

**EXPERIMENTAL METHODS APPLIED TO  
THE COMPUTATION OF INTEGER SEQUENCES**

**BY ERIC SAMUEL ROWLAND**

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and approved by

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## ABSTRACT OF THE DISSERTATION

### Experimental methods applied to the computation of integer sequences

by Eric Samuel Rowland

Dissertation Director: Doron Zeilberger

We apply techniques of experimental mathematics to certain problems in number theory and combinatorics. The goal in each case is to understand certain integer sequences, where foremost we are interested in computing a sequence faster than by its definition. Often this means taking a sequence of integers that is defined recursively and rewriting it without recursion as much as possible. The benefits of doing this are twofold. From the view of computational complexity, one obtains an algorithm for computing the system that is faster than the original; from the mathematical view, one obtains new information about the structure of the system.

Two particular topics are studied with the experimental method. The first is the recurrence

$$a(n) = a(n - 1) + \gcd(n, a(n - 1)),$$

which is shown to generate primes in a certain sense. The second is the enumeration of binary trees avoiding a given pattern and extensions of this problem. In each of these problems, computing sequences quickly is intimately connected to understanding the structure of the objects and being able to prove theorems about them.

## Acknowledgements

I greatly thank Doron Zeilberger for his help over the past few years. As an advisor he has been a source of challenging problems and valuable assistance drawn from his comprehensive knowledge of symbolics. As a mathematician he has influenced my philosophy and methodology, and he has provided a practical model for discovering and proving theorems by computer. And as a member of academia he has shown me that rules aren't to be taken too seriously.

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Thanks are due to an anonymous referee, whose critical comments greatly improved the exposition of the material in Chapter 2.

Regarding the material in Chapter 3, I thank Phillippe Flajolet for helping me understand the relation of the work to existing literature, and I thank Lou Shapiro for suggestions which clarified some points.

I am also indebted to Elizabeth Kupin for much valuable feedback. Her comments greatly improved the exposition and readability of Chapter 3. In addition, the idea of looking for bijections between trees avoiding  $s$  and trees avoiding  $t$  that do not extend to bijections on the full set of binary trees is hers, and this turned out to be an important generalization of the two-rule bijections I had been considering.

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# Chapter 1

## Introduction

### 1.1 Overview

This thesis applies techniques of automatic data generation, analysis, form-fitting, and proof to problems in discrete mathematics — in particular to the problem of speeding up the computation of terms in certain integer sequences.

This chapter is devoted to a description of the experimental methodology used throughout the thesis and to the notion of an ansatz.

In Chapter 2 I discuss the recurrence

$$a(n) = a(n - 1) + \gcd(n, a(n - 1))$$

with initial condition  $a(1) = 7$  and prove that  $a(n) - a(n - 1)$  takes on only 1s and primes, making this recurrence a rare “naturally occurring” generator of primes. Toward a generalization of this result to an arbitrary initial condition, we also study the limiting behavior of  $a(n)/n$  and a transience property of the evolution. This work was published in the *Journal of Integer Sequences* [25].

Chapter 3 considers the enumeration of trees avoiding a contiguous pattern. We provide an algorithm for computing the generating function that counts the  $n$ -leaf binary trees avoiding a given binary tree pattern  $t$ . Equipped with this counting mechanism, we study the analogue of Wilf equivalence in which two tree patterns are equivalent if the respective  $n$ -leaf trees that avoid them are equinumerous. We investigate the equivalence classes combinatorially, finding some relationships to Dyck words avoiding a given subword. Toward establishing bijective proofs of tree pattern equivalence, we develop a general method of restructuring trees that conjecturally succeeds to produce an explicit bijection. This work has been submitted for publication [26].

Results in mathematics are generally presented as static works, where evidence of the dynamic discovery process has been removed. Aside from being the current cultural norm, one reason for this is that conveying the history of a result is difficult and messy. However, I believe that the human process that led to the discovery of a conjecture or theorem or proof is the best way for another human to develop an understanding of that material (short of recreating it from scratch). Therefore, possibly at the expense of some elegance and brevity, I have attempted to indicate how the results in this thesis were found.

The software used for this work was predominantly *Mathematica*. Several packages developed by the author are available from <http://math.rutgers.edu/~erowland/programs.html>. In particular, the package TREEPATTERNS [27] accompanies Chapter 3. Additionally, the algebra software Singular was used via an interface package by Manuel Kauers and Viktor Levandovskyy [18] to compute Gröbner bases for systems of polynomial equations in Chapter 3.

Sequence numbers such as [A000108](#) refer to entries in the Encyclopedia of Integer Sequences [29].

## 1.2 Experimental methodology

Experimental mathematics is not a new way of doing mathematics. In fact, it is the oldest way of doing mathematics, the idea being that by naively generating explicit *numeric* examples of a mathematical structure one can eventually perceive the general *symbolic* structure. In practice, the methodology is as follows. Generate data in the form of a sequence of integers or a graph or an image, etc. Then manipulate the data until it takes a recognizable form, e.g., the Thue–Morse sequence or the 4-dimensional hypercube graph or the Sierpiński sieve. Then undo the manipulations symbolically to arrive at an algorithm for computing the original data. Most often this algorithm represents a compression of the data in which its structure is revealed and by which it may be computed more quickly.

For example, if we compute a function  $f(n)$  for  $n = 1, 2, \dots, 8$  and find that the

values are 1, 1, 2, 3, 5, 8, 13, 21 then (without requiring much analysis in this case) we generally suspect that  $f(n)$  is the  $n$ th Fibonacci number.

Although this principle is quite old, what is relatively new is the use of computers to assist in mathematics research. There are major advantages that computers provide in both the stages of data generation and data analysis.

The advantage in generating data is the obvious one — that machines can simply compute faster and more accurately than humans, so any algorithmic task can be done on a much larger scale by machine. Sometimes the time or space needed to compute more data grows quickly, making it infeasible to compute by hand. Sometimes small values of the data do not fit into the general pattern (e.g., the first few terms of an eventually periodic sequence), and the transience may in fact be long. In both these cases it is clearly desirable to compute by machine.

The advantage in using modern mathematical software to study empirical data is that the ease of setting up and executing computations with these systems allows the mathematician to search for structure in real time. One can process the data in many different ways fairly quickly — applying transformations of all sorts, looking for patterns visually in the form of a plot or a graph, attempting fits to known ansatzes (as discussed below), etc. Since the software is doing all the computation, there is little overhead for the human, who is free to experiment with the data as much as it wishes. This naturally increases the likelihood that significant patterns will be discovered.

### 1.3 The notion of ansatz

Humans are quite good at identifying some patterns. For example, it is easy for a human (at least a human who has seen them before) to guess a general form for each of the following sequences.

$$1, 4, 9, 16, \dots$$

$$2, 3, 5, 7, 11, 13, 17, 19, \dots$$

$$1, 2, 1, 3, 1, 2, 1, 4, 1, 2, 1, 3, 1, 2, 1, 5, \dots$$

However, this process of identification by human familiarity is not very robust. The following sequences are of roughly the same complexity, in a certain mathematical sense, as the preceding sequences, but they are not as immediately identifiable (especially out of context of the preceding sequences).

$$2, 7, 14, 23, \dots$$

$$3, 7, 13, 19, 29, 37, 43, 53, \dots$$

$$1, 1, 2, 1, 2, 2, 3, 1, 2, 2, 4, 2, 3, 3, 4, 1, \dots$$

That is, these sequences are not of the same complexity, in the sense of some humans, as the first sequences. Consequently, we do not want to relegate pattern recognition to humans alone.

Lookup tables such as the Encyclopedia of Integer Sequences [29] and analogous databases for leading digits of real numbers [2, 23] provide one type of systematic pattern recognition. In essence they extend the basic “recognizable primitives”.

How can we potentially recognize infinitely many different objects? We might start by applying a finite set of transformations to all of our recognizable primitives. However, no finite list will get us there. (We may of course iterate the transformations, but then in attempting to identify an object we never know when to stop applying the inverse transformations.)

We must work symbolically. To get software to “find a pattern” in empirical data, we specify precisely the general form — the *ansatz* — of the pattern we are looking for. The *ansatz* is the symbolic structure behind a class of objects, where each object in the class is realized for certain values of the parameters.

Let us focus on *ansatzes* of integer sequences, with the understanding that the principles apply equally well to other objects. (For example, in Chapter 3 we consider several *ansatzes* of bijections on binary trees.) Frequently in discrete mathematics the answer to a question can be rendered as a sequence of integers, and because they are so universal there is much that we know about them.

Some historically successful *ansatzes* of integer sequences include (in roughly increasing sophistication) periodic functions, polynomials, rational functions, quasi-polynomials,

C-recursive sequences (solutions of linear recurrences with constant coefficients),  $k$ -regular sequences as introduced by Allouche and Shallit [1], sequences whose generating functions are algebraic, and holonomic sequences (solutions of linear recurrences with polynomial coefficients). Zeilberger [33] discusses many of these in greater detail. Each of these ansatzes is useful in sequence identification problems because of its ubiquity in mathematics. The sequences of Chapter 3, for instance, are all algebraic.

Given an ansatz and some data, it is generally routine to find (if it exists) an object in that ansatz that represents the data. If the empirical data can be generated by a function with fewer degrees of freedom than the data, then most likely the sequence has been identified. A familiar example is the interpolation of polynomials: If a polynomial of degree 2 correctly reproduces 4 terms of a sequence, this indicates some redundancy in those terms.

Certainly one comes across objects in mathematics that do not fit a known ansatz. When this happens it is the role of the human to study the object until its structure becomes clear. That is, the human is the creator/identifier of new ansatzes, and this is the not-yet-routine mathematics being done in the context of the experimental method. Such was the case with the integer sequences in Chapter 2 and with the bijections in Chapter 3; these new classes were introduced to answer particular number theoretic and combinatorial questions.

## Chapter 2

### A natural prime-generating recurrence

#### 2.1 Introduction

Since antiquity it has been intuited that the distribution of primes among the natural numbers is in many ways random. For this reason, functions that reliably generate primes have been revered for their apparent traction on the set of primes.

Ribenboim [24, page 179] provides three classes into which certain prime-generating functions fall:

- (a)  $f(n)$  is the  $n$ th prime  $p_n$ .
- (b)  $f(n)$  is always prime, and  $f(n) \neq f(m)$  for  $n \neq m$ .
- (c) The set of positive values of  $f$  is equal to the set of prime numbers.

Known functions in these classes are generally infeasible to compute in practice. For example, both Gandhi's formula

$$p_n = \left\lfloor 1 - \log_2 \left( -\frac{1}{2} + \sum_{d|P_{n-1}} \frac{\mu(d)}{2^d - 1} \right) \right\rfloor$$

[11], where  $P_n = p_1 p_2 \cdots p_n$ , and Willans' formula

$$p_n = 1 + \sum_{i=1}^{2^n} \left\lfloor \left( \frac{n}{\sum_{j=1}^i \left\lfloor \left( \cos \frac{(j-1)! + 1}{j} \pi \right)^2 \right\rfloor} \right)^{1/n} \right\rfloor$$

[31] satisfy condition (a) but are essentially versions of the sieve of Eratosthenes [12, 13]. Gandhi's formula depends on properties of the Möbius function  $\mu(d)$ , while Willans' formula is built on Wilson's theorem. Jones [16] provided another formula for  $p_n$  using Wilson's theorem.

