

Mutation effects in ordered trees

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Abstract

A mutation will affect an individual and some or all of its descendants. In this paper, we investigate ordered trees with a distinguished vertex called the mutator. We describe various mutations in ordered trees, and find the generating functions for statistics concerning trees with those mutations. The examples give new interpretations to several known sequences and also introduce many new sequences and their combinatorial interpretations.

AMS classifications: Primary: 05A15; secondary: 05C05

Key words: mutation, ordered trees, short lived mutation, toggle tree, right path tree.

1 Introduction

A mutation is a change in the genome of an organism as well as a genotype that exhibits high rates of mutation. It can result in several different types of change in the nucleotide sequences. For instance, mutations in genes can either have no effect, alter the product of a gene, or prevent the gene from functioning properly or completely. These phenomena may be reflected in a family tree which is an example of ordered tree where its subtrees are usually ordered by date of birth but could be ordered by some other attribute such as height.

*This work was supported by the National Research Foundation of Korea Grant funded by the Korean Government (NRF-2012-007648)

†This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology (2013R1A6A3A03024342)

In the present paper, we consider ordered trees with one distinguished vertex called the *mutator*. The vertices changed by the mutator are said to be of a *new type*. We include the mutator itself as being of the new type. Ordered trees with a mutation may reflect many biological or social structures where changes occur. There are an abundant literature on applications. For instance, if the mutator represents a genetic mutation in a family then the new type vertices are those carrying this mutation. If an ordered tree represents a river network then a mutator could be a spot where pollution has been detected and the vertices above it could be the possible source of the pollution.

It is well-known that the number of ordered trees with n edges is counted by the n th Catalan number $C_n = \frac{1}{n+1} \binom{2n}{n}$, and its generating function is $C = \sum_{n \geq 0} C_n z^n = \frac{1 - \sqrt{1-4z}}{2z}$ resulting from $C = 1 + zC^2 = \frac{1}{1-zC}$. In particular, the number of the ordered trees with a distinguished vertex is counted by the n th central binomial coefficient $B_n = \binom{2n}{n}$ with $B = \sum_{n \geq 0} B_n z^n = \frac{1}{\sqrt{1-4z}}$. A key fact directly obtained from the uplift principle (see Proposition 2.1) provides the generating function B/C for the ordered trees with a distinguished leaf (i.e. terminal vertex).

The purpose of this paper is to investigate five kinds of ordered trees with mutations according to some conditions on the children of the mutator. In particular, we postulate that such conditions are given or can be explained in terms of generating functions. We then enumerate the numbers of such trees and their vertices as well as vertices of each new type. The asymptotic behavior of those numbers will be also discussed. Finally in Section 3 we change from ordered trees to complete binary trees.

2 Ordered trees with various mutations

Throughout this section, a tree means an ordered tree. Let us begin with trees affected by a mutation. By the children we shall mean the vertices directly connected to the mutator, and by the descendants we shall mean all subsequent vertices above the mutator. There are a variety of types of conditions that we could set for the children or the descendants of the mutator.

At one extreme the mutation causes sterility. In this case the generating function for the number of trees is $T_M := L = B/C$ and we have only one new type vertex, the mutator per tree. At the other extreme all the descendants of the mutator are of the new type. As an intermediate case once a new type child appears all subsequent descendants are new type. This could model a case where the mutator is a person who moves to a new country. Other possibilities include exactly one new and sterile child. We also consider what happens if the new type vertices are all on the right most branch or on the right most path.

There are many further variations possible. In one direction we could look at different kinds of trees such as complete (or incomplete) binary trees, Motzkin 0-1-2 trees, even trees, Riordan trees, and spoiled child trees. A second direction would allow a variety of new types, and a third would allow more than one mutator. All of mutation possibilities can be considered with these variations, but to keep this paper focused we discuss these only briefly.

