)

Output: $m = 219, (mq) = 3285,$

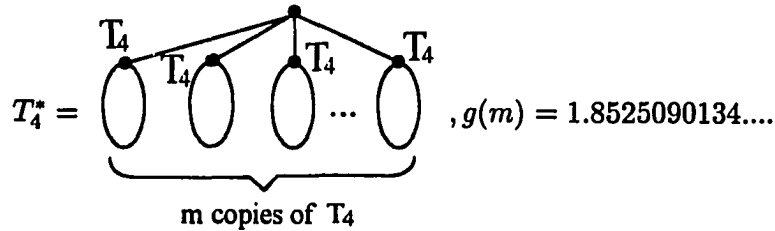


(The tree T_3^* is the suspected "best" tree of height 3.)

Input: $T = T_4, q = 3046.$

(Note T_4 is the suspected "best" maximum b -tree of height 4.)

Output: $m = 79\ 171\ 813\ 495\ 757\ 148\ 510\ 957\ 659\ 415\ 989,$
 $(mq) = 241\ 157\ 343\ 908\ 076\ 274\ 364\ 377\ 030\ 581\ 102\ 494,$



(The tree T_4^* is the suspected "best" tree of height 4.)

The tree T_4^* has the size about 2×10^{35} , so it is a huge tree.

By using the *PE*-processor, we get a sequence $\{T_h^*\}$ of trees. Since T_h^* is built from the "best" maximum b -tree of height h and in the "best" combination we may think T_h^* as the "best" tree of height h . By observation of data (see Figure 17) we see that T_1^* and T_2^* are the "best" trees of height 1 and 2 respectively in the sense that there exists no other tree of height 1 (or height 2) has the larger value of $(a + c)^{1/q}$. And hence we have the following conjecture:

Conjecture 2 *Every member of $\{T_h^*\}$ is indeed a maximum tree.*

The data we have tells us that T_1^* and T_2^* are maximum trees (see Figure 17).

As a consequence, we have the basic picture of the structure of maximum trees. In particular, we have the following:

Conjecture 3 1.) *The diameter of T_q^* approaches ∞ as $q \rightarrow \infty$.*

2.) *The maximum degree of T_q^* approaches ∞ as $q \rightarrow \infty$.*

We have conjectured the basic structure of maximum trees for those sizes that happen to appear in our processor. But what about the structure maximum trees for other sizes? It might be impossible to get the structure for each single maximum tree. But we believe that every maximum tree of height h is built from the maximum b -trees of height at most h . There are not many maximum b -trees of height at most 3, and we use only 12 maximum b -trees (see Figure 15) to generate all “conjectured” maximum trees of size q for $17 \leq q \leq 3375$.

The following gives conjectured maximum trees for $17 \leq q \leq 30$.

$q = 17$: “Maximum Tree” = {4, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 18$: “Maximum Tree” = {9, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 19$: “Maximum Tree” = {4, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 20$: “Maximum Tree” = {10, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 21$: “Maximum Tree” = {5, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 22$: “Maximum Tree” = {11, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 23$: “Maximum Tree” = {5, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0}

$q = 24$: “Maximum Tree” = {12, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

$q = 25$: “Maximum Tree” = {6, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0}

$q = 26$: “Maximum Tree” = {8, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}

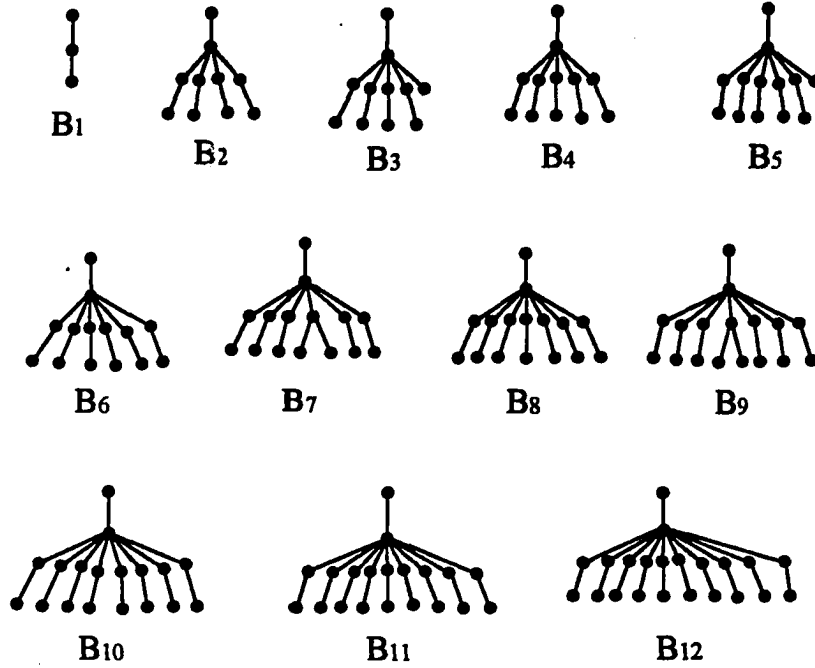


Figure 15. Twelve Maximum b-Trees in Conjecture 2.

$q = 27$: "Maximum Tree" = $\{6, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0\}$

$q = 28$: "Maximum Tree" = $\{4, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$

$q = 29$: "Maximum Tree" = $\{7, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0\}$

$q = 30$: "Maximum Tree" = $\{5, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$

The conjectured "Maximum Tree" T is represented by an array of dimension 12. If the i th entry of the array has value k , then k copies of B_i are merged at the root of T . For example, $q = 28$: "Maximum Tree" = $\{4, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0\}$ means four copies of B_1 , one copy of B_2 , and one copy of B_4 are merged at the root of T , where T is the conjectured maximum tree of size 28. See Figure 16.

Conjectured maximum trees for $31 \leq q \leq 300$ are reported in Table 10.