Functions satisfying (b) are interesting from a theoretical point of view, although all known members of this class are not practical generators of primes. The first example was provided by Mills [21], who proved the existence of a real number  $A$  such that  $\lfloor A^{3^n} \rfloor$  is prime for  $n \geq 1$ . The only known way of finding an approximation to a suitable  $A$  is by working backward from known large primes. Several relatives of Mills' function can be constructed similarly [7].

The peculiar condition (c) is tailored to a class of multivariate polynomials constructed by Matiyasevich [20] and Jones et al. [17] with this property. These results are implementations of primality tests in the language of polynomials and thus also cannot be used to generate primes in practice.

It is evidently quite rare for a prime-generating function to not have been expressly *engineered* for this purpose. One might wonder whether there exists a nontrivial prime-generating function that is “naturally occurring” in the sense that it was not constructed to generate primes but simply *discovered* to do so.

Euler's polynomial  $n^2 - n + 41$  of 1772 is presumably an example; it is prime for  $1 \leq n \leq 40$ . Of course, in general there is no known simple characterization of those  $n$  for which  $n^2 - n + 41$  is prime. So, let us revise the question: Is there a naturally occurring function that always generates primes?

The subject of this chapter is such a function. It is recursively defined and produces a prime at each step, although the primes are not distinct as required by condition (b).

The recurrence was discovered in 2003 at the NKS Summer School<sup>1</sup>, at which I was a participant. Primary interest at the Summer School is in systems with simple definitions that exhibit complex behavior. In a live computer experiment led by Stephen Wolfram, we searched for complex behavior in a class of nested recurrence equations. A group led by Matt Frank followed up with additional experiments, somewhat simplifying the structure of the equations and introducing different components. One of the recurrences they considered is

$$a(n) = a(n - 1) + \gcd(n, a(n - 1)). \quad (2.1)$$

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<sup>1</sup> The NKS Summer School (<http://www.wolframscience.com/summerschool>) is a three-week program in which participants conduct original research informed by *A New Kind of Science* [32].



the following sequence of primes (sequence [A137613](#)).

5, 3, 11, 3, 23, 3, 47, 3, 5, 3, 101, 3, 7, 11, 3, 13, 233, 3, 467, 3, 5, 3, 941, 3, 7, 1889, 3, 3779, 3, 7559, 3, 13, 15131, 3, 53, 3, 7, 30323, 3, 60647, 3, 5, 3, 101, 3, 121403, 3, 242807, 3, 5, 3, 19, 7, 5, 3, 47, 3, 37, 5, 3, 17, 3, 199, 53, 3, 29, 3, 486041, 3, 7, 421, 23, 3, 972533, 3, 577, 7, 1945649, 3, 163, 7, 3891467, 3, 5, 3, 127, 443, 3, 31, 7783541, 3, 7, 15567089, 3, 19, 29, 3, 5323, 7, 5, 3, 31139561, 3, 41, 3, 5, 3, 62279171, 3, 7, 83, 3, 19, 29, 3, 1103, 3, 5, 3, 13, 7, 124559609, 3, 107, 3, 911, 3, 249120239, 3, 11, 3, 7, 61, 37, 179, 3, 31, 19051, 7, 3793, 23, 3, 5, 3, 6257, 3, 43, 11, 3, 13, 5, 3, 739, 37, 5, 3, 498270791, 3, 19, 11, 3, 41, 3, 5, 3, 996541661, 3, 7, 37, 5, 3, 67, 1993083437, 3, 5, 3, 83, 3, 5, 3, 73, 157, 7, 5, 3, 13, 3986167223, 3, 7, 73, 5, 3, 7, 37, 7, 11, 3, 13, 17, 3, ...

It certainly seems to be the case that larger and larger primes appear fairly frequently. Unfortunately, these primes do not come for free: If we compute terms of the sequence without the aforementioned shortcut, then a prime  $p$  appears only after  $\frac{p-3}{2}$  consecutive 1s, and indeed the primality of  $p$  is being established essentially by trial division. As we will see, the shortcut is much better, but it requires an external primality test, and in general it requires finding the smallest prime divisor of an integer  $\Delta$ . So although it is naturally occurring, the recurrence, like its artificial counterparts, is not a magical generator of large primes.

We mention that Benoit Cloitre [4] has considered variants of Equation (2.1) and has discovered several interesting results. A striking parallel to the main result of this chapter is that if

$$b(n) = b(n-1) + \text{lcm}(n, b(n-1))$$

with  $b(1) = 1$ , then  $b(n)/b(n-1) - 1$  (sequence [A135506](#)) is either 1 or prime for each  $n \geq 2$ .

## 2.2 Initial observations

In order to reveal several key features, it is worth recapitulating the experimental process that led to the discovery of the proof that  $a(n) - a(n-1)$  is always 1 or prime.

$n$	$\Delta(n)$	$g(n)$	$a(n)$	$a(n)/n$	$n$	$\Delta(n)$	$g(n)$	$a(n)$	$a(n)/n$
1			7	7	54	101	1	156	2.88889
2	5	1	8	4	55	101	1	157	2.85455
3	5	1	9	3	56	101	1	158	2.82143
4	5	1	10	2.5	57	101	1	159	2.78947
5	5	5	15	3	58	101	1	160	2.75862
6	9	3	18	3	59	101	1	161	2.72881
7	11	1	19	2.71429	60	101	1	162	2.7
8	11	1	20	2.5	61	101	1	163	2.67213
9	11	1	21	2.33333	62	101	1	164	2.64516
10	11	1	22	2.2	63	101	1	165	2.61905
11	11	11	33	3	64	101	1	166	2.59375
12	21	3	36	3	65	101	1	167	2.56923
13	23	1	37	2.84615	66	101	1	168	2.54545
14	23	1	38	2.71429	67	101	1	169	2.52239
15	23	1	39	2.6	68	101	1	170	2.5
16	23	1	40	2.5	69	101	1	171	2.47826
17	23	1	41	2.41176	70	101	1	172	2.45714
18	23	1	42	2.33333	71	101	1	173	2.43662
19	23	1	43	2.26316	72	101	1	174	2.41667
20	23	1	44	2.2	73	101	1	175	2.39726
21	23	1	45	2.14286	74	101	1	176	2.37838
22	23	1	46	2.09091	75	101	1	177	2.36
23	23	23	69	3	76	101	1	178	2.34211
24	45	3	72	3	77	101	1	179	2.32468
25	47	1	73	2.92	78	101	1	180	2.30769
26	47	1	74	2.84615	79	101	1	181	2.29114
27	47	1	75	2.77778	80	101	1	182	2.275
28	47	1	76	2.71429	81	101	1	183	2.25926
29	47	1	77	2.65517	82	101	1	184	2.2439
30	47	1	78	2.6	83	101	1	185	2.22892
31	47	1	79	2.54839	84	101	1	186	2.21429
32	47	1	80	2.5	85	101	1	187	2.2
33	47	1	81	2.45455	86	101	1	188	2.18605
34	47	1	82	2.41176	87	101	1	189	2.17241
35	47	1	83	2.37143	88	101	1	190	2.15909
36	47	1	84	2.33333	89	101	1	191	2.14607
37	47	1	85	2.2973	90	101	1	192	2.13333
38	47	1	86	2.26316	91	101	1	193	2.12088
39	47	1	87	2.23077	92	101	1	194	2.1087
40	47	1	88	2.2	93	101	1	195	2.09677
41	47	1	89	2.17073	94	101	1	196	2.08511
42	47	1	90	2.14286	95	101	1	197	2.07368
43	47	1	91	2.11628	96	101	1	198	2.0625
44	47	1	92	2.09091	97	101	1	199	2.05155
45	47	1	93	2.06667	98	101	1	200	2.04082
46	47	1	94	2.04348	99	101	1	201	2.0303
47	47	47	141	3	100	101	1	202	2.02
48	93	3	144	3	101	101	101	303	3
49	95	1	145	2.95918	102	201	3	306	3
50	95	5	150	3	103	203	1	307	2.98058
51	99	3	153	3	104	203	1	308	2.96154
52	101	1	154	2.96154	105	203	7	315	3
53	101	1	155	2.92453	106	209	1	316	2.98113

Table 2.1: The first few terms for  $a(1) = 7$ .

For brevity, let  $g(n) = a(n) - a(n-1) = \gcd(n, a(n-1))$  so that  $a(n) = a(n-1) + g(n)$ . Table 2.1 lists the first few values of  $a(n)$  and  $g(n)$  as well as of the quantities  $\Delta(n) = a(n-1) - n$  and  $a(n)/n$ , whose motivation will become clear presently. Additional features of Table 2.1 not vital to the main result are discussed in Section 2.5.

One observes from the data that  $g(n)$  contains long runs of consecutive 1s. On such a run, say if  $g(n) = 1$  for  $n_1 < n < n_1 + k$ , we have

$$a(n) = a(n_1) + \sum_{i=1}^{n-n_1} g(n_1 + i) = a(n_1) + (n - n_1), \quad (2.2)$$

so the difference  $a(n) - n = a(n_1) - n_1$  is invariant in this range. When the next nontrivial gcd does occur, we see in Table 2.1 that it has some relationship to this difference. Indeed, it appears to divide

$$\Delta(n) := a(n-1) - n = a(n_1) - 1 - n_1.$$

For example  $3 \mid 21$ ,  $23 \mid 23$ ,  $3 \mid 45$ ,  $47 \mid 47$ , etc. This observation is easy to prove and is a first hint of the shortcut mentioned in Section 2.1.

Restricting attention to steps where the gcd is nontrivial, one notices that  $a(n) = 3n$  whenever  $g(n) \neq 1$ . This fact is the central ingredient in the proof of the lemma, and it suggests that  $a(n)/n$  may be worthy of study. We pursue this in Section 2.4.

Another important observation can be discovered by plotting the values of  $n$  for which  $g(n) \neq 1$ , as in Figure 2.1. They occur in clusters, each cluster initiated by a large prime and followed by small primes interspersed with 1s. The ratio between the index  $n$  beginning one cluster and the index ending the previous cluster is very nearly 2, which causes the regular vertical spacing seen when plotted logarithmically. With further experimentation one discovers the reason for this, namely that when  $2n - 1 = p$  is prime for  $g(n) \neq 1$ , such a “large gap” between nontrivial gcds occurs (demarcating two clusters) and the next nontrivial gcd is  $g(p) = p$ . This suggests looking at the quantity  $2n - 1$  (which is  $\Delta(n+1)$  when  $a(n) = 3n$ ), and one guesses that in general the next nontrivial gcd is the smallest prime divisor of  $2n - 1$ .

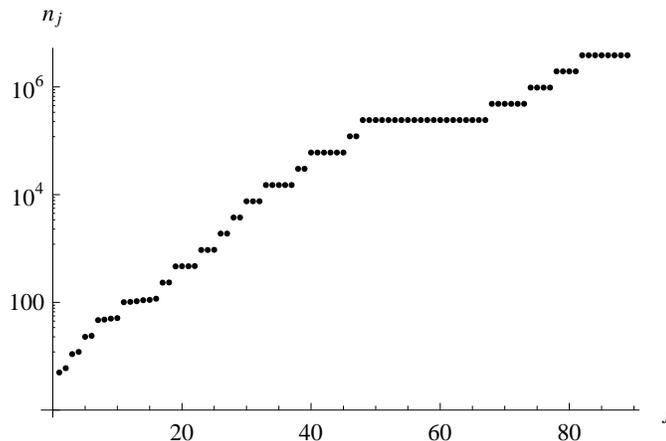


Figure 2.1: Logarithmic plot of  $n_j$ , the  $j$ th value of  $n$  for which  $a(n) - a(n - 1) \neq 1$ , for the initial condition  $a(1) = 7$ . The regularity of the vertical gaps between clusters indicates local structure in the sequence.