In this section, we consider five kinds of trees with mutations arising from different conditions on the children or descendants. We compute the number of vertices of each

new type by the following procedure. First we find the generating function for such trees, designate this generating function as T_M . Since each tree with n edges has $n + 1$ vertices, the generating function for the vertices is the derivative $(zT_M)'$. We then find the generating function V_N for vertices of the new type. In this step, the uplift principle can be used for transferring results established at the root to an arbitrary vertex. We note that a mutator does not change the conditions on its children wherever it appears as is usual.

Proposition 2.1 (The uplift principle, [1]) *First, find the generating function for whatever is being counted at the root. Then uplift the result at the root to an arbitrary vertex by multiplying by the leaf generating function $L = B/C$.*

Next, we compute the proportion of new type vertices among all the vertices. For this step we use a few asymptotic results depending on Stirling's approximation or the ratio test. These are

- (i) $\binom{2n}{n} \sim \frac{4^n}{\sqrt{\pi n}}$ or $4^n \sim \binom{2n}{n} \sqrt{\pi n}$, $\binom{2n}{n} \sim 4 \binom{2n-2}{n-1}$;
- (ii) $C_n \sim 4C_{n-1}$, $B_n \sim 4B_{n-1}$;

We also adopt a singularity analysis for few complicated cases. In addition here are some other facts we will use:

- (i) $L = B/C$, $C' = BC^2$, $B' = 2B^3$;
- (ii) $B = 1 + 2zBC = \frac{1}{1-2zC} = \frac{C}{1-zC^2}$ so that $\frac{B-1}{2} = zBC$;
- (iii) $[z^n]C^s = \frac{s}{2n+s} \binom{2n+s}{n}$ and $[z^n]BC^s = \binom{2n+s}{n}$.

where $[z^n]$ is the coefficient extraction operator.

Let us now describe first example of ordered trees with a mutation under the variation of an extreme case. Here the rightmost child of the mutator is of the new type. The mutator has no more children of the new type and the child of the new type has no children. In this sense, we call such mutation the *short lived mutation*. As an example if a male donkey mates with a female horse, it stops reproducing and the child, a mule, is sterile. The horse, traumatized by the experience, has no more offspring.

Every such tree has exactly two vertices of the new type so the question of interest is the number of such trees. The generating function is

$$L \cdot C \cdot z = \frac{B}{C} \cdot C \cdot z = zB = \frac{z}{\sqrt{1-4z}} = z + 2z^2 + 6z^3 + 20z^4 + \dots \quad (A000984).$$

To illustrate with $n = 3$ edges, we consider the ordered trees with a short lived mutator and three edges. There are 6 trees as shown in Figure 1. From now on, 'x' denotes the root and the mutator is circled. Along with the mutator, we will mark the edges above the vertices of the new type as this is easier to see.

We note that the total number of vertices is $(n + 1) \binom{2n-2}{n-1}$ for $n \geq 1$ and the proportion of new type vertices $\frac{2}{(n+1) \binom{2n-2}{n-1}}$ approaches 0 when n gets larger as is obvious.

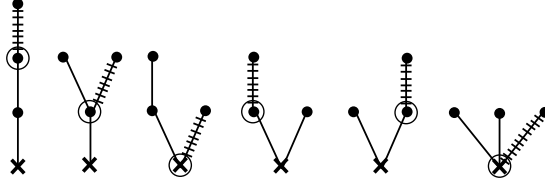


Figure 1. Trees with the short lived mutation

However, if the horse should resume an active social life the generating function for the trees becomes zBC .

For the second example we look at *toggle trees*. Once the mutator has a child of the new type, all the later descendants are also new type. In other words, the first child of the mutator of the new type plays a role of a ‘toggle’ that divides all children of the mutator into two groups, those on the left are normal, those on the right are new type.

Theorem 2.2 *The number of toggle trees with n edges is $\binom{2n+1}{n}$. In particular, the proportion of new type vertices is asymptotically $\frac{1}{2}\sqrt{\frac{\pi}{n}}$.*

Proof. The number of toggle trees with a mutator at the root has the generating function C^2 , where each of the first family and the new family contributes a C .