Table 10

Conjectured Maximum Trees ($31 \leq q \leq 300$)

q	Maximum Tree	q	Maximum Tree
31	{8, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0}	61	{8, 0, 0, 0, 0, 0, 0, 3, 0, 0, 0, 0}
32	{5, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0}	62	{6, 0, 0, 1, 0, 3, 0, 0, 0, 0, 0, 0}
33	{8, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0}	63	{8, 0, 0, 0, 0, 0, 0, 2, 0, 1, 0, 0}
34	{6, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0}	64	{6, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0}
35	{8, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0}	65	{8, 0, 0, 0, 0, 0, 0, 1, 0, 2, 0, 0}
36	{6, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0}	66	{7, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0}
37	{9, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0}	67	{8, 0, 0, 0, 0, 0, 0, 0, 0, 3, 0, 0}
38	{6, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0}	68	{7, 0, 0, 0, 0, 3, 0, 1, 0, 0, 0, 0}
39	{9, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1}	69	{9, 0, 0, 0, 0, 0, 0, 0, 0, 3, 0, 0}
40	{7, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0}	70	{7, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 0}
41	{10, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1}	71	{9, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1, 0}
42	{7, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0}	72	{7, 0, 0, 0, 0, 1, 0, 3, 0, 0, 0, 0}
43	{5, 0, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0}	73	{6, 0, 0, 2, 0, 3, 0, 0, 0, 0, 0, 0}
44	{7, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0}	74	{7, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0}
45	{6, 0, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0}	75	{6, 0, 0, 1, 0, 4, 0, 0, 0, 0, 0, 0}
46	{8, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0}	76	{8, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0}
47	{6, 0, 0, 2, 0, 1, 0, 0, 0, 0, 0, 0}	77	{6, 0, 0, 0, 0, 5, 0, 0, 0, 0, 0, 0}
48	{8, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0}	78	{8, 0, 0, 0, 0, 0, 0, 3, 0, 1, 0, 0}
49	{6, 0, 0, 1, 0, 2, 0, 0, 0, 0, 0, 0}	79	{7, 0, 0, 0, 0, 5, 0, 0, 0, 0, 0, 0}
50	{8, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0}	80	{8, 0, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0}
51	{6, 0, 0, 0, 0, 3, 0, 0, 0, 0, 0, 0}	81	{7, 0, 0, 0, 0, 4, 0, 1, 0, 0, 0, 0}
52	{9, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0}	82	{8, 0, 0, 0, 0, 0, 0, 1, 0, 3, 0, 0}
53	{7, 0, 0, 0, 0, 3, 0, 0, 0, 0, 0, 0}	83	{7, 0, 0, 0, 0, 3, 0, 2, 0, 0, 0, 0}
54	{9, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0}	84	{8, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0}
55	{7, 0, 0, 0, 0, 2, 0, 1, 0, 0, 0, 0}	85	{7, 0, 0, 0, 0, 2, 0, 3, 0, 0, 0, 0}
56	{9, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0}	86	{9, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0}
57	{7, 0, 0, 0, 0, 1, 0, 2, 0, 0, 0, 0}	87	{7, 0, 0, 0, 0, 1, 0, 4, 0, 0, 0, 0}
58	{6, 0, 0, 3, 0, 1, 0, 0, 0, 0, 0, 0}	88	{6, 0, 0, 1, 0, 5, 0, 0, 0, 0, 0, 0}
59	{7, 0, 0, 0, 0, 0, 0, 3, 0, 0, 0, 0}	89	{7, 0, 0, 0, 0, 0, 0, 5, 0, 0, 0, 0}
60	{6, 0, 0, 2, 0, 2, 0, 0, 0, 0, 0, 0}	90	{6, 0, 0, 0, 0, 6, 0, 0, 0, 0, 0, 0}