### 2.3 Recurring structure

We now establish the observations of the previous section, treating the recurrence (2.1) as a discrete dynamical system on pairs  $(n, a(n))$  of integers. We no longer assume  $a(1) = 7$ ; a general initial condition for the system specifies integer values for  $n_1$  and  $a(n_1)$ .

Accordingly, we may broaden the result: In the previous section we observed that  $a(n)/n = 3$  is a significant recurring event; it turns out that  $a(n)/n = 2$  plays the same role for other initial conditions (for example,  $a(3) = 6$ ). The following lemma explains the relationship between one occurrence of this event and the next, allowing the elimination of the intervening run of 1s. We need only know the smallest prime divisor of  $\Delta(n_1 + 1)$ .

**Lemma 2.1.** *Let  $r \in \{2, 3\}$  and  $n_1 \geq \frac{3}{r-1}$ . Let  $a(n_1) = rn_1$ , and for  $n > n_1$  let*

$$a(n) = a(n - 1) + \gcd(n, a(n - 1))$$

*and  $g(n) = a(n) - a(n - 1)$ . Let  $n_2$  be the smallest integer greater than  $n_1$  such that  $g(n_2) \neq 1$ . Let  $p$  be the smallest prime divisor of*

$$\Delta(n_1 + 1) = a(n_1) - (n_1 + 1) = (r - 1)n_1 - 1.$$

Then

$$(a) \ n_2 = n_1 + \frac{p-1}{r-1},$$

$$(b) \ g(n_2) = p, \text{ and}$$

$$(c) \ a(n_2) = rn_2.$$

Brief remarks on the condition  $(r-1)n_1 \geq 3$  are in order. Foremost, this condition guarantees that the prime  $p$  exists, since  $(r-1)n_1 - 1 \geq 2$ . However, we can also interpret it as a restriction on the initial condition. We stipulate  $a(n_1) = rn_1 \neq n_1 + 2$  because otherwise  $n_2$  does not exist; note however that among positive integers this excludes only the two initial conditions  $a(2) = 4$  and  $a(1) = 3$ . A third initial condition,  $a(1) = 2$ , is eliminated by the inequality; most of the conclusion holds in this case (since  $n_2 = g(n_2) = a(n_2)/n_2 = 2$ ), but because  $(r-1)n_1 - 1 = 0$  it is not covered by the following proof.

*Proof.* Let  $k = n_2 - n_1$ . We show that  $k = \frac{p-1}{r-1}$ . Clearly  $\frac{p-1}{r-1}$  is an integer if  $r = 2$ ; if  $r = 3$  then  $(r-1)n_1 - 1$  is odd, so  $\frac{p-1}{r-1}$  is again an integer.

By Equation (2.2), for  $1 \leq i \leq k$  we have  $g(n_1 + i) = \gcd(n_1 + i, rn_1 - 1 + i)$ . Therefore,  $g(n_1 + i)$  divides both  $n_1 + i$  and  $rn_1 - 1 + i$ , so  $g(n_1 + i)$  also divides both their difference

$$(rn_1 - 1 + i) - (n_1 + i) = (r-1)n_1 - 1$$

and the linear combination

$$r \cdot (n_1 + i) - (rn_1 - 1 + i) = (r-1)i + 1.$$

We use these facts below.

$k \geq \frac{p-1}{r-1}$ : Since  $g(n_1 + k)$  divides  $(r-1)n_1 - 1$  and by assumption  $g(n_1 + k) \neq 1$ , we have  $g(n_1 + k) \geq p$ . Since  $g(n_1 + k)$  also divides  $(r-1)k + 1$ , we have

$$p \leq g(n_1 + k) \leq (r-1)k + 1.$$

$k \leq \frac{p-1}{r-1}$ : Now that  $g(n_1 + i) = 1$  for  $1 \leq i < \frac{p-1}{r-1}$ , we show that  $i = \frac{p-1}{r-1}$  produces a nontrivial gcd. We have

$$\begin{aligned} g(n_1 + \frac{p-1}{r-1}) &= \gcd\left(n_1 + \frac{p-1}{r-1}, rn_1 - 1 + \frac{p-1}{r-1}\right) \\ &= \gcd\left(\frac{((r-1)n_1 - 1) + p}{r-1}, \frac{r \cdot ((r-1)n_1 - 1) + p}{r-1}\right). \end{aligned}$$

By the definition of  $p$ ,  $p \mid ((r-1)n_1 - 1)$  and  $p \nmid (r-1)$ . Thus  $p$  divides both arguments of the gcd, so  $g(n_1 + \frac{p-1}{r-1}) \geq p$ .

Therefore  $k = \frac{p-1}{r-1}$ , and we have shown (a). On the other hand,  $g(n_1 + \frac{p-1}{r-1})$  divides  $(r-1) \cdot \frac{p-1}{r-1} + 1 = p$ , so in fact  $g(n_1 + \frac{p-1}{r-1}) = p$ , which is (b). We now have  $g(n_2) = p = (r-1)k + 1$ , so to obtain (c) we compute

$$\begin{aligned} a(n_2) &= a(n_2 - 1) + g(n_2) \\ &= (rn_1 - 1 + k) + ((r-1)k + 1) \\ &= r(n_1 + k) \\ &= rn_2. \end{aligned} \quad \square$$

We immediately obtain the following result for  $a(1) = 7$ ; one simply computes  $g(2) = g(3) = 1$ , and  $a(3)/3 = 3$  so the lemma applies inductively thereafter.

**Theorem 2.2.** *Let  $a(1) = 7$ . For each  $n \geq 2$ ,  $a(n) - a(n-1)$  is 1 or prime.*

Similar results can be obtained for many other initial conditions, such as  $a(1) = 4$ ,  $a(1) = 8$ , etc. Indeed, most small initial conditions quickly produce a state in which the lemma applies.

## 2.4 Transience

However, the statement of the theorem is false for general initial conditions. Two examples of non-prime gcDs are  $g(18) = 9$  for  $a(1) = 532$  and  $g(21) = 21$  for  $a(1) = 801$ . With additional experimentation one does however come to suspect that  $g(n)$  is eventually 1 or prime for every initial condition.

**Conjecture 2.3.** *If  $n_1 \geq 1$  and  $a(n_1) \geq 1$ , then there exists an  $N$  such that  $a(n) - a(n-1)$  is 1 or prime for each  $n > N$ .*

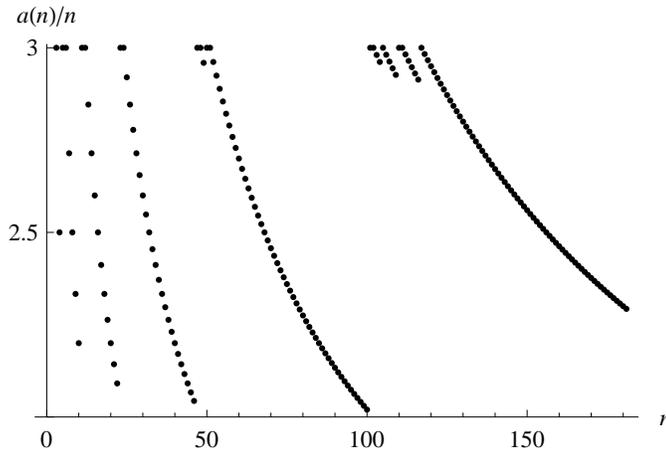


Figure 2.2: Plot of  $a(n)/n$  for  $a(1) = 7$ . Proposition 2.5 establishes that  $a(n)/n > 2$ .

The conjecture asserts that the states for which the lemma of Section 2.3 does not apply are transient. To prove the conjecture, it would suffice to show that if  $a(n_1) \neq n_1 + 2$  then  $a(N)/N$  is 1, 2, or 3 for some  $N$ : If  $a(N) = N + 2$  or  $a(N)/N = 1$ , then  $g(n) = 1$  for  $n > N$ , and if  $a(N)/N$  is 2 or 3, then the lemma applies inductively. Thus we should try to understand the long-term behavior of  $a(n)/n$ . We give two propositions in this direction.

Empirical data show that when  $a(n)/n$  is large, it tends to decrease. The first proposition states that  $a(n)/n$  can never cross over an integer from below.

**Proposition 2.4.** *If  $n_1 \geq 1$  and  $a(n_1) \geq 1$ , then  $a(n)/n \leq \lceil a(n_1)/n_1 \rceil$  for all  $n \geq n_1$ .*

*Proof.* Let  $r = \lceil a(n_1)/n_1 \rceil$ . We proceed inductively; assume that  $a(n-1)/(n-1) \leq r$ .

Then

$$rn - a(n-1) \geq r \geq 1.$$

Since  $g(n)$  divides the linear combination  $r \cdot n - a(n-1)$ , we have

$$g(n) \leq rn - a(n-1);$$

thus

$$a(n) = a(n-1) + g(n) \leq rn. \quad \square$$

From Equation (2.2) in Section 2.2 we see that  $g(n_1 + i) = 1$  for  $1 \leq i < k$  implies that  $a(n_1 + i)/(n_1 + i) = (a(n_1) + i)/(n_1 + i)$ , and so  $a(n)/n$  is strictly decreasing in this range if  $a(n_1) > n_1$ . Moreover, if the nontrivial gcds are overall sufficiently few and sufficiently small, then we would expect  $a(n)/n \rightarrow 1$  as  $n$  gets large; indeed the hyperbolic segments in Figure 2.2 have the line  $a(n)/n = 1$  as an asymptote.

However, in practice we rarely see this occurring. Rather,  $a(n_1)/n_1 > 2$  seems to almost always imply that  $a(n)/n > 2$  for all  $n \geq n_1$ . Why is this the case?

Suppose the sequence of ratios crosses 2 for some  $n$ :  $a(n)/n > 2 \geq a(n+1)/(n+1)$ . Then

$$2 \geq \frac{a(n+1)}{n+1} = \frac{a(n) + \gcd(n+1, a(n))}{n+1} \geq \frac{a(n) + 1}{n+1},$$

so  $a(n) \leq 2n + 1$ . Since  $a(n) > 2n$ , we are left with  $a(n) = 2n + 1$ ; and indeed in this case we have

$$\frac{a(n+1)}{n+1} = \frac{2n+1 + \gcd(n+1, 2n+1)}{n+1} = \frac{2n+2}{n+1} = 2.$$

The task at hand, then, is to determine whether  $a(n) = 2n + 1$  can happen in practice. That is, if  $a(n_1) > 2n_1 + 1$ , is there ever an  $n > n_1$  such that  $a(n) = 2n + 1$ ? Working backward, let  $a(n) = 2n + 1$ . We will consider possible values for  $a(n-1)$ .