If we allow a mutator to be anywhere, applying the uplift principle gives

$$T_M = \frac{B}{C} \cdot C^2 = BC = \sum_{n \geq 0} \binom{2n+1}{n} z^n = 1 + 3z + 10z^2 + 35z^3 + \dots \quad (\text{A001700}).$$

Then the generating function for vertices is

$$(zT_M)' = \left(\frac{B-1}{2}\right)' = B^3 = \sum_{n \geq 0} (2n+1) \binom{2n}{n} z^n.$$

To count new type vertices we see that if the mutator is at the root, we have $C \cdot (zC)' = CB$ possibilities with C for the pretoggle subtree and $(zC)' = B$ counting the new type vertices. Multiplying by $L = B/C$ allows the mutator to be anywhere and our generating function is $V_N = \frac{B}{C} \cdot CB = B^2 = 1 + 4z + 16z^2 + 64z^3 + \dots$.

To estimate the proportion of new type vertices, we apply the Stirling’s approximation and get

$$\frac{[z^n]B^2}{[z^n]B^3} = \frac{4^n}{(2n+1)\binom{2n}{n}} \sim \frac{\sqrt{\pi n} \binom{2n}{n}}{(2n+1)\binom{2n}{n}} \sim \frac{1}{2} \sqrt{\frac{\pi}{n}}. \quad (1)$$

■

Figure 2 illustrates the ten toggle trees with 30 vertices of which 16 are of the new type. The result (1) is reasonable since a mutator high up will usually have few descendants. If, by way of contrast, we specify that the mutator be at height 1 then the number of toggle trees is counted by

$$zC^4 = \sum_{n \geq 1} \frac{4}{n+3} \binom{2n+1}{n-1} z^n = z + 4z^2 + 14z^3 + 48z^4 + 165z^5 + \dots$$

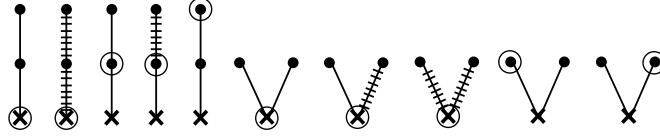


Figure 2. Toggle trees with 16 new type vertices.

The number of vertices has the generating function $(z^2 C^4)' = 2z C^4 B = 2 \sum_{n \geq 1} \binom{2n+2}{n-1} z^n = 2z + 12z^2 + 56z^3 + 240z^4 + 990z^5 + \dots$. The generating function for vertices of the new type is

$$z C^3 B = \sum_{n \geq 1} \binom{2n+1}{n-1} z^n = z + 5z^2 + 21z^3 + 84z^4 + \dots$$

For instance, there are $4 \cdot 14 = 56$ vertices of which 21 vertices are of the new type, see Figure 3.

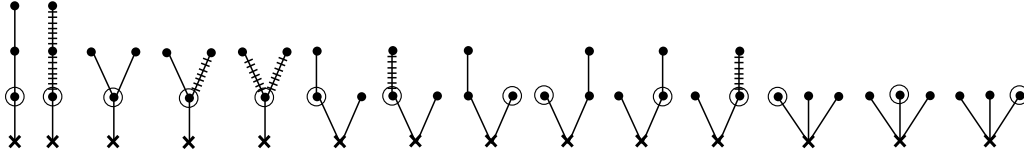


Figure 3. Toggle trees with a mutator at height 1.

We note that the proportion of new type vertices in this height 1 case is

$$\frac{\binom{2n+1}{n-1}}{\frac{4n+4}{n+3} \binom{2n+1}{n-1}} = \frac{n+3}{4n+4} \rightarrow \frac{1}{4}.$$

In a toggle tree, if a child of the new type of the mutator appears, all later offspring of the mutator and their descendants are of the new type. Suppose instead that every child of the mutator and recursively every child of a new type vertex has a 50% chance of being new type. We call such trees *embedded new type (ENT) trees* since the result is a tree with a subtree of new type vertices. This concept coincides with an autosomal dominant mutation when we assume that we only keep track of genetic history of a single family, and every member met a spouse not having a mutant gene so that appearance of a mutation only depends on a member of the family. Figure 4 illustrates the 12 possible trees with 2 edges.