Table 10 — Continued

q	Maximum Tree	q	Maximum Tree
91	{8, 0, 0, 0, 0, 0, 0, 5, 0, 0, 0, 0}	126	{7, 0, 0, 0, 0, 4, 0, 4, 0, 0, 0, 0}
92	{7, 0, 0, 0, 0, 0, 6, 0, 0, 0, 0, 0}	127	{8, 0, 0, 0, 0, 0, 0, 4, 0, 3, 0, 0}
93	{8, 0, 0, 0, 0, 0, 0, 4, 0, 1, 0, 0}	128	{7, 0, 0, 0, 0, 3, 0, 5, 0, 0, 0, 0}
94	{7, 0, 0, 0, 0, 5, 0, 1, 0, 0, 0, 0}	129	{8, 0, 0, 0, 0, 0, 0, 3, 0, 4, 0, 0}
95	{8, 0, 0, 0, 0, 0, 0, 3, 0, 2, 0, 0}	130	{7, 0, 0, 0, 0, 2, 0, 6, 0, 0, 0, 0}
96	{7, 0, 0, 0, 0, 4, 0, 2, 0, 0, 0, 0}	131	{8, 0, 0, 0, 0, 0, 0, 2, 0, 5, 0, 0}
97	{8, 0, 0, 0, 0, 0, 0, 2, 0, 3, 0, 0}	132	{7, 0, 0, 0, 0, 1, 0, 7, 0, 0, 0, 0}
98	{7, 0, 0, 0, 0, 3, 0, 3, 0, 0, 0, 0}	133	{8, 0, 0, 0, 0, 0, 0, 1, 0, 6, 0, 0}
99	{8, 0, 0, 0, 0, 0, 0, 1, 0, 4, 0, 0}	134	{7, 0, 0, 0, 0, 0, 0, 8, 0, 0, 0, 0}
100	{7, 0, 0, 0, 0, 2, 0, 4, 0, 0, 0, 0}	135	{7, 0, 0, 0, 0, 7, 0, 2, 0, 0, 0, 0}
101	{8, 0, 0, 0, 0, 0, 0, 0, 0, 5, 0, 0}	136	{8, 0, 0, 0, 0, 0, 0, 8, 0, 0, 0, 0}
102	{7, 0, 0, 0, 0, 1, 0, 5, 0, 0, 0, 0}	137	{7, 0, 0, 0, 0, 6, 0, 3, 0, 0, 0, 0}
103	{6, 0, 0, 0, 0, 7, 0, 0, 0, 0, 0, 0}	138	{8, 0, 0, 0, 0, 0, 0, 7, 0, 1, 0, 0}
104	{7, 0, 0, 0, 0, 0, 0, 6, 0, 0, 0, 0}	139	{7, 0, 0, 0, 0, 5, 0, 4, 0, 0, 0, 0}
105	{7, 0, 0, 0, 0, 7, 0, 0, 0, 0, 0, 0}	140	{8, 0, 0, 0, 0, 0, 0, 6, 0, 2, 0, 0}
106	{8, 0, 0, 0, 0, 0, 0, 6, 0, 0, 0, 0}	141	{7, 0, 0, 0, 0, 4, 0, 5, 0, 0, 0, 0}
107	{7, 0, 0, 0, 0, 6, 0, 1, 0, 0, 0, 0}	142	{8, 0, 0, 0, 0, 0, 0, 5, 0, 3, 0, 0}
108	{8, 0, 0, 0, 0, 0, 0, 5, 0, 1, 0, 0}	143	{7, 0, 0, 0, 0, 3, 0, 6, 0, 0, 0, 0}
109	{7, 0, 0, 0, 0, 5, 0, 2, 0, 0, 0, 0}	144	{8, 0, 0, 0, 0, 0, 0, 4, 0, 4, 0, 0}
110	{8, 0, 0, 0, 0, 0, 0, 4, 0, 2, 0, 0}	145	{7, 0, 0, 0, 0, 2, 0, 7, 0, 0, 0, 0}
111	{7, 0, 0, 0, 0, 4, 0, 3, 0, 0, 0, 0}	146	{8, 0, 0, 0, 0, 0, 0, 3, 0, 5, 0, 0}
112	{8, 0, 0, 0, 0, 0, 0, 3, 0, 3, 0, 0}	147	{7, 0, 0, 0, 0, 1, 0, 8, 0, 0, 0, 0}
113	{7, 0, 0, 0, 0, 3, 0, 4, 0, 0, 0, 0}	148	{6, 0, 0, 0, 0, 7, 0, 3, 0, 0, 0, 0}
114	{8, 0, 0, 0, 0, 0, 0, 2, 0, 4, 0, 0}	149	{7, 0, 0, 0, 0, 0, 0, 9, 0, 0, 0, 0}
115	{7, 0, 0, 0, 0, 2, 0, 5, 0, 0, 0, 0}	150	{7, 0, 0, 0, 0, 7, 0, 3, 0, 0, 0, 0}
116	{8, 0, 0, 0, 0, 0, 0, 1, 0, 5, 0, 0}	151	{8, 0, 0, 0, 0, 0, 0, 9, 0, 0, 0, 0}
117	{7, 0, 0, 0, 0, 1, 0, 6, 0, 0, 0, 0}	152	{7, 0, 0, 0, 0, 6, 0, 4, 0, 0, 0, 0}
118	{8, 0, 0, 0, 0, 0, 0, 0, 0, 6, 0, 0}	153	{8, 0, 0, 0, 0, 0, 0, 8, 0, 1, 0, 0}
119	{7, 0, 0, 0, 0, 0, 0, 7, 0, 0, 0, 0}	154	{7, 0, 0, 0, 0, 5, 0, 5, 0, 0, 0, 0}
120	{7, 0, 0, 0, 0, 7, 0, 1, 0, 0, 0, 0}	155	{8, 0, 0, 0, 0, 0, 0, 7, 0, 2, 0, 0}
121	{8, 0, 0, 0, 0, 0, 0, 7, 0, 0, 0, 0}	156	{7, 0, 0, 0, 0, 4, 0, 6, 0, 0, 0, 0}
122	{7, 0, 0, 0, 0, 6, 0, 2, 0, 0, 0, 0}	157	{8, 0, 0, 0, 0, 0, 0, 6, 0, 3, 0, 0}
123	{8, 0, 0, 0, 0, 0, 0, 6, 0, 1, 0, 0}	158	{7, 0, 0, 0, 0, 3, 0, 7, 0, 0, 0, 0}
124	{7, 0, 0, 0, 0, 5, 0, 3, 0, 0, 0, 0}	159	{8, 0, 0, 0, 0, 0, 0, 5, 0, 4, 0, 0}
125	{8, 0, 0, 0, 0, 0, 0, 5, 0, 2, 0, 0}	160	{7, 0, 0, 0, 0, 2, 0, 8, 0, 0, 0, 0}