If  $a(n-1) = 2n$ , then

$$2n + 1 = a(n) = 2n + \gcd(n, 2n) = 3n,$$

so  $n = 1$ . The state  $a(1) = 3$  is produced after one step by the initial condition  $a(0) = 2$  but is a moot case if we restrict to positive initial conditions.

If  $a(n-1) < 2n$ , then  $a(n-1) = 2n - j$  for some  $j \geq 1$ . Then

$$2n + 1 = a(n) = 2n - j + \gcd(n, 2n - j),$$

so  $j + 1 = \gcd(n, 2n - j)$  divides  $2 \cdot n - (2n - j) = j$ . This is a contradiction.

Thus for  $n > 1$  the state  $a(n) = 2n + 1$  only occurs as an initial condition, and we have proved the following.

**Proposition 2.5.** *If  $n_1 \geq 1$  and  $a(n_1) > 2n_1 + 1$ , then  $a(n)/n > 2$  for all  $n \geq n_1$ .*

In light of these propositions, the largest obstruction to the conjecture is showing that  $a(n)/n$  cannot remain above 3 indefinitely. Unfortunately, this is a formidable obstruction:

The only distinguishing feature of the values  $r = 2$  and  $r = 3$  in the lemma is the guarantee that  $\frac{p-1}{r-1}$  is an integer, where  $p$  is again the smallest prime divisor of  $(r-1)n_1 - 1$ . If  $r \geq 4$  is an integer and  $(r-1) \mid (p-1)$ , then the proof goes through, and indeed it is possible to find instances of an integer  $r \geq 4$  persisting for some time; in fact a repetition can occur even without the conditions of the lemma. Searching in the range  $1 \leq n_1 \leq 10^4$ ,  $4 \leq r \leq 20$ , one finds the example  $n_1 = 7727$ ,  $r = 7$ ,  $a(n_1) = rn_1 = 54089$ , in which  $a(n)/n = 7$  reoccurs eleven times (the last at  $n = 7885$ ).

The evidence suggests that there are arbitrarily long such repetitions of integers  $r \geq 4$ . With the additional lack of evidence of global structure that might control the number of these repetitions, it is possible that, when phrased as a parameterized decision problem, the conjecture becomes undecidable. Perhaps this is not altogether surprising, since the experience with discrete dynamical systems (not least of all the Collatz  $3n+1$  problem) is frequently one of presumed inability to significantly shortcut computations.

The next best thing we can do, then, is speed up computation of the transient region so that one may quickly establish the conjecture for specific initial conditions. It is a pleasant fact that the shortcut of the lemma can be generalized to give the location of the next nontrivial gcd without restriction on the initial condition, although naturally we lose some of the benefits as well.

In general one can interpret the evolution of Equation (2.1) as repeatedly computing for various  $n$  and  $a(n-1)$  the minimal  $k \geq 1$  such that  $\gcd(n+k, a(n-1)+k) \neq 1$ , so let us explore this question in isolation. Let  $a(n-1) = n + \Delta$  (with  $\Delta \geq 1$ ); we seek  $k$ . (The lemma determines  $k$  for the special cases  $\Delta = n-1$  and  $\Delta = 2n-1$ .)

Clearly  $\gcd(n+k, n+\Delta+k)$  divides  $\Delta$ .

Suppose  $\Delta = p$  is prime; then we must have  $\gcd(n+k, n+p+k) = p$ . This is equivalent to  $k \equiv -n \pmod{p}$ . Since  $k \geq 1$  is minimal, then  $k = \text{mod}_1(-n, p)$ , where  $\text{mod}_j(a, b)$  is the unique number  $x \equiv a \pmod{b}$  such that  $j \leq x < j+b$ .

Now consider a general  $\Delta$ . A prime  $p$  divides  $\gcd(n+i, n+\Delta+i)$  if and only if it divides both  $n+i$  and  $\Delta$ . Therefore

$$\{i : \gcd(n+i, n+\Delta+i) \neq 1\} = \bigcup_{p|\Delta} (-n+p\mathbb{Z}).$$

Calling this set  $I$ , we have

$$k = \min \{i \in I : i \geq 1\} = \min \{\text{mod}_1(-n, p) : p \mid \Delta\}.$$

Therefore (as we record in slightly more generality)  $k$  is the minimum of  $\text{mod}_1(-n, p)$  over all primes dividing  $\Delta$ .

**Proposition 2.6.** *Let  $n \geq 0$ ,  $\Delta \geq 2$ , and  $j$  be integers. Let  $k \geq j$  be minimal such that  $\gcd(n+k, n+\Delta+k) \neq 1$ . Then*

$$k = \min \{\text{mod}_j(-n, p) : p \text{ is a prime dividing } \Delta\}.$$

## 2.5 Primes

We conclude with several additional observations that can be deduced from the lemma regarding the prime  $p$  that occurs as  $g(n_2)$  under various conditions.

We return to the large gaps observed in Figure 2.1. A large gap occurs when  $(r-1)n_1 - 1 = p$  is prime, since then  $n_2 - n_1 = \frac{p-1}{r-1}$  is maximal. In this case we have  $n_2 = \frac{2p}{r-1}$ , so since  $n_2$  is an integer and  $p > r-1$  we also see that  $(r-1)n_1 - 1$  can only be prime if  $r$  is 2 or 3. Thus large gaps only occur for  $r \in \{2, 3\}$ .

Table 2.1 suggests two interesting facts about the beginning of each cluster of primes after a large gap:

- $p = g(n_2) \equiv 5 \pmod{6}$ .
- The next nontrivial gcd after  $p$  is always  $g(n_2 + 1) = 3$ .

The reason is that when  $r = 3$ , eventually we have  $a(n) \equiv n \pmod{6}$ , with exceptions only when  $g(n) \equiv 5 \pmod{6}$  (in which case  $a(n) \equiv n + 4 \pmod{6}$ ). In the range  $n_1 <$

$n < n_2$  we have  $g(n) = 1$ , so  $p = 2n_1 - 1 = \Delta(n) = a(n-1) - n \equiv 5 \pmod{6}$  and

$$\begin{aligned} g(n_2 + 1) &= \gcd(n_2 + 1, a(n_2)) \\ &= \gcd(p + 1, 3p) \\ &= 3. \end{aligned}$$

An analogous result holds for  $r = 2$  and  $n_1 - 1 = p$  prime:  $g(n_2) = p \equiv 5 \pmod{6}$ ,  $g(n_2 + 1) = 1$ , and  $g(n_2 + 2) = 3$ .

In fact, this analogy suggests a more general similarity between the two cases  $r = 2$  and  $r = 3$ : An evolution for  $r = 2$  can generally be emulated (and actually computed twice as quickly) by  $r' = 3$  under the transformation

$$\begin{aligned} n' &= n/2, \\ a'(n') &= a(n) - n/2 \end{aligned}$$

for even  $n$  (discarding odd  $n$ ). One verifies that the conditions and conclusions of the lemma are preserved; in particular

$$\frac{a'(n')}{n'} = 2 \cdot \frac{a(n)}{n} - 1.$$

For example, the evolution from initial condition  $a(4) = 8$  is emulated by the evolution from  $a'(1) = 7$  for  $n = 2n' \geq 6$ .

One wonders whether  $g(n)$  takes on all primes. For  $r = 3$ , clearly the case  $p = 2$  never occurs since  $2n_1 - 1$  is odd. Furthermore, for  $r = 2$ , the case  $p = 2$  can only occur once for a given initial condition: A simple checking of cases shows that  $n_2$  is even, so applying the lemma to  $n_2$  we find  $n_2 - 1$  is odd (at which point the evolution can be emulated by  $r' = 3$ ).

We conjecture that all other primes occur. After ten thousand applications of the shortcut starting from the initial condition  $a(1) = 7$ , the smallest odd prime that has not yet appeared is 587.

For general initial conditions the results are similar, and one quickly notices that evolutions from different initial conditions frequently converge to the same evolution after some time, reducing the number that must be considered. For example,  $a(1) = 4$

and  $a(1) = 7$  converge after two steps to  $a(3) = 9$ . One can use the shortcut to feasibly track these evolutions for large values of  $n$  and thereby estimate the density of distinct evolutions. In the range  $2^2 \leq a(1) \leq 2^{13}$  one finds that there are only 203 equivalence classes established below  $n = 2^{23}$ , and no two of these classes converge below  $n = 2^{60}$ . It therefore appears that disjoint evolutions are quite sparse. Sequence [A134162](#) is the sequence of minimal initial conditions for these equivalence classes.

## Chapter 3

### Pattern avoidance in binary trees

#### 3.1 Introduction

Determining the number of words of length  $n$  on a given alphabet that avoid a certain (contiguous) subword is a classical combinatorial problem that can be solved, for example, by the principle of inclusion–exclusion. An approach to this question using generating functions is provided by the Goulden–Jackson cluster method [14, 22], which utilizes only the self-overlaps (or “autocorrelations”) of the word being considered. A natural question is “When do two words have the same avoiding generating function?” That is, when are the  $n$ -letter words avoiding (respectively)  $w_1$  and  $w_2$  equinumerous for all  $n$ ? The answer is simple: precisely when their self-overlaps coincide. For example, the equivalence classes of length-4 words on the alphabet  $\{0, 1\}$  are as follows.

equivalence class	self-overlap lengths
{0001, 0011, 0111, 1000, 1100, 1110}	{4}
{0010, 0100, 0110, 1001, 1011, 1101}	{1, 4}
{0101, 1010}	{2, 4}
{0000, 1111}	{1, 2, 3, 4}

In this chapter we consider the analogous questions for plane trees. All trees are rooted and ordered. The *depth* of a vertex is the length of the minimal path to that vertex from the root, and  $\text{depth}(T)$  is the maximum vertex depth in the tree  $T$ .

Our focus will be on *binary trees* — trees in which each vertex has 0 or 2 (ordered) children. A vertex with 0 children is a *leaf*, and a vertex with 2 children is an *internal* vertex. A binary tree with  $n$  leaves has  $n - 1$  internal vertices, and the number of such trees is the Catalan number  $C_{n-1}$ . The first few binary trees are depicted in

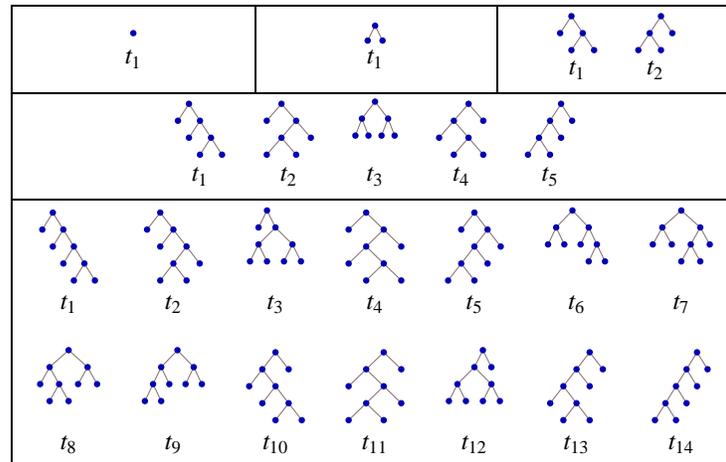


Figure 3.1: The binary trees with at most 5 leaves.

Figure 3.1. We use an indexing for  $n$ -leaf binary trees that arises from the natural recursive construction of all  $n$ -leaf binary trees by pairing each  $k$ -leaf binary tree with each  $(n - k)$ -leaf binary tree, for all  $1 \leq k \leq n - 1$ . In practice it will be clear from context which tree we mean by, for example, ‘ $t_1$ ’.