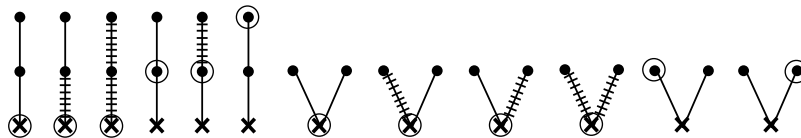


Figure 4. The embedded new type trees with 2 edges.

Theorem 2.3 *The number of embedded new type trees with n edges is $\sum_{k=0}^n \frac{1}{k+1} \binom{2n}{n-k} \binom{2k}{k}$. In particular, the proportion of new type vertices is asymptotically $\frac{3}{5}$.*

Proof. Let T_0 be the generating function for ENT trees having a mutator at the root. If a mutator has k children, there are 2^k possible distributions of the mutation over the children where each normal child and child of the new type are the roots of subtrees described by C and T_0 , respectively. It then follows that the generating function for ENT trees having a mutator at the root of updegree k is $z^k(C + T_0)^k$. So T_0 satisfies

$$T_0 = \frac{1}{1 - z(C + T_0)}$$

and solving the functional equation gives

$$T_0 = \frac{1 - \sqrt{5 - 4C}}{2zC} = 1 + 2z + 7z^2 + 29z^3 + 131z^4 + \dots \quad (\text{A007852}).$$

A simple computation shows $T_0 = C \cdot (C \circ zC^2)$. By the uplift principle,

$$T_M = \frac{B}{C} \cdot T_0 = B \cdot (C \circ zC^2) = 1 + 3z + 12z^2 + 52z^3 + 236z^4 + \dots$$

This is (A007856) in the OEIS [4] and is also known [3] to count the number of subtrees in ordered trees with n edges. It can be shown that $[z^n]T_M = \sum_{k=0}^n C_k \binom{2n}{n-k}$. The singular expansion of C at the dominant singularity $z = \frac{4}{25}$ of $C \circ zC^2$ gives $[z^n]T_M \sim \frac{5\sqrt{15}}{9} \frac{1}{\sqrt{\pi n^3}} \left(\frac{25}{4}\right)^n$, which implies the asymptotic number of vertices of ENT trees with n edges is $\frac{5\sqrt{15}}{9} \frac{1}{\sqrt{\pi n}} \left(\frac{25}{4}\right)^n$.

In order to count the vertices of the new type, first consider ENT trees with a mutator at the root. Let \tilde{V}_N be the generating function for such ENT trees where we have marked one of the new type vertices. Suppose the root degree is k of which j are new type. The marked vertex, if not the root itself, is in one of the j new type subtrees. The other $j - 1$ subtrees are themselves ENT trees with the mutator at the root. Thus

$$\begin{aligned} \tilde{V}_N &= T_0 + z\tilde{V}_N + 2z^2\tilde{V}_N(C + T_0) + 3z^3\tilde{V}_N(C + T_0)^2 + \dots \\ &= T_0 + \frac{z\tilde{V}_N}{(1 - z(C + T_0))^2} \end{aligned}$$

with T_0 counting the case where the marked vertex is the root. Solving the functional equation yields

$$\begin{aligned} V_N &= L \cdot \tilde{V}_N = \frac{B}{C} \cdot T_0 \cdot \left(1 - \frac{z}{(1 - z(C + T_0))^2}\right)^{-1} = \sqrt{\frac{2 - 5z + 2\sqrt{1 - 4z}}{(4 - 25z)(1 - 4z)}} \\ &= 1 + 4z + 20z^2 + 106z^3 + 580z^4 + \dots \end{aligned}$$

It follows from $V_N \sim \frac{\sqrt{15}}{3} \left(1 - \frac{25}{4}z\right)^{-1/2}$ that $[z^n]V_N \sim \frac{\sqrt{15}}{3} \frac{1}{\sqrt{\pi n}} \left(\frac{25}{4}\right)^n$. Thus the proportion of vertices of the new type is asymptotically equal to

$$\frac{\frac{\sqrt{15}}{3} \frac{1}{\sqrt{\pi n}} \left(\frac{25}{4}\right)^n}{\frac{5\sqrt{15}}{9} \frac{1}{\sqrt{\pi n}} \left(\frac{25}{4}\right)^n} = \frac{3}{5}.$$