Table 10 — Continued

q	Maximum Tree	q	Maximum Tree
161	{8, 0, 0, 0, 0, 0, 0, 4, 0, 5, 0, 0}	196	{7, 0, 0, 0, 0, 0, 0, 11, 0, 1, 0, 0}
162	{7, 0, 0, 0, 0, 0, 1, 0, 9, 0, 0, 0}	197	{6, 0, 0, 0, 0, 0, 5, 0, 8, 0, 0, 0}
163	{6, 0, 0, 0, 0, 0, 7, 0, 4, 0, 0, 0}	198	{7, 0, 0, 0, 0, 0, 0, 10, 0, 2, 0, 0}
164	{7, 0, 0, 0, 0, 0, 0, 10, 0, 0, 0, 0}	199	{6, 0, 0, 0, 0, 0, 4, 0, 9, 0, 0, 0}
165	{6, 0, 0, 0, 0, 0, 6, 0, 5, 0, 0, 0}	200	{8, 0, 0, 0, 0, 0, 0, 10, 0, 2, 0, 0}
166	{8, 0, 0, 0, 0, 0, 0, 10, 0, 0, 0, 0}	201	{7, 0, 0, 0, 0, 0, 4, 0, 9, 0, 0, 0}
167	{7, 0, 0, 0, 0, 0, 6, 0, 5, 0, 0, 0}	202	{8, 0, 0, 0, 0, 0, 0, 9, 0, 3, 0, 0}
168	{8, 0, 0, 0, 0, 0, 0, 9, 0, 1, 0, 0}	203	{7, 0, 0, 0, 0, 3, 0, 10, 0, 0, 0, 0}
169	{7, 0, 0, 0, 0, 5, 0, 6, 0, 0, 0, 0}	204	{8, 0, 0, 0, 0, 0, 0, 8, 0, 4, 0, 0}
170	{8, 0, 0, 0, 0, 0, 0, 8, 0, 2, 0, 0}	205	{7, 0, 0, 0, 0, 2, 0, 11, 0, 0, 0, 0}
171	{7, 0, 0, 0, 0, 4, 0, 7, 0, 0, 0, 0}	206	{8, 0, 0, 0, 0, 0, 0, 7, 0, 5, 0, 0}
172	{8, 0, 0, 0, 0, 0, 0, 7, 0, 3, 0, 0}	207	{7, 0, 0, 0, 0, 1, 0, 12, 0, 0, 0, 0}
173	{7, 0, 0, 0, 0, 3, 0, 8, 0, 0, 0, 0}	208	{6, 0, 0, 0, 0, 7, 0, 7, 0, 0, 0, 0}
174	{8, 0, 0, 0, 0, 0, 0, 6, 0, 4, 0, 0}	209	{7, 0, 0, 0, 0, 0, 0, 13, 0, 0, 0, 0}
175	{7, 0, 0, 0, 0, 2, 0, 9, 0, 0, 0, 0}	210	{6, 0, 0, 0, 0, 6, 0, 8, 0, 0, 0, 0}
176	{8, 0, 0, 0, 0, 0, 0, 5, 0, 5, 0, 0}	211	{7, 0, 0, 0, 0, 0, 0, 12, 0, 1, 0, 0}
177	{7, 0, 0, 0, 0, 1, 0, 10, 0, 0, 0, 0}	212	{6, 0, 0, 0, 0, 5, 0, 9, 0, 0, 0, 0}
178	{6, 0, 0, 0, 0, 7, 0, 5, 0, 0, 0, 0}	213	{7, 0, 0, 0, 0, 0, 0, 11, 0, 2, 0, 0}
179	{7, 0, 0, 0, 0, 0, 0, 11, 0, 0, 0, 0}	214	{6, 0, 0, 0, 0, 4, 0, 10, 0, 0, 0, 0}
180	{6, 0, 0, 0, 0, 6, 0, 6, 0, 0, 0, 0}	215	{7, 0, 0, 0, 0, 0, 0, 10, 0, 3, 0, 0}
181	{8, 0, 0, 0, 0, 0, 0, 11, 0, 0, 0, 0}	216	{6, 0, 0, 0, 0, 3, 0, 11, 0, 0, 0, 0}
182	{6, 0, 0, 0, 0, 5, 0, 7, 0, 0, 0, 0}	217	{7, 0, 0, 0, 0, 0, 0, 9, 0, 4, 0, 0}
183	{8, 0, 0, 0, 0, 0, 0, 10, 0, 1, 0, 0}	218	{7, 0, 0, 0, 0, 3, 0, 11, 0, 0, 0, 0}
184	{7, 0, 0, 0, 0, 5, 0, 7, 0, 0, 0, 0}	219	{8, 0, 0, 0, 0, 0, 0, 9, 0, 4, 0, 0}
185	{8, 0, 0, 0, 0, 0, 0, 9, 0, 2, 0, 0}	220	{7, 0, 0, 0, 0, 2, 0, 12, 0, 0, 0, 0}
186	{7, 0, 0, 0, 0, 4, 0, 8, 0, 0, 0, 0}	221	{8, 0, 0, 0, 0, 0, 0, 8, 0, 5, 0, 0}
187	{8, 0, 0, 0, 0, 0, 0, 8, 0, 3, 0, 0}	222	{7, 0, 0, 0, 0, 1, 0, 13, 0, 0, 0, 0}
188	{7, 0, 0, 0, 0, 3, 0, 9, 0, 0, 0, 0}	223	{6, 0, 0, 0, 0, 7, 0, 8, 0, 0, 0, 0}
189	{8, 0, 0, 0, 0, 0, 0, 7, 0, 4, 0, 0}	224	{7, 0, 0, 0, 0, 0, 0, 14, 0, 0, 0, 0}
190	{7, 0, 0, 0, 0, 2, 0, 10, 0, 0, 0, 0}	225	{6, 0, 0, 0, 0, 6, 0, 9, 0, 0, 0, 0}
191	{8, 0, 0, 0, 0, 0, 0, 6, 0, 5, 0, 0}	226	{7, 0, 0, 0, 0, 0, 0, 13, 0, 1, 0, 0}
192	{7, 0, 0, 0, 0, 1, 0, 11, 0, 0, 0, 0}	227	{6, 0, 0, 0, 0, 5, 0, 10, 0, 0, 0, 0}
193	{6, 0, 0, 0, 0, 7, 0, 6, 0, 0, 0, 0}	228	{7, 0, 0, 0, 0, 0, 0, 12, 0, 2, 0, 0}
194	{7, 0, 0, 0, 0, 0, 0, 12, 0, 0, 0, 0}	229	{6, 0, 0, 0, 0, 4, 0, 11, 0, 0, 0, 0}
195	{6, 0, 0, 0, 0, 6, 0, 7, 0, 0, 0, 0}	230	{7, 0, 0, 0, 0, 0, 0, 11, 0, 3, 0, 0}