Conceptually, a binary tree  $T$  *avoids* a tree pattern  $t$  if there is no instance of  $t$  anywhere inside  $T$ . Steyaert and Flajolet [30] were interested in such patterns in vertex-labeled trees. They were mainly concerned with the asymptotic probability of avoiding a pattern, whereas our focus is on enumeration. However, they establish in Section 2.2 that the total number of occurrences of an  $m$ -leaf binary tree pattern  $t$  in all  $n$ -leaf binary trees is

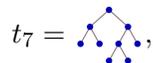
$$2 \binom{2n - m - 1}{n - m - 1}.$$

In this sense, all  $m$ -leaf binary trees are indistinguishable; the results of this chapter may be thought of as a refinement of this statement.

We remark that a different notion of tree pattern was later considered by Flajolet, Sipala, and Steyaert [9], in which every leaf of the pattern must be matched by a leaf of the tree. Such patterns are only matched at the bottom of a tree, so they arise naturally in the problem of compactly representing in memory an expression containing repeated subexpressions. The enumeration of trees avoiding such a pattern is simple, since no

two instances of the pattern can overlap: The number of  $n$ -leaf binary trees avoiding  $t$  depends only on the number of leaves in  $t$ . See also Flajolet and Sedgewick [8, Note III.40].

The reason for us studying patterns in binary trees as opposed to rooted, ordered trees in general is that it is straightforward to determine what it should mean for a binary tree to avoid, for example,



whereas *a priori* it is ambiguous to say that a general tree avoids



Namely, for general trees, ‘matches a vertex with  $i$  children’ for  $i \geq 1$  could mean either ‘has exactly  $i$  children’ or ‘has at least  $i$  children’. For binary trees, these are the same for  $i = 2$ .

However, it turns out that the notion of pattern avoidance for binary trees induces a well-defined notion of pattern avoidance for general trees. This arises via the Harary–Prins–Tutte bijection  $\beta$  (defined in Section 3.2.1) between the set of  $n$ -vertex trees and the set of  $n$ -leaf binary trees.

A main theoretical purpose of this chapter is to provide an algorithm for computing the generating function that counts the trees avoiding a certain binary tree pattern. This algorithm easily generalizes to count the trees containing a prescribed number of occurrences of a certain pattern, and additionally we consider the number of trees containing several patterns each a prescribed number of times. All of these generating functions are algebraic. Section 3.5 is devoted to these algorithms, which are implemented in TREEPATTERNS [27], a *Mathematica* package available from the author’s website.

By contrast, another main purpose of this chapter is quite concrete, and that is to determine equivalence classes of binary trees. We say that two tree patterns  $s$  and  $t$  are *equivalent* if for all  $n \geq 1$  the number of  $n$ -leaf binary trees avoiding  $s$  is equal to the number of  $n$ -leaf binary trees avoiding  $t$ . In other words, equivalent trees have

the same generating function with respect to avoidance. This is the analogue of Wilf equivalence in permutation patterns. Each tree is trivially equivalent to its left–right reflection, but there are other equivalences as well. The first few classes are presented in Section 3.3. The appendix contains a complete list of equivalence classes of binary trees with at most 7 leaves, from which we draw examples throughout the chapter. Classes are named with the convention that class  $m.i$  is the  $i$ th class of  $m$ -leaf binary trees.

We seek to understand equivalence classes of binary trees combinatorially, and this is the third purpose of the chapter. As discussed in Section 3.4, in a few cases there is a bijection between  $n$ -leaf binary trees avoiding a certain pattern and Dyck  $(n - 1)$ -words avoiding a certain (contiguous) subword. In general, when  $s$  and  $t$  are equivalent tree patterns, we would like to provide a bijection between trees avoiding  $s$  and trees avoiding  $t$ . Conjecturally, all classes of binary trees can be established bijectively by *top-down* and *bottom-up* replacements; this is the topic of Section 3.6. Nearly all bijections in the chapter are implemented in the package TREEPATTERNS.

Aside from mathematical interest, a general study of pattern avoidance in trees has applications to any collection of objects related by a tree structure, such as people in a family tree or species in a phylogenetic tree. In particular, this chapter answers the following question. Given  $n$  related objects (e.g., species) for which the exact relationships aren’t known, how likely is it that some prescribed (e.g., evolutionary) relationship exists between some subset of them? (Unfortunately, it probably will not lead to insight regarding the practical question “What is the probability of avoiding a mother-in-law?”) Alternatively, we can think of trees as describing the syntax of sentences in natural language or of fragments of computer code; in this context the chapter answers questions about the occurrence and frequency of given phrase substructures.

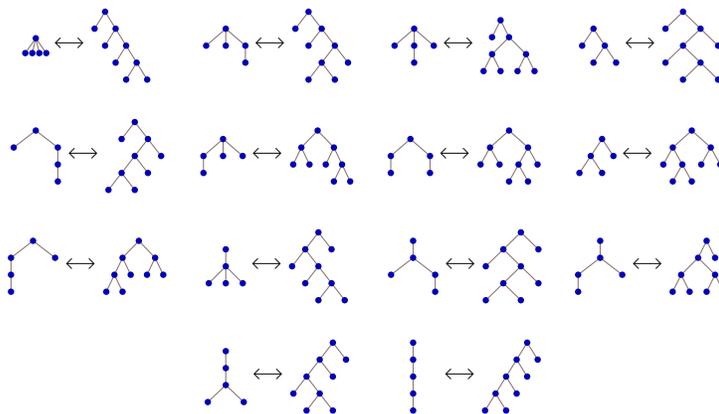


Figure 3.2: The Harary–Prins–Tutte correspondence  $\beta$  between trees with 5 vertices and binary trees with 5 leaves.

## 3.2 Definitions

### 3.2.1 The Harary–Prins–Tutte bijection

We first recall a fundamental bijection between  $n$ -leaf binary trees and general (rooted, ordered)  $n$ -vertex trees. The bijection was given by Harary, Prins, and Tutte [15] and simplified by de Bruijn and Morselt [3]. Following Knuth [19, Section 2.3.2], we use a modified version in which the trees are de-planted. (An extra vertex is used by those authors because they think of these objects as trivalent trees.) The correspondence for  $n = 5$  is shown in Figure 3.2. Throughout the chapter we shall call this bijection  $\beta$ . That is,

$$\beta : (\text{set of all trees}) \rightarrow (\text{set of binary trees}).$$

To obtain the  $n$ -leaf binary tree  $\beta(T)$  associated with a given  $n$ -vertex tree  $T$ :

1. Delete the root vertex.
2. For each remaining vertex, let its new left child be its original leftmost child (if it exists), and let its new right child be its original immediate right sibling (if it exists).
3. Add children to the existing vertices so that each has two children. (If a vertex has only one child, the new child is added in place of the child missing in step 2.)

Note that the leaves of the final binary tree are precisely the vertices added in this step.

For example,

$$T = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \xrightarrow{(1)} \begin{array}{c} \bullet \\ | \\ \bullet \end{array} \quad \begin{array}{c} \bullet \\ | \\ \bullet \end{array} \xrightarrow{(2)} \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \xrightarrow{(3)} \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = \beta(T).$$

If  $T$  is an  $n$ -vertex tree, then clearly  $\beta(T)$  is a binary tree, and  $\beta(T)$  has  $n$  leaves because the  $n - 1$  vertices present in step 2 are precisely the internal vertices of  $\beta(T)$ . Constructing the inverse map  $\beta^{-1}$  is not difficult; one simply reverses the algorithm. A quick way to visualize the inverse is by contracting every rightward edge to a single vertex.

Of course,  $\beta$  is chiral in the sense that there is another, equally good bijection  $\rho\beta\rho \neq \beta$ , where  $\rho$  is left-right reflection (which acts by reversing the order of the children of each vertex); but it suffices to employ just one of these bijections.

### 3.2.2 Avoidance

The more formal way to think of an  $n$ -vertex tree is as a particular arrangement of  $n$  pairs of parentheses, where each vertex is represented by the pair of parentheses containing its children. For example, the tree

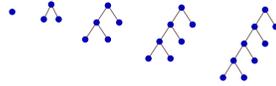
$$T = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

is represented by  $((()((())))$ . This is the word representation of this tree in the alphabet  $\{(,)\}$ . We do not formally distinguish between the graphical representation of a tree and the word representation, and it is the latter that is useful in manipulating trees algorithmically. (*Mathematica's* pattern matching capabilities provide a convenient tool for working with trees represented as nested lists, so this is the convention used by TREEPATTERNS.)

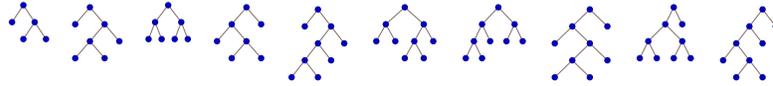
Informally, our concept of containment is as follows. A binary tree  $T$  *contains*  $t$  if there is a (contiguous, rooted, ordered) subtree of  $T$  that is a copy of  $t$ . For example, consider

$$t = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

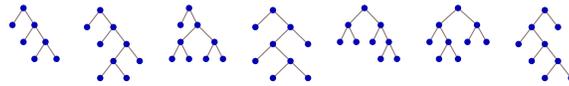
None of the trees



contains a copy of  $t$ , while each of the trees



contains precisely one copy of  $t$ , each of the trees



contains precisely two (possibly overlapping) copies of  $t$ , and the tree



contains precisely three copies of  $t$ . This is a classification of binary trees with at most 5 leaves according to the number of copies of  $t$ .

We might formalize this concept with a graph theoretic definition as follows. Let  $t$  be a binary tree. A *copy* of  $t$  in  $T$  is a subgraph of  $T$  (obtained by removing vertices) that is isomorphic to  $t$  (preserving edge directions and the order of children). Naturally,  $T$  *avoids*  $t$  if the number of copies of  $t$  in  $T$  is 0.

An equivalent but much more useful definition is a language theoretic one, and to provide this we first distinguish a *tree pattern* from a tree.

By ‘tree pattern’, informally we mean a tree whose leaves are “blanks” that can be filled (matched) by any tree, not just a single vertex. More precisely, let  $\Sigma = \{ (, ) \}$ , and let  $L$  be the language on  $\Sigma$  containing (the word representation of) every binary tree. Consider a binary tree  $\tau$ , and let  $t$  be the word on the three symbols  $(, ), L$  obtained by replacing each leaf  $()$  in  $\tau$  by  $L$ . We call  $t$  the *tree pattern* of  $\tau$ . This tree pattern naturally generates a language  $L_t$  on  $\Sigma$ , which we obtain by interpreting the word  $t$  as a product of the three languages  $( = \{ (, ) = \} \}$ ,  $L$ . Informally,  $L_t$  is the set of words that match  $t$ . We think of  $t$  and  $L_t$  interchangeably. (Note that a tree is a tree pattern matched only by itself.)

For example, let

$$\tau = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = ((() (()) ());$$

then the corresponding tree pattern is  $t = (L(LL))$ , and the language  $L_t$  consists of all trees of the form  $(T(UV))$ , where  $T, U, V$  are binary trees.