■

In fact, we see for example that

$$\frac{[z^{50}]V_N}{[z^{50}](zT_M)'} = \frac{642784246122173091957609761927581466320}{1086960365349865718238126127455484769220} \doteq 0.59135942.$$

One instance where ENT trees occur is classical. These were family names as in England. The mutator, often the root, passes his name to his male children (these would be new type) whereas the female children would not carry on the family name, see [5].

In a *right branch new type (RBNT) tree*, the rightmost branch from the mutator is nontrivial and all the vertices of the new type constitute this branch including the mutator.

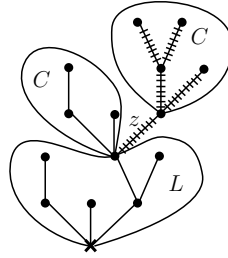


Figure 5. A right branch new type tree with a mutator.

Theorem 2.4 *The number of right branch new type trees with n edges is $\binom{2n-1}{n}$. In particular, the proportion of new type vertices is asymptotically $2\sqrt{\frac{\pi}{n}}$.*

Proof. The generating function for RBNT trees follows from Figure 5:

$$T_M = L \cdot C \cdot zC = \frac{B}{C} \cdot C \cdot zC = zBC = \frac{B-1}{2} = \sum_{n \geq 1} \binom{2n-1}{n} z^n.$$

The number of vertices involved are then counted by

$$(zT_M)' = \frac{B-1}{2} + zB^3 = \sum_{n \geq 1} (n+1) \binom{2n-1}{n} z^n = 2z + 9z^2 + 40z^3 + 175z^4 + \dots \quad (2)$$

for (A097070). It also counts the number of parts equal to 1 over all weak compositions of $n+1$ into $n+1$ parts. Since the right branch from the mutator contains all vertices of the new type, it follows from Figure 5 that

$$V_N = L \cdot C \cdot (z(zC))' = B \cdot (z^2C)' = B \cdot (2zC + z^2BC^2) = 2 + 7z^2 + 26z^3 + 99z^4 + \dots$$

This is (A114121) in [4] except for the initial term. We would like to find the proportion of new type vertices among all the vertices. For $n \geq 1$, the denominator is $[z^n](zT_M)' = (n+1)\binom{2n-1}{n} = \frac{n+1}{2}\binom{2n}{n}$ and the numerator is

$$\begin{aligned} [z^n]V_N &= [z^n](2zBC + z^2B^2C^2) = [z^n] \left(B-1 + \left(\frac{B-1}{2} \right)^2 \right) \\ &= \binom{2n}{n} + \frac{1}{4} \left(4^n - 2\binom{2n}{n} \right) = 4^{n-1} + \frac{1}{2} \binom{2n}{n}. \end{aligned}$$

Thus the proportion of new type vertices is

$$\frac{4^{n-1} + \frac{1}{2} \binom{2n}{n}}{\frac{n+1}{2} \binom{2n}{n}} \sim \frac{\sqrt{\pi n} + \frac{1}{2}}{\frac{n+1}{2}} \sim 2\sqrt{\frac{\pi}{n}}.$$

■

Another intermediate case of mutations in trees is obtained by assuming that the vertices of the new type for trees go from the mutator to the rightmost leaf above the mutator. For instance, Figure 6 shows a tree with 5 vertices of the new type. We call trees involving such mutation the *right path trees*.

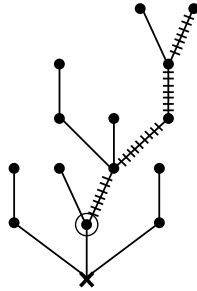


Figure 6. A right path tree with 5 new type vertices.