Table 10 — Continued

q	Maximum Tree	q	Maximum Tree
231	{6, 0, 0, 0, 0, 3, 0, 12, 0, 0, 0, 0}	266	{7, 0, 0, 0, 0, 0, 0, 10, 0, 6, 0, 0}
232	{7, 0, 0, 0, 0, 0, 0, 10, 0, 4, 0, 0}	267	{6, 0, 0, 0, 0, 0, 0, 17, 0, 0, 0, 0}
233	{6, 0, 0, 0, 0, 2, 0, 13, 0, 0, 0, 0}	268	{6, 0, 0, 0, 0, 7, 0, 11, 0, 0, 0, 0}
234	{7, 0, 0, 0, 0, 0, 0, 9, 0, 5, 0, 0}	269	{7, 0, 0, 0, 0, 0, 0, 17, 0, 0, 0, 0}
235	{6, 0, 0, 0, 0, 1, 0, 14, 0, 0, 0, 0}	270	{6, 0, 0, 0, 0, 6, 0, 12, 0, 0, 0, 0}
236	{7, 0, 0, 0, 0, 0, 0, 8, 0, 6, 0, 0}	271	{7, 0, 0, 0, 0, 0, 0, 16, 0, 1, 0, 0}
237	{7, 0, 0, 0, 0, 1, 0, 14, 0, 0, 0, 0}	272	{6, 0, 0, 0, 0, 5, 0, 13, 0, 0, 0, 0}
238	{6, 0, 0, 0, 0, 7, 0, 9, 0, 0, 0, 0}	273	{7, 0, 0, 0, 0, 0, 0, 15, 0, 2, 0, 0}
239	{7, 0, 0, 0, 0, 0, 0, 15, 0, 0, 0, 0}	274	{6, 0, 0, 0, 0, 4, 0, 14, 0, 0, 0, 0}
240	{6, 0, 0, 0, 0, 6, 0, 10, 0, 0, 0, 0}	275	{7, 0, 0, 0, 0, 0, 0, 14, 0, 3, 0, 0}
241	{7, 0, 0, 0, 0, 0, 0, 14, 0, 1, 0, 0}	276	{6, 0, 0, 0, 0, 3, 0, 15, 0, 0, 0, 0}
242	{6, 0, 0, 0, 0, 5, 0, 11, 0, 0, 0, 0}	277	{7, 0, 0, 0, 0, 0, 0, 13, 0, 4, 0, 0}
243	{7, 0, 0, 0, 0, 0, 0, 13, 0, 2, 0, 0}	278	{6, 0, 0, 0, 0, 2, 0, 16, 0, 0, 0, 0}
244	{6, 0, 0, 0, 0, 4, 0, 12, 0, 0, 0, 0}	279	{7, 0, 0, 0, 0, 0, 0, 12, 0, 5, 0, 0}
245	{7, 0, 0, 0, 0, 0, 0, 12, 0, 3, 0, 0}	280	{6, 0, 0, 0, 0, 1, 0, 17, 0, 0, 0, 0}
246	{6, 0, 0, 0, 0, 3, 0, 13, 0, 0, 0, 0}	281	{7, 0, 0, 0, 0, 0, 0, 11, 0, 6, 0, 0}
247	{7, 0, 0, 0, 0, 0, 0, 11, 0, 4, 0, 0}	282	{6, 0, 0, 0, 0, 0, 0, 18, 0, 0, 0, 0}
248	{6, 0, 0, 0, 0, 2, 0, 14, 0, 0, 0, 0}	283	{6, 0, 0, 0, 0, 7, 0, 12, 0, 0, 0, 0}
249	{7, 0, 0, 0, 0, 0, 0, 10, 0, 5, 0, 0}	284	{7, 0, 0, 0, 0, 0, 0, 18, 0, 0, 0, 0}
250	{6, 0, 0, 0, 0, 1, 0, 15, 0, 0, 0, 0}	285	{6, 0, 0, 0, 0, 6, 0, 13, 0, 0, 0, 0}
251	{7, 0, 0, 0, 0, 0, 0, 9, 0, 6, 0, 0}	286	{7, 0, 0, 0, 0, 0, 0, 17, 0, 1, 0, 0}
252	{6, 0, 0, 0, 0, 0, 0, 16, 0, 0, 0, 0}	287	{6, 0, 0, 0, 0, 5, 0, 14, 0, 0, 0, 0}
253	{6, 0, 0, 0, 0, 7, 0, 10, 0, 0, 0, 0}	288	{7, 0, 0, 0, 0, 0, 0, 16, 0, 2, 0, 0}
254	{7, 0, 0, 0, 0, 0, 0, 16, 0, 0, 0, 0}	289	{6, 0, 0, 0, 0, 4, 0, 15, 0, 0, 0, 0}
255	{6, 0, 0, 0, 0, 6, 0, 11, 0, 0, 0, 0}	290	{7, 0, 0, 0, 0, 0, 0, 15, 0, 3, 0, 0}
256	{7, 0, 0, 0, 0, 0, 0, 15, 0, 1, 0, 0}	291	{6, 0, 0, 0, 0, 3, 0, 16, 0, 0, 0, 0}
257	{6, 0, 0, 0, 0, 5, 0, 12, 0, 0, 0, 0}	292	{7, 0, 0, 0, 0, 0, 0, 14, 0, 4, 0, 0}
258	{7, 0, 0, 0, 0, 0, 0, 14, 0, 2, 0, 0}	293	{6, 0, 0, 0, 0, 2, 0, 17, 0, 0, 0, 0}
259	{6, 0, 0, 0, 0, 4, 0, 13, 0, 0, 0, 0}	294	{7, 0, 0, 0, 0, 0, 0, 13, 0, 5, 0, 0}
260	{7, 1, 0, 0, 0, 0, 0, 13, 0, 3, 0, 0}	295	{6, 0, 0, 0, 0, 1, 0, 18, 0, 0, 0, 0}
261	{6, 0, 0, 0, 0, 3, 0, 14, 0, 0, 0, 0}	296	{7, 0, 0, 0, 0, 0, 0, 12, 0, 6, 0, 0}
262	{7, 0, 0, 0, 0, 0, 0, 12, 0, 4, 0, 0}	297	{6, 0, 0, 0, 0, 0, 0, 19, 0, 0, 0, 0}
263	{6, 0, 0, 0, 0, 2, 0, 15, 0, 0, 0, 0}	298	{6, 0, 0, 0, 0, 7, 0, 13, 0, 0, 0, 0}
264	{7, 0, 0, 0, 0, 0, 0, 11, 0, 5, 0, 0}	299	{7, 0, 0, 0, 0, 0, 0, 19, 0, 0, 0, 0}
265	{6, 0, 0, 0, 0, 1, 0, 16, 0, 0, 0, 0}	300	{6, 0, 0, 0, 0, 6, 0, 14, 0, 0, 0, 0}