Let  $\Sigma^*$  denote the set of all finite words on  $\Sigma$ . The language  $\Sigma^*L_t\Sigma^* \cap L$  is the set of all binary trees whose word has a subword in  $L_t$ . Therefore we say that a binary tree  $T$  *contains* the tree pattern  $t$  if  $T$  is in the language  $\Sigma^*L_t\Sigma^* \cap L$ . We can think of this language as a multiset, where a given tree  $T$  occurs with multiplicity equal to the number of ways that it matches  $\Sigma^*L_t\Sigma^*$ . Then the *number of copies* of  $t$  in  $T$  is the multiplicity of  $T$  in  $\Sigma^*L_t\Sigma^* \cap L$ .

Continuing the example from above, the tree

$$T = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = ((() (()) (()) (()))$$

contains 2 copies of  $t$  since it matches  $\Sigma^*L_t\Sigma^*$  in 2 ways:  $(T(UV))$  with  $T = ()$  and  $U = V = (()())$ , and  $((() (T(UV))))$  with  $T = (()())$  and  $U = V = ()$ .

Our notation distinguishes tree patterns from trees: Tree patterns are represented by lowercase variables, and trees are represented by uppercase variables. To be absolutely precise, we would graphically distinguish between terminal leaves  $()$  of a tree and blank leaves  $L$  of a tree pattern, but this gets in the way of speaking about them as the same objects, which is quite convenient.

In Sections 3.5 and 3.6 we will be interested in taking the intersection  $p \cap q$  of tree patterns  $p$  and  $q$  (by which we mean the intersection of the corresponding languages  $L_p$  and  $L_q$ ). The intersection of two or more explicit tree patterns can be computed recursively:  $p \cap L = p$ , and  $(p_l p_r) \cap (q_l q_r) = ((p_l \cap q_l)(p_r \cap q_r))$ .

### 3.2.3 Generating functions

Our primary goal is to determine the number  $a_n$  of binary trees with  $n$  vertices that avoid a given binary tree pattern  $t$ , and more generally to determine the number  $a_{n,m}$  of binary trees with  $n$  vertices and precisely  $m$  copies of  $t$ . Thus we consider two

generating functions associated with  $t$ : the *avoiding generating function*

$$\text{Av}_t(x) = \sum_{T \text{ avoids } t} x^{\text{number of vertices in } T} = \sum_{n=0}^{\infty} a_n x^n$$

and the *enumerating generating function*

$$\begin{aligned} \text{En}_{L,t}(x, y) &= \sum_T x^{\text{number of vertices in } T} y^{\text{number of copies of } t \text{ in } T} \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_{n,m} x^n y^m. \end{aligned}$$

The avoiding generating function is the special case  $\text{Av}_t(x) = \text{En}_{L,t}(x, 0)$ .

**Theorem 3.1.**  $\text{En}_{L,t}(x, y)$  is algebraic.

The proof is constructive, so it enables us to compute  $\text{En}_{L,t}(x)$ , and in particular  $\text{Av}_t(x)$ , for explicit tree patterns. We postpone the proof until Section 3.5.2 to address a natural question that arises: Which trees have the same generating function? That is, for which pairs of binary tree patterns  $s$  and  $t$  are the  $n$ -leaf trees avoiding (or containing  $m$  copies of) these patterns equinumerous?

We say that  $s$  and  $t$  are *avoiding-equivalent* if  $\text{Av}_s(x) = \text{Av}_t(x)$ . We say they are *enumerating-equivalent* if the seemingly stronger condition  $\text{En}_{L,s}(x, y) = \text{En}_{L,t}(x, y)$  holds. We can compute these equivalence classes explicitly by computing  $\text{Av}_t(x)$  and  $\text{En}_{L,t}(x, y)$  for, say, all  $m$ -leaf binary tree patterns  $t$ . In doing this for binary trees with up to 7 leaves, one comes to suspect that these conditions are actually equivalent.

**Conjecture 3.2.** *If  $s$  and  $t$  are avoiding-equivalent, then they are also enumerating-equivalent.*

In light of this experimental result, we focus attention in the remainder of the chapter on classes of avoiding-equivalence, since conjecturally they are the same as classes of enumerating-equivalence.

### 3.3 Initial inventory and some special bijections

In this section we undertake an analysis of small patterns. We determine  $\text{Av}_t(x)$  for binary tree patterns with at most 4 leaves using methods specific to each. This allows us to establish the equivalence classes in this range.

### 3.3.1 1-leaf trees

There is only one binary tree pattern with a single leaf, namely

$$t = \bullet = L.$$

Every binary tree contains at least one vertex, so  $\text{Av}_t(x) = 0$ . The number of binary trees with  $2n - 1$  vertices is  $C_{n-1}$ , so

$$\text{En}_L(x) = x + x^3 + 2x^5 + 5x^7 + 14x^9 + 42x^{11} + \dots = \sum_{n=1}^{\infty} C_{n-1} x^{2n-1}.$$

### 3.3.2 2-leaf trees

There is also only one binary tree pattern with precisely 2 leaves:

$$t = \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array} = (LL).$$

However,  $t$  is a fairly fundamental structure in binary trees; the only tree avoiding it is the 1-vertex tree  $()$ . Thus  $\text{Av}_t(x) = x$ , and

$$\text{En}_{L,t}(x, y) = \sum_{n=1}^{\infty} C_{n-1} x^{2n-1} y^{n-1} = \frac{1 - \sqrt{1 - 4x^2y}}{2xy}.$$

### 3.3.3 3-leaf trees

There are  $C_2 = 2$  binary trees with 3 leaves, and they are equivalent by left–right reflection:

$$\begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array} \quad \text{and} \quad \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \end{array}.$$

There is only one binary tree with  $n$  leaves avoiding

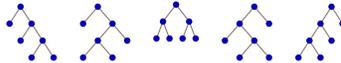
$$\begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \end{array} = ((LL)L),$$

namely the “right comb”  $((()((()((()((\dots))))))$ ). Therefore for these trees

$$\text{Av}_t(x) = x + x^3 + x^5 + x^7 + x^9 + x^{11} + \dots = \frac{x}{1 - x^2}.$$

### 3.3.4 4-leaf trees

Among 4-leaf binary trees we find more interesting behavior. There are  $C_3 = 5$  such trees, pictured as follows.



They comprise 2 equivalence classes.

#### Class 4.1

The first equivalence class consists of the trees

$$t_1 = \text{[tree diagram]} \quad \text{and} \quad t_5 = \text{[tree diagram]}.$$

The avoiding generating function  $\text{Av}_t(x)$  for each of these trees satisfies

$$x^3 f^2 + (x^2 - 1)f + x = 0$$

because the number of  $n$ -leaf binary trees avoiding  $t_1$  is the Motzkin number  $M_{n-1}$  (sequence [A001006](#)):

$$\text{Av}_t(x) = x + x^3 + 2x^5 + 4x^7 + 9x^9 + 21x^{11} + \dots = \sum_{n=1}^{\infty} M_{n-1} x^{2n-1}.$$

This fact is presented in a slightly different form by Donaghey and Shapiro [6] as their final example of objects counted by the Motzkin numbers. They provide a bijective proof which we reformulate here. Specifically, there is a natural bijection between the set of  $n$ -leaf binary trees avoiding  $t_1$  and the set of Motzkin paths of length  $n - 1$  — paths from  $(0, 0)$  to  $(n - 1, 0)$  composed of steps  $\langle 1, -1 \rangle$ ,  $\langle 1, 0 \rangle$ ,  $\langle 1, 1 \rangle$  that do not go below the  $x$ -axis. We represent a Motzkin path as a word on  $\{-1, 0, 1\}$  encoding the sequence of steps under  $\langle 1, \Delta y \rangle \mapsto \Delta y$ . The bijection is as follows.

To obtain the Motzkin path associated with a binary tree  $T$  avoiding  $t_1$ :

1. Let  $T' = \beta^{-1}(T)$ . No vertex in  $T'$  has more than 2 children, since

$$\beta^{-1}(t_1) = \text{[tree diagram]}$$

and  $T$  avoids  $t_1$ .

2. Create a word  $w$  on  $\{0, 1, 2\}$  by traversing the tree  $T'$  depth-first (i.e., for each subtree first visit the root vertex, then visit its children trees in order), recording the number of children of each vertex. Delete the last 0. The word  $w$  contains the same number of 0s and 2s, and every prefix of  $w$  contains at least as many 2s as 0s.
3. Apply the morphism

$$0 \rightarrow -1, 1 \rightarrow 0, 2 \rightarrow 1$$

to  $w$ .

The resulting word on  $\{-1, 0, 1\}$  is a Motzkin path because of the two properties of  $w$  stated in step 2. The steps are easily reversed to provide the inverse map from Motzkin paths to binary trees avoiding  $t_1$ .

#### Class 4.2

The second equivalence class consists of the three trees

$$t_2 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \quad t_3 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \quad \text{and} \quad t_4 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

and provides the smallest example of nontrivial equivalence. Symmetry gives  $\text{Av}_{t_2}(x) = \text{Av}_{t_4}(x)$ . To establish  $\text{Av}_{t_2}(x) = \text{Av}_{t_3}(x)$ , for each of these trees  $t$  we give a bijection between  $n$ -leaf binary trees avoiding  $t$  and binary words of length  $n - 2$ . By composing these two maps we obtain a bijection between trees avoiding  $t_2$  and trees avoiding  $t_3$ .

First consider

$$t_3 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}.$$

If  $T$  avoids  $t_3$ , then no vertex of  $T$  has four grandchildren; that is, at most one of a vertex's children has children of its own. This implies that at each generation at most one vertex has children. Since there are two vertices at each generation after the first, the number of such  $n$ -leaf trees is  $2^{n-2}$  for  $n \geq 2$ :

$$\text{Av}_{t_3}(x) = x + x^3 + 2x^5 + 4x^7 + 8x^9 + 16x^{11} + \dots = x + \sum_{n=2}^{\infty} 2^{n-2} x^{2n-1} = \frac{x(1-x^2)}{1-2x^2}.$$



### 3.4 Bijections to Dyck words

In Section 3.2.2 we assigned a word on the alphabet  $\{(,)\}$  to each tree. In this section we use a slight variant of this word that is more widely used in the literature. This is the *Dyck word* on the alphabet  $\{0,1\}$ , which differs from the aforementioned word on  $\{(,)\}$  in that the root vertex is omitted. For example, the Dyck word of



is 01001011. Omitting the root allows consistency with the definition of a Dyck word as a word consisting of  $n$  0s and  $n$  1s such that no prefix contains more 1s than 0s. It is mnemonically useful to think of the letters in the Dyck word as the directions (down or up) taken along the edges in the depth-first traversal of the tree.

Because trees and Dyck words are essentially the same objects, one expects questions about pattern avoidance in trees to have an interpretation as questions about pattern avoidance in Dyck words. Specifically, the set of trees avoiding a certain tree pattern corresponds to the set of Dyck words avoiding a (not necessarily contiguous) “word pattern”. This is simply a consequence of the bijection between trees and Dyck words.

However, in some cases there is a stronger relationship: The set of trees avoiding a certain pattern is in natural bijection to the set of Dyck words avoiding a certain contiguous subword. This relationship is the subject of the current section, in which we give several such bijections. For each equivalence class of trees we will be content with one bijection to Dyck words, although in many cases there are several.