Theorem 2.5 *The number of right path trees with n edges is $\binom{2n}{n}$. In particular, the proportion of new type vertices is asymptotically $\frac{1}{2n}$.*

Proof. It can be easily seen that the generating function for right path trees is

$$T_M = L \cdot (1 + zC + z^2C^2 + \dots) = \frac{B}{C} \cdot \frac{1}{1 - zC} = \frac{B}{C} \cdot C = B.$$

Hence the number of vertices in right path trees is counted by $(zB)' = B + 2zB^3 = \sum_{n \geq 0} (n+1) \binom{2n}{n} z^n = 1 + 4z + 18z^2 + 80z^3 + \dots$. Next we want to compute the number of new type vertices. If the right path from the mutator has length k , we have $k+1$ new type vertices and the generating function for vertices $(k+1)z^k C^k$ since a subtree can be attached to the left of all vertices except the last. Including the location of the mutator and summing over k gives the generating function

$$V_N = L \cdot (1 + 2zC + 3z^2C^2 + \dots) = \frac{B}{C} \cdot \frac{1}{(1 - zC)^2} = \frac{B}{C} \cdot C^2 = BC = \sum_{n \geq 0} \binom{2n+1}{n} z^n.$$

Thus the proportion of new type vertices is

$$\frac{\frac{1}{2} \binom{2n}{n}}{(n+1) \binom{2n}{n}} = \frac{1}{2(n+1)} \sim \frac{1}{2n}.$$

■

A common situation is that the mutator is not known until the child appears in the new state. So we want to look at this rightmost path from the mutator to the new type leaf but now requiring the mutator to have at least one descendant. Such mutation will be called the *right path** mutation.

The number of right path* trees has the generating function

$$L \cdot (zC + z^2C^2 + \dots) = \frac{B}{C} \cdot \frac{zC}{1 - zC} = zB \cdot \frac{1}{1 - zC} = zBC = \sum_{n \geq 1} \binom{2n-1}{n} z^n,$$

which is the same as T_M of right branch new type trees. So the generating function for vertices is given by (2).

For the number of vertices of the new type we have

$$\begin{aligned} L \cdot (2zC + 3(zC)^2 + \dots) &= \frac{B}{C} \cdot \left(\frac{1}{(1 - zC)^2} - 1 \right) = \frac{B}{C} \cdot (C^2 - 1) = BC - \frac{B}{C} \\ &= \sum_{n \geq 1} \frac{3n+1}{2n+2} \binom{2n}{n} z^n = 2z + 7z^2 + 25z^3 + 91z^4 + \dots \end{aligned}$$

This is (A097613) in [4] except for the initial term. The proportion of new type vertices out of all vertices is

$$\frac{\frac{3n+1}{2n+2} \binom{2n}{n}}{\frac{n+1}{2} \binom{2n}{n}} = \frac{3n+1}{(n+1)^2} \sim \frac{3}{n}.$$

Here is an illustration for the 10 right path* trees on 3 edges. There are 40 vertices of which 25 are of the new type.

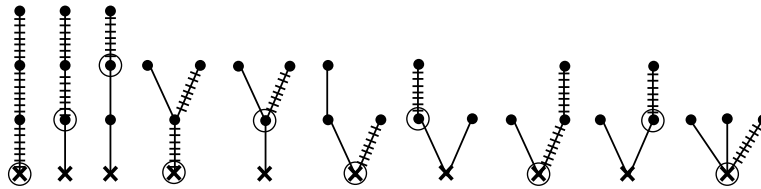


Figure 7. Right path trees with a mutator having at least one child.

The following table summarizes the main results in this section.