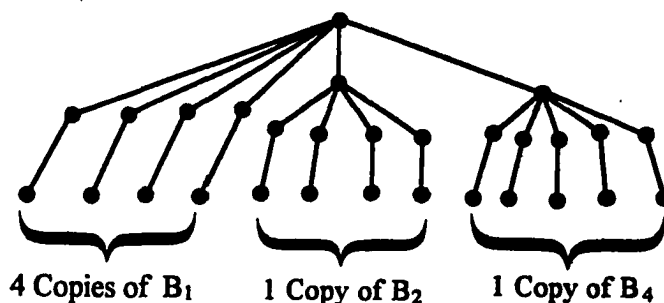


Figure 16. Conjectured Maximum Tree of Size 28.

The data we have so far tells us that the diameter of maximum trees for $1 \leq q \leq 22$ is at most 5; on the other hand the conjecture implies the diameter of maximum trees approaches ∞ . But since the “best” maximum tree of height 3 is T_3^* which has size 3285; the “best” maximum tree of height 4 is T_4^* which has size about 2×10^{35} . We believe that the diameter of maximum trees would not exceed 6 until the size q is about 3000, and the diameter of maximum trees would not exceed 8 until the size q is about 2×10^{35} . So the diameter of maximum trees seems to be increasing extremely slowly as the size q goes to infinity.

Among all maximum trees, we may think T_1 is the basic unit for maximum tree of height 1; T_2 is the basic unit for maximum tree of height 2 and so on, and it appears that nearly all branches in all maximum trees are those T_i^* s.

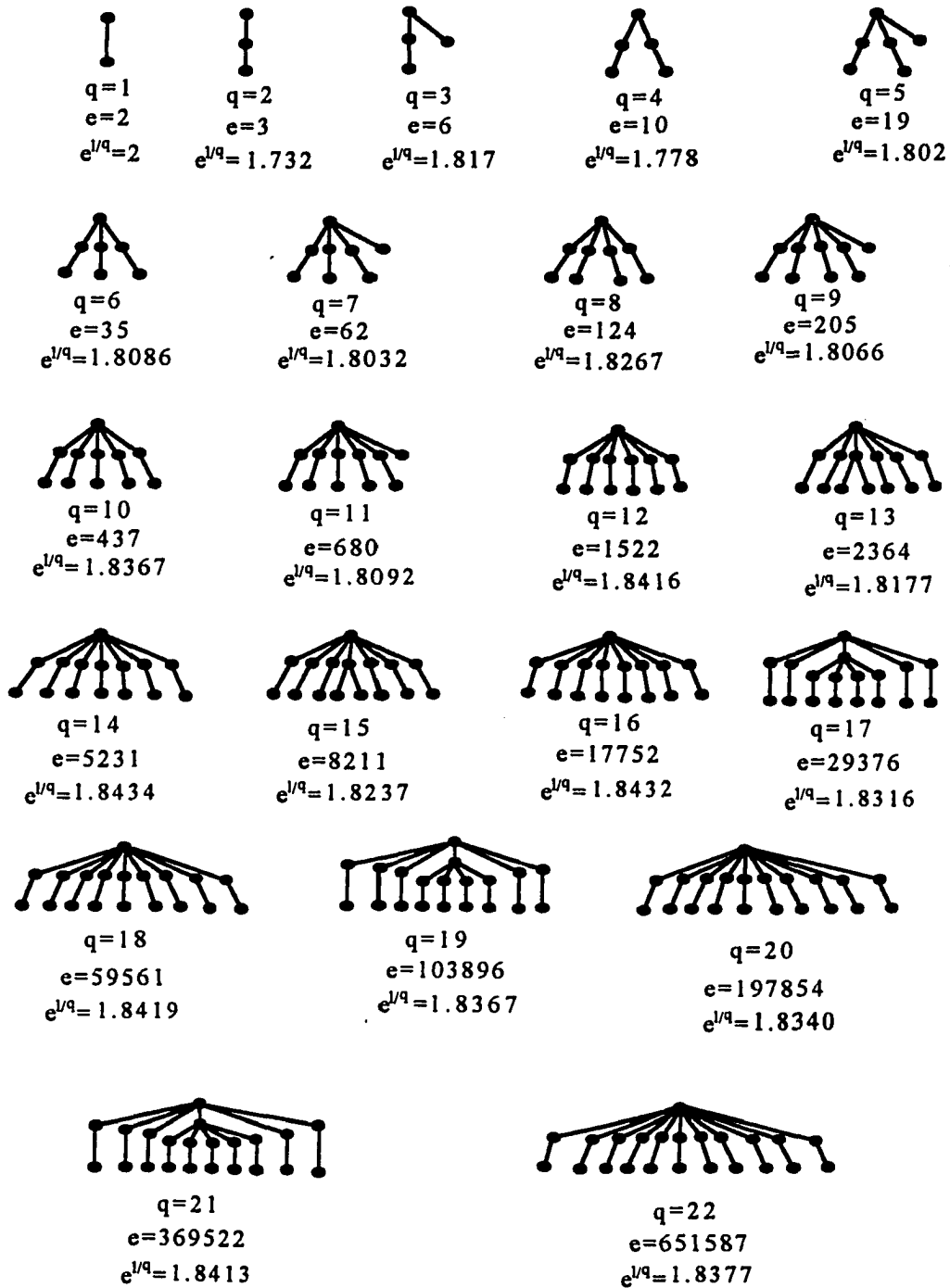


Figure 17. Maximum Trees of Size q for Each q up to 22.