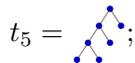
The first of these results were discovered by looking up the coefficients of various  $Av_t(x)$  in the Encyclopedia of Integer Sequences [29], where notes on sequences counting the number of Dyck words avoiding a subword (specifically, sequences [A005773](#), [A036765](#), and [A036766](#)) have been contributed by David Callan and Emeric Deutsch. The subject appears to have begun with Deutsch [5, Section 6.17], who enumerated Dyck words according to the number of occurrences of the subword 100. Sapounakis, Tasoulas, and Tsikouras [28] have considered additional subwords. Via the bijections described below, their results provide additional derivations of the generating functions  $Av_t(x)$ .

In Section 3.3.4 we observed that trees avoiding a tree pattern in class 4.1 are in bijection to Motzkin paths. From here it is easy to establish a bijection to Dyck words avoiding the subword 000. Simply apply the morphism

$$1 \rightarrow 001, 0 \rightarrow 01, -1 \rightarrow 1$$

to the Motzkin path. Clearly the resulting word has no instance of 000, and it is a Dyck word because 1 and  $-1$  occur in pairs in a Motzkin path, with every prefix containing at least as many 1s as  $-1$ s.

A different and more direct bijection to Dyck words avoiding 000 (and the one that we will generalize to other tree patterns) can be obtained as follows. Consider the 4-leaf binary tree



then

$$\beta^{-1}(t_5) = \begin{array}{c} \bullet \\ \vdots \\ \bullet \end{array},$$

whose Dyck word is 000111.

The inverse of the map  $\beta$  of Section 3.2.1 preserves a certain feature of any binary tree  $T$  containing  $t_5$ :  $\beta^{-1}(T)$  contains a sequence of four vertices in which each of the lower three is the first child of the previous. In other words, let  $T$  be a tree obtained by replacing the leaves of  $t_5$  with any binary trees. Then  $\beta^{-1}(T)$  is obtained from  $\beta^{-1}(t_5)$  by adding vertices as either children or right siblings — never as left siblings — to those in  $\beta^{-1}(t_5)$ . Therefore 000 is characteristic of  $t_5$  in the sense that  $T$  contains  $t_5$  if and only if the Dyck word of  $\beta^{-1}(T)$  contains 000.

And of course this bijection works for any left comb (i.e., class  $m.1$  for all  $m$ ): The binary trees avoiding the  $m$ -leaf left comb are in bijection to Dyck words avoiding  $0^{m-1}$ . Binary trees avoiding patterns in classes 5.1 and 6.1 are counted by sequences [A036765](#) and [A036766](#).

In general there is a natural bijection between  $n$ -leaf binary trees avoiding  $t$  and  $(n-1)$ -Dyck words avoiding  $w$  whenever  $w$  is a minimal characteristic feature of  $\beta^{-1}(t)$  (that is, some feature of the tree that is preserved locally by  $\beta^{-1}$ ).

For example, for the binary trees in class 4.2 we have

$$\beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \quad \beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \quad \beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}.$$

Which of these patterns have a bijection to Dyck words? Consider the third tree,

$$\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = 001011.$$

While it is true that any tree containing this tree must contain 001, the converse is not true, so this tree does not admit a bijection to Dyck words. However, the two trees

$$\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = 010011 \quad \text{and} \quad \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} = 001101$$

contain the word 100 and its reverse complement 110 respectively, and containing one of these subwords is a necessary and sufficient condition for the corresponding tree to contain the respective tree pattern. Thus binary trees avoiding a tree pattern in class 4.2 are in bijection to Dyck words avoiding 100, and they are counted by sequence [A011782](#).

Bijections for other patterns can be found similarly. Binary trees avoiding a tree pattern in class 5.2 (sequence [A086581](#)) are in bijection to Dyck words avoiding 1100, via

$$\beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}.$$

Class 5.3 (sequence [A005773](#)) corresponds to 1000 via

$$\beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}.$$

Class 6.3 corresponds to 11000 and class 6.6 to 10000 via

$$\beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \quad \text{and} \quad \beta^{-1} \left( \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \right) = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}.$$

respectively.

It is apparent that results of this kind involve “two-pronged” trees because avoidance for these trees corresponds to a local condition on Dyck words. It should not be surprising then that not all equivalence classes of binary trees have a corresponding Dyck word class. For example, classes 6.2, 6.4, 6.5, and 6.7 do not. The lack of a Dyck

word class can be proven in each case by exhibiting an  $n$  such that the number of  $n$ -leaf binary trees avoiding  $t$  is not equal to the number of  $(n-1)$ -Dyck words avoiding  $w$  for all  $w$ ; only a finite amount of computation is required because all  $C_{n-1}$   $(n-1)$ -Dyck words avoid  $w$  for  $|w| > 2(n-1)$ . For example,  $n = 8$  suffices for classes 6.2 and 6.5.

### 3.5 Algorithms

In this section we provide algorithms for computing algebraic equations satisfied by  $\text{Av}_t(x)$ ,  $\text{En}_{L,t}(x, y)$ , and the more general  $\text{En}_{L,p_1,\dots,p_k}(x_L, x_{p_1}, \dots, x_{p_k})$  defined in Section 3.5.3. Computing  $\text{Av}_t(x)$  or  $\text{En}_{L,t}(x, y)$  for all  $m$ -leaf binary tree patterns  $t$  allows one to automatically determine the equivalence classes given in the appendix.

We draw upon the notation and results described in Section 3.2.2. In particular, the intersection  $p \cap p'$  of two tree patterns plays a central role.

#### 3.5.1 Avoiding a single tree

Fix a binary tree pattern  $t$  we wish to avoid. For a given tree pattern  $p$ , we will make use of the generating function

$$\text{weight}(p) = \text{weight}(L_p) := \sum_{T \in L_p} \text{weight}(T),$$

where

$$\text{weight}(T) = \begin{cases} x^{\text{number of vertices in } T} & \text{if } T \text{ avoids } t; \\ 0 & \text{if } T \text{ contains } t. \end{cases}$$

The case  $t = L$  was covered in Section 3.3.1, so we assume  $t \neq L$ . Then  $t = (t_l t_r)$  for some tree patterns  $t_l$  and  $t_r$ . Since  $(T_l T_r)$  avoids  $t$  precisely when  $(T_l$  avoids  $t)$  and  $(T_r$  avoids  $t)$  and  $((T_l$  doesn't match  $t_l)$  or  $(T_r$  doesn't match  $t_r))$ , we have

$$\begin{aligned} \text{weight}((p_l p_r)) &= \\ x \cdot (\text{weight}(p_l) \cdot \text{weight}(p_r) - \text{weight}(p_l \cap t_l) \cdot \text{weight}(p_r \cap t_r)). \end{aligned} \quad (3.1)$$

The coefficient  $x$  is the weight of the root vertex of  $(p_l p_r)$  that we destroy in separating this pattern into its two subpatterns.

We now construct a polynomial (with coefficients that are polynomials in  $x$ ) that is satisfied by  $\text{Av}_t(x) = \text{weight}(L)$ , the weight of the language of binary trees. The algorithm is as follows.

Begin with the equation

$$\text{weight}(L) = \text{weight}(\circ) + \text{weight}((LL)).$$

The variable  $\text{weight}((LL))$  is “new”; we haven’t yet written it in terms of other variables. So use Equation (3.1) to rewrite  $\text{weight}((LL))$ . For each expression  $\text{weight}(p \cap p')$  that is introduced, we compute the intersection  $p \cap p'$ . This allows us to write  $\text{weight}(p \cap p')$  as  $\text{weight}(q)$  for some pattern  $q$  that is simply a word on  $\{(\circ, \cdot), L\}$  (i.e., does not contain the  $\cap$  operator).

For each new variable  $\text{weight}(q)$ , obtain a new equation by making it the left side of Equation (3.1), and then as before we eliminate  $\cap$  by explicitly computing intersections.

We continue in this manner until there are no new variables produced. This must happen because  $\text{depth}(p \cap p') \leq \max(\text{depth}(p), \text{depth}(p'))$ , so since there are only finitely many trees that are shallower than  $t$ , there are only finitely many variables in this system of polynomial equations.

Finally, compute a Gröbner basis for the system in which all variables except  $\text{weight}(\circ) = x$  and  $\text{weight}(L) = \text{Av}_t(x)$  are eliminated. This gives a single polynomial equation in these variables, which provides an algebraic equation satisfied by  $\text{Av}_t(x)$ .

Let us work out an example. We use the graphical representation of tree patterns with the understanding that the leaves are blanks. Consider the tree pattern

$$t = \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \bullet \quad \bullet \quad \bullet \quad \bullet \end{array} = (L(L((LL)L)))$$

from class 5.2. The first equation is

$$\text{weight}(\cdot) = x + \text{weight}(\blacktriangle).$$

We have  $t_l = \cdot$  and  $t_r = \blacktriangle$ , so Equation (3.1) gives

$$\begin{aligned} \text{weight}(\blacktriangle) &= x \cdot (\text{weight}(\cdot) \cdot \text{weight}(\cdot) - \text{weight}(\cdot \cap \cdot) \cdot \text{weight}(\cdot \cap \blacktriangle)) \\ &= x \cdot (\text{weight}(\cdot)^2 - \text{weight}(\cdot) \cdot \text{weight}(\blacktriangle \cap \cdot)) \end{aligned}$$

since  $L \cap p = p$  for any tree pattern  $p$ . The variable  $\text{weight}(\hat{\triangleleft}) = \text{weight}(t_r)$  is new, so we put it into Equation (3.1):

$$\begin{aligned} \text{weight}(\hat{\triangleleft}) &= x \cdot (\text{weight}(\cdot) \cdot \text{weight}(\triangleleft) - \text{weight}(\cdot \cap \cdot) \cdot \text{weight}(\triangleleft \cap \hat{\triangleleft})) \\ &= x \cdot (\text{weight}(\cdot) \cdot \text{weight}(\triangleleft) - \text{weight}(\cdot) \cdot \text{weight}(\triangleleft \hat{\triangleleft})). \end{aligned}$$

There are two new variables:

$$\begin{aligned} \text{weight}(\triangleleft) &= x \cdot (\text{weight}(\triangleleft) \cdot \text{weight}(\cdot) - \text{weight}(\triangleleft \cap \cdot) \cdot \text{weight}(\cdot \cap \hat{\triangleleft})) \\ &= x \cdot (\text{weight}(\triangleleft) \cdot \text{weight}(\cdot) - \text{weight}(\triangleleft) \cdot \text{weight}(\hat{\triangleleft})); \\ \text{weight}(\triangleleft \hat{\triangleleft}) &= x \cdot (\text{weight}(\triangleleft) \cdot \text{weight}(\hat{\triangleleft}) - \text{weight}(\triangleleft \cap \cdot) \cdot \text{weight}(\hat{\triangleleft} \cap \hat{\triangleleft})) \\ &= x \cdot (\text{weight}(\triangleleft) \cdot \text{weight}(\hat{\triangleleft}) - \text{weight}(\triangleleft) \cdot \text{weight}(\hat{\triangleleft} \hat{\triangleleft})). \end{aligned}$$

We have no new variables, so we eliminate the four auxiliary variables

$$\text{weight}(\triangleleft), \text{weight}(\hat{\triangleleft}), \text{weight}(\hat{\triangleleft}), \text{weight}(\hat{\triangleleft} \hat{\triangleleft})$$

from this system of five equations to obtain

$$x^3 \text{weight}(\cdot)^2 - (x^2 - 1)^2 \text{weight}(\cdot) - x(x^2 - 1) = 0.$$

### 3.5.2 Enumerating with respect to a single tree

To prove Theorem 3.1, we make a few modifications in order to compute  $\text{En}_{L,t}(x, y)$  instead of  $\text{Av}_t(x)$ . Again

$$\text{weight}(p) := \sum_{T \in L_p} \text{weight}(T),$$

but now  $\text{weight}(T) = x^{\text{number of vertices in } T} y^{\text{number of copies of } t \text{ in } T}$  for all  $T$ . We modify Equation (3.1) to become

$$\begin{aligned} \text{weight}((p_l p_r)) &= \\ &= x \cdot (\text{weight}(p_l) \cdot \text{weight}(p_r) + (y - 1) \cdot \text{weight}(p_l \cap t_l) \cdot \text{weight}(p_r \cap t_r)) \quad (3.2) \end{aligned}$$

since in addition to accounting for the trees that avoid  $t$  we also account for those that match  $t$ , in which case  $y$  is contributed.