Mutation	Number of trees with the mutation	Asymptotic ratio of vertices of the new type
Short lived	$\binom{2n-2}{n-1}$	$2/((n+1)\binom{2n-2}{n-1})$
Toggle	$\binom{2n+1}{n}$	$\frac{1}{2}\sqrt{\frac{\pi}{n}}$
Embedded new type	$\sum_{k=0}^n \frac{1}{k+1} \binom{2n}{n-k} \binom{2k}{k}$	$\frac{3}{5}$
Right branch new type	$\binom{2n-1}{n}$	$2\sqrt{\frac{\pi}{n}}$
Right path	$\binom{2n}{n}$	$\frac{1}{2n}$
Right path*	$\binom{2n-1}{n}$	$\frac{3}{n}$

3 Another class of ordered trees

What if a mutation occurs in another class of ordered trees instead of the usual ordered trees? We end this paper with the complete binary trees with a simple mutation in which a mutator changes all of its descendants to the new type. A complete binary tree has every vertex with updegree 0 or 2. It is known that there are C_n complete binary trees with n internal vertices. To have the coefficient of z^n count edges instead of internal vertices, the appropriate generating function is $\sum_{n \geq 0} C_n z^{2n} = C(z^2) = \frac{1 - \sqrt{1 - 4z^2}}{2z^2}$. This change brings about various other small changes. By setting $\tilde{C}(z) = \tilde{C} = C(z^2)$ and $\tilde{B}(z) = \tilde{B} = B(z^2)$, we have $\tilde{C}' = 2z\tilde{B}\tilde{C}^2$, $\tilde{B}' = 4z\tilde{B}^3$ and $\tilde{B} = 1 + 2z^2\tilde{B}\tilde{C}$. The vertex and leaf generating functions V and L are

$$V = (z\tilde{C})' = \tilde{C} \cdot (1 + 2z^2\tilde{B}\tilde{C}) = \tilde{C}\tilde{B} \quad \text{and} \quad L = \frac{\tilde{C}\tilde{B}}{\tilde{C}} = \tilde{B}.$$

Let T_M be the generating function for complete binary trees with a mutator, where all the descendants of the mutator are of the new type. Then $T_M = V = \tilde{C}\tilde{B} = 1 + 3z^2 + 10z^4 + 35z^6 + \dots$. The number of vertices of these mutator enhanced trees has the generating function

$$\begin{aligned} \tilde{V} &= (z\tilde{T})' = \tilde{T} + z\tilde{T}' = \tilde{B}\tilde{C} + z(\tilde{B}\tilde{C})' = \tilde{B}\tilde{C} + z(\tilde{B} \cdot 2z\tilde{B}\tilde{C}^2 + 4z\tilde{B}^3\tilde{C}) \\ &= \tilde{B}\tilde{C} \cdot (1 + 2z^2\tilde{B}\tilde{C} + 4z^2\tilde{B}^2) = \tilde{B}\tilde{C} \cdot \left(\tilde{B} + \frac{4z^2}{1 - 4z^2} \right) \\ &= \sum_{n \geq 0} (2n + 1)^2 C_n z^{2n} = 1 + 9z^2 + 50z^4 + 245z^6 + \dots \end{aligned}$$

This is a new entry in the OEIS [4].

To figure out the number of new type vertices, we apply the uplift principle again and get the generating function

$$L\tilde{V} = \tilde{B} \cdot \tilde{B}\tilde{C} = \tilde{B}^2\tilde{C} = \sum_{n \geq 0} \left(2^{2n-1} - \frac{1}{2} \binom{2n}{n} \right) z^{2n} = 1 + 5z^2 + 22z^4 + 93z^6 + \dots$$

The proportion of new type vertices is

$$\frac{[z^n]\tilde{B}^2\tilde{C}}{[z^n]\tilde{V}} = \frac{2^{2n-1} - \frac{1}{2} \binom{2n}{n}}{(2n+1)^2 \frac{1}{n+1} \binom{2n}{n}} \sim \frac{\frac{1}{2} \binom{2n}{n} \sqrt{\pi n} - \frac{1}{2} \binom{2n}{n}}{\frac{(2n+1)^2}{n+1} \binom{2n}{n}} = \frac{\frac{1}{2} \sqrt{\pi n} - \frac{1}{2}}{\frac{(2n+1)^2}{n+1}} \sim \frac{1}{8} \sqrt{\frac{\pi}{n}}.$$

Complete binary trees and ordered trees are both examples of trees satisfying a uniform updegree requirement. The methods used in this paper generalize to all such trees but that will be the subject of a separate manuscript.

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