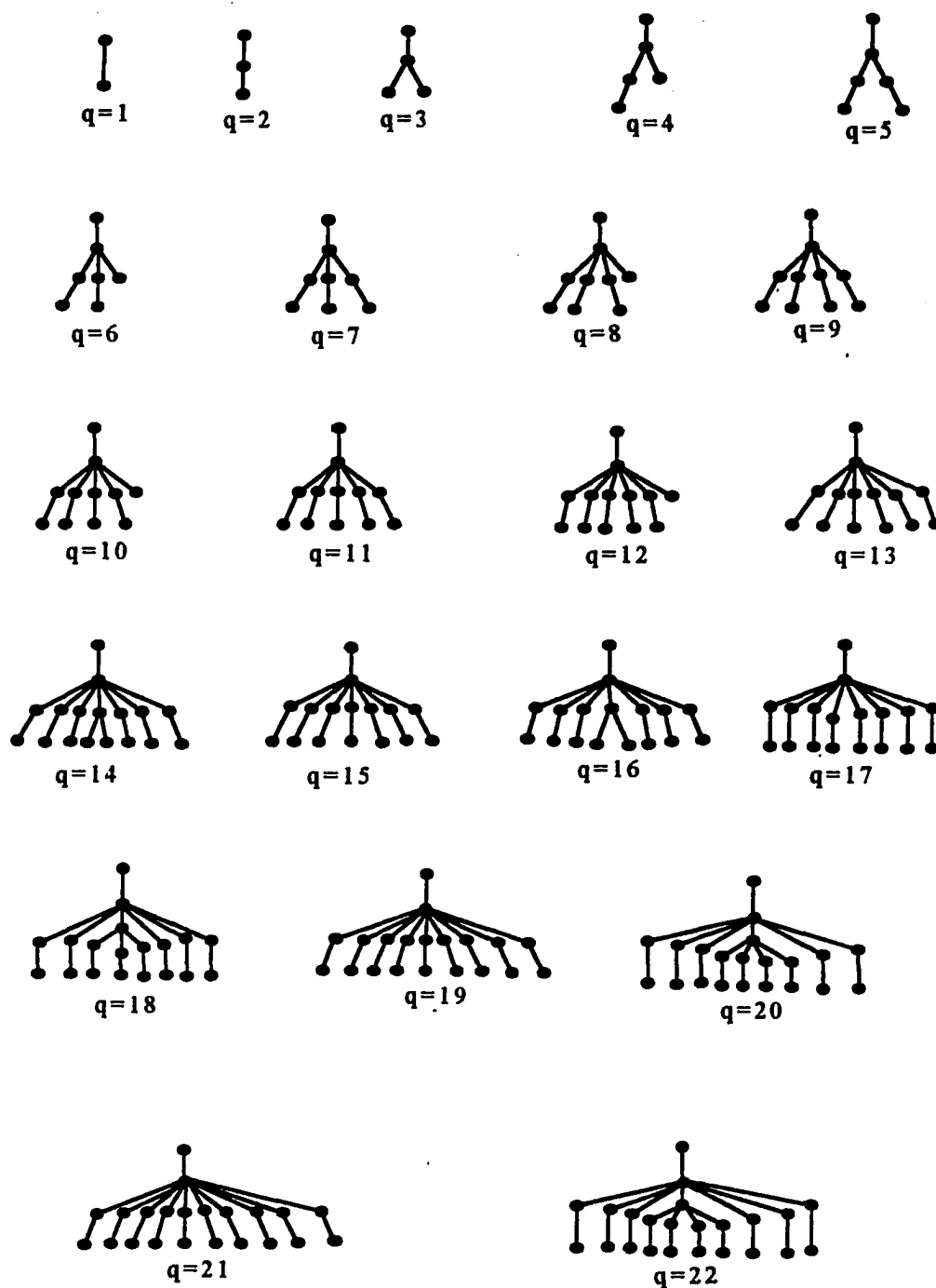


Figure 18. Maximum b-Trees of Size q for Each q up to 22.

CHAPTER V

SOME OPEN PROBLEMS

In this chapter, we include some open problems for further study.

1. In Chapter IV, we discussed some properties of maximum trees and conjectured the q th root of the number of efficient dominating sets of maximum tree of size q $e^{1/q}(T_q^*)$ has the limit of 1.852509....Can we indeed prove it? Further, can we find an asymptotic formula for $e^{1/q}(T_q^*)$?

2. We can show that there exist ties of the number of efficient dominating sets among all trees of size q if q is large enough ($q \geq 13$ approximately), that is, there will be two nonisomorphic trees of the same size q having the same number of efficient dominating sets if q is large enough. On the other hand, by investigating the data we notice that there is no ties for maximum trees of size q for $1 \leq q \leq 22$, that is we have not found two nonisomorphic trees of the same size q having the largest possible number of efficient dominating sets for $1 \leq q \leq 22$. Is this true for any q ?

3. In Chapter IV, we defined the maximum tree of size q to be a tree with the largest possible number of efficient dominating sets among all labeled trees of the same size q . And this maximum tree is the same for the rooted or unrooted version. We can define the maximum tree of size q for other alternate two versions. The maximum tree of size q of unlabeled rooted trees is the rooted tree with the largest possible number of efficient dominating sets among all unlabeled rooted trees of the same size q ; the maximum tree of size q of unlabeled unrooted trees can be defined similarly. In Figure 19, a tree has the different number of efficient

dominating sets for different versions.

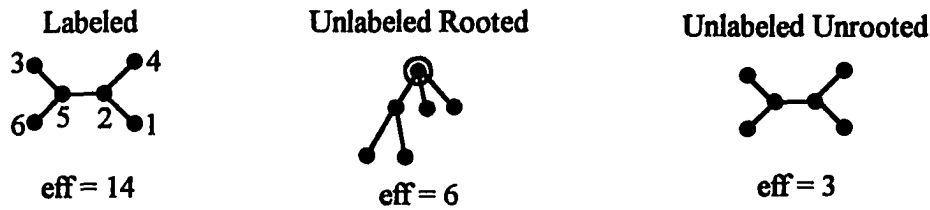


Figure 19. Efficient Dominating Sets of the Same Tree for Different Version.

We have obtained the algorithms to search maximum trees for each of these two alternate versions. Many questions can be asked for these two alternate versions. In particular, we would like to know the structures of maximum trees for these two versions. Are there any ties of maximum trees in these two versions? Does the q th root of the number of efficient dominating sets of maximum trees of each these two versions exist? If it dose, what is the limit? And if both limits exist, are they the same? Can we find asymptotic formulas for these two versions?

Appendix A
Programs Written in C

Generating the code of the next rooted tree

```

/* *****
* These two functions generate the code of next tree from
* the code of previous tree.
***** */

# include <stdio.h>

next_tree (tree, p)
int *tree;
int p;
{
    if (tree[p-1]>1) -tree[p-1]; /* Last entry decreased by 1 */
    else special (tree, p); /* Use the function "special" for this case */
}

# include <stdio.h>

special (tree, p)
int *tree;
int p;
{
    int j1=1; int js1;
    int j; int k;
    int search;
    while (tree[p-j1-1]==1) ++j1;
    search = -tree[p-j1-1];
    j=1;

```

```
while (tree[p-j1-j-1]!=search) ++j;
js1=j1;
while (j1>=j)
{
    for (k=0; k<j; ++k) tree[p-j1+k] = tree[p-js1-j+k];
    j1 -=j;
}
for (k=0; k<j1; ++k) tree[p-j1+k] = tree[p-js1-j+k];
}
```

Finding maximum trees (Main program)

```

/* *****
* p: The order of a tree
* q: The size of a tree
* tree[p]: An array of dimension p; indexing from 0 to p-1
* max_tree[p]: An array storing the maximum tree
* a[p], b[p], c[p]: Arrays of dimension p; indexing from 0 to p-1
* count: Count the number of trees computed
* max: Store the maximum number of efficient dominating sets
* height: Store the height of a tree
* compute ( ): The function computing the (a, b, c) of a tree;
    The triple (a, b, c) for the tree is stored in a[0], b[0], c[0]
* eq ( ): The function replacing one array by another
* print ( ): The function printing a tree
* next_tree: The function generating the code of the next tree
* ***** */

#include <stdio.h>
#include <math.h>

#define p 22 /* Give the order of the trees to be searched*/

main( ) /* main program with no arguments*/
{
    int q=p-1;
    int tree[p];
    int max_tree[p];
    long max, t_max;

```

```

long a[p], b[p], c[p];
int h, height;
int count, j;
/* ***** Initializing ***** */
for (j=0; j<p; ++j) tree[j]=j; /* Initial tree is the path */
for (j=0; j<p; ++j) a[j]=1, b[j]=1, c[j]=0; /*Initializing the
    triple (a, b, c) */
count=0;
max=0;
/* ***** */
next:
++count;
compute (tree, p, a, b);
t_max = a[0] + c[0];
if (t_max>=max)
{
    h = height_tree (tree, p);
    if (t_max>max)
    {
        max = t_max;
        eq (max_tree, tree, p); /* Replace max_tree by tree */
        height = h;
    }
    else if (h < height) /* Minimizing height */
    {
        eq (max_tree, tree, p); /* Replace max_tree by tree */
    }
}

```

```

        height = h;
    }
}
if (tree[2]>1) /* If the tree is not the star */
{
    next_tree (tree, p);
    a[0] = 1; b[0] = 1; c[0] = 0; /* Re-initializing the root */
    goto next; /* Go to the next_tree */
}
/* ***** If the tree is the star then print out ***** */
printf ("\n # of rooted trees of size %d computed = %d\n\n", q, count);
printf ("maximum # efficient dominating sets %d = %d", q, max);
printf ("maximum tree of size %d: ", q);
print (max_tree, p);
printf ("\n\n\n");
/* ***** */
}

```

Computing the triple (a, b, c)

```

/* *****
*This function is computing the triple (a, b, c) of a tree
* and store the triple in (a[0], b[0], c[0]).
* ***** */
# include <stdio.h>

```

```

compute (tree, p, a, b, c)
int *tree; int p;
long *a, *b, *c;
{
    int i=p-1;
    long a2c;
    while (i>0) /* If not reaches the root */
    {
        /* ***** Compute the triple of the parent ***** */
        a[tree[i]] = a[tree[i]]*(b[0] + c[0]);
        a2c = a[0] + c[0] +c[0];
        c[tree[i]] = c[tree[i]]*a2c + b[tree[i]]*a[0];
        b[tree[i]] = b[tree[i]]*a2c;
        /* ***** */
        if (tree[i-1] < tree[i]) /* If tree[i-1] is the parent of tree[i] */
        {
            a[0] = a[tree[i]];
            b[0] = b[tree[i]];
            c[0] = c[tree[i]];

            a[tree[i]] = 1;
            b[tree[i]] = 1;
            c[tree[i]] = 0;
        }
        else /* If tree[i-1] is not the parent of tree[i] */

```

```

    {
        a[0] = 1;
        b[0] = 1;
        c[0] = 0;
    }
    - -i;
}
}

/* *****
* This function replaces the vector v1 by v2
***** */

# include <stdio.h>

eq (v1, v2, n)
int *v1, *v2;
int n;
{
    int i=0;
    while (i<n) v1[i] = v2[i], ++i;
}

/* *****
* This function prints the code for a tree
***** */

# include <stdio.h>

print (tree, p)
int *tree;

```

```

int p;
{
    int j;
    for (j=0; j<p; ++j) printf ("%d ", tree[j]);
}

/* *****
* This function is used to find the height of a tree
***** */
#include <stdio.h>
int height_tree (tree, p)
int *tree, p;
{
    int i=0;
    while (i<p && tree[i+1]>tree[i]) ++i;
    return (i);
}

```


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