The rest of the algorithm carries over unchanged, and we obtain a polynomial equation in  $x$ ,  $y$ , and  $\text{En}_{L,t}(x, y) = \text{weight}(L)$ .

### 3.5.3 Enumerating with respect to multiple trees

A more general question is the following. Given several binary tree patterns  $p_1, \dots, p_k$ , what is the number  $a_{n_0, n_1, \dots, n_k}$  of binary trees containing precisely  $n_0$  vertices,  $n_1$  copies of  $p_1, \dots, n_k$  copies of  $p_k$ ? We consider the enumerating generating function

$$\begin{aligned} \text{En}_{L, p_1, \dots, p_k}(x_L, x_{p_1}, \dots, x_{p_k}) &= \sum_T x_L^{\alpha_0} x_{p_1}^{\alpha_1} \cdots x_{p_k}^{\alpha_k} \\ &= \sum_{n_0=0}^{\infty} \sum_{n_1=0}^{\infty} \cdots \sum_{n_k=0}^{\infty} a_{n_0, n_1, \dots, n_k} x_L^{n_0} x_{p_1}^{n_1} \cdots x_{p_k}^{n_k}, \end{aligned}$$

where  $p_0 = L$  and  $\alpha_i$  is the number of copies of  $p_i$  in  $T$ . (We need not assume that the  $p_i$  are distinct.) This generating function can be used to obtain information about how correlated a family of tree patterns is. We have the following generalization of Theorem 3.1.

**Theorem 3.3.**  $\text{En}_{L, p_1, \dots, p_k}(x_L, x_{p_1}, \dots, x_{p_k})$  is algebraic.

Keeping track of multiple tree patterns  $p_1, \dots, p_k$  is not much more complicated than handling a single pattern, and the algorithm for doing so has the same outline.

Let

$$\text{weight}(p) := \sum_{T \in L_p} \text{weight}(T)$$

with

$$\text{weight}(T) = x_L^{\alpha_0} x_{p_1}^{\alpha_1} \cdots x_{p_k}^{\alpha_k},$$

where  $\alpha_i$  is the number of copies of  $p_i$  in  $T$ . Let  $d = \max_{1 \leq i \leq k} \text{depth}(p_i)$ . First we describe what to do with each new variable  $\text{weight}(q)$  that arises. The approach used is different than that for one tree pattern; in particular, we do not make use of intersections. Consequently, it is less efficient.

Let  $l$  be the number of leaves in  $q$ . If  $T$  is a tree matching  $q$ , then for each leaf  $L$  of  $q$  there are two possibilities: Either  $L$  is matched by a terminal vertex  $()$  in  $T$ , or  $L$  is matched by a tree matching  $(LL)$ . For each leaf we make this choice independently, thus partitioning the language  $L_q$  into  $2^l$  disjoint sets represented by  $2^l$  tree patterns that are disjoint in the sense that each tree matching  $q$  matches precisely one of these

patterns. For example, partitioning the pattern  $(LL)$  into  $2^2$  patterns gives

$$\begin{aligned} \text{weight}((LL)) &= \text{weight}((())()) + \text{weight}((())(LL)) \\ &\quad + \text{weight}(((LL)())) + \text{weight}(((LL)(LL))). \end{aligned}$$

We need an analogue of Equation (3.2) for splitting a pattern  $(p_l p_r)$  into the two subpatterns  $p_l$  and  $p_r$ . For this, examine each of the  $2^l$  patterns that arose in partitioning  $q$ . For each pattern  $p = (p_l p_r)$  whose language is infinite (that is, the word  $p$  contains the symbol  $L$ ) and has  $\text{depth}(p) \geq d$ , rewrite

$$\text{weight}(p) = \text{weight}(p_l) \cdot \text{weight}(p_r) \cdot \prod_{\substack{0 \leq i \leq k \\ p \text{ matches } p_i}} x_{p_i},$$

where ‘ $p$  matches  $p_i$ ’ means that every tree in  $L_p$  matches  $p_i$  (so  $L_p \subset L_{p_i}$ ). If  $p$  has an infinite language but  $\text{depth}(p) < d$ , keep  $\text{weight}(p)$  intact as a variable.

Finally, for all tree patterns  $p$  whose language is finite (i.e.,  $p$  is a tree), rewrite

$$\text{weight}(p) = \prod_{0 \leq i \leq k} x_{p_i}^{\text{number of copies of } p_i \text{ in } p}.$$

The algorithm is as follows. As before, begin with the equation

$$\text{weight}(L) = \text{weight}(( )) + \text{weight}((LL)).$$

At each step, take each new variable  $\text{weight}(q)$  and obtain another equation by performing the procedure described: Write it as the sum of  $2^l$  other variables, split the designated patterns into subpatterns, and explicitly compute the weights of any trees appearing. Continue in this manner until there are no new variables produced; this must happen because we break up  $\text{weight}(p)$  whenever  $\text{depth}(p) \geq d$ , so there are only finitely many possible variables. Eliminate from this system of polynomial equations all but the  $k + 2$  variables  $\text{weight}(( )) = x_L$ ,  $x_{p_1}, \dots, x_{p_k}$ , and  $\text{weight}(L) = \text{En}_{L, p_1, \dots, p_k}(x_L, x_{p_1}, \dots, x_{p_k})$  to obtain a polynomial equation satisfied by  $\text{weight}(L)$ .

### 3.6 Replacement bijections

In this section we address the question of providing systematic bijective proofs of avoiding-equivalence. Given two equivalent binary tree patterns  $s$  and  $t$ , we would

like to produce an explicit bijection between binary trees avoiding  $s$  and binary trees avoiding  $t$ . It turns out that this can often be achieved by structural replacements on trees. We start by describing an example in full, and later generalize.

### 3.6.1 An example replacement bijection

Consider the trees

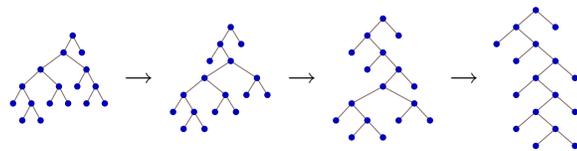
$$t_2 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \quad \text{and} \quad t_3 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

in class 4.2. The idea is that since  $n$ -leaf trees avoiding  $t_2$  are in bijection to  $n$ -leaf trees avoiding  $t_3$ , then somehow swapping all occurrences of these tree patterns should produce a bijection. However, since the patterns may overlap, it is necessary to specify an order in which to perform the replacements. A natural order is to start with the root and work down the tree. More precisely, a *top-down replacement* is a restructuring of a tree  $T$  in which we iteratively apply a set of transformation rules to subtrees of  $T$ , working downward from the root.

Take the replacement rule to be

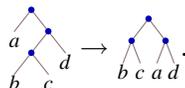
$$\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ a \quad b \quad c \quad d \end{array} \rightarrow \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ a \quad b \quad d \quad c \end{array}$$

where the variables represent trees attached at the leaves, rearranged according to the permutation 3124. (Most permutations are not viable; we discuss this in the next section.) Begin at the root: If  $T$  itself matches the left side of the rule, then we restructure  $T$  according to the rule; if not, we leave  $T$  unchanged. Then we repeat the procedure on the root's (new) children, then on their children, etc., so that each vertex in the tree is taken to be the root of a subtree which is possibly transformed by the rule. For example,



shows the three replacements required to compute the image (on the right) of the left tree via two intermediate trees.

This top-down replacement is invertible. The inverse map is a *bottom-up replacement* with the inverse replacement rule,



Rather than starting at the root and working down the tree, start at the leaves and work up the tree.

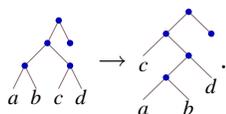
We now show that the top-down replacement is in fact a bijection from trees avoiding  $t_2$  to trees avoiding  $t_3$ . It turns out to be the same bijection given in Section 3.3.4 via words in  $\{0, 1\}^{n-2}$ .

Assume  $T$  avoids  $t_2$ ; we show that the image of  $T$  under the top-down replacement avoids  $t_3$ . It is helpful to think of  $T$  as broken up into (possibly overlapping) “spheres of influence” — subtrees which are maximal with respect to the replacement rule in the sense that performing the top-down replacement on the subtree does not introduce instances of the relevant tree patterns containing vertices outside of the subtree. It suffices to consider each sphere of influence separately. A natural focal point for each sphere of influence is the highest occurrence of  $t_3$ . We verify that restructuring this  $t_3$  to  $t_2$  under the top-down replacement produces no  $t_3$  above, at, or below the root of the new  $t_2$  in the image of  $T$ .

above: Since  $t_3$  has depth 2,  $t_3$  can occur at most one level above the root of the new  $t_2$  while overlapping it. Thus it suffices to consider all subtrees with  $t_3$  occurring at level 1. There are two cases,



The first case does not avoid  $t_2$ , so it does not occur in  $T$ . The second case may occur in  $T$ . However, we do not want the subtree itself to match  $t_3$  (because we assume that the  $t_3$  at level 1 is the highest  $t_3$  in this sphere of influence), so we must have  $e = ()$ . Thus this subtree is transformed by the top-down replacement as





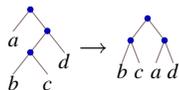
**Conjecture 3.4.** *Two binary tree patterns  $s$  and  $t$  are equivalent if and only if there is a sequence of top-down replacements, bottom-up replacements, and left-right reflections that produces a bijection from binary trees avoiding  $s$  to binary trees avoiding  $t$ .*

In this section we discuss qualitative results regarding this conjecture.

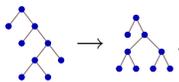
Given two  $m$ -leaf tree patterns  $s$  and  $t$ , one can ask which permutations of the leaves give rise to a top-down replacement that induces a bijection from trees avoiding  $s$  to trees avoiding  $t$ . Candidate permutations can be found experimentally by simply testing all  $m!$  permutations of leaves on a set of randomly chosen binary trees avoiding  $s$ ; one checks that the image avoids  $t$  and that composing the top-down replacement with the inverse bottom-up replacement produces the original tree. This approach is feasible for small  $m$ , but it is slow and does not provide any insight into why certain trees are equivalent. A question unresolved at present is to efficiently find all such bijections. The naive method was used to find the examples in this section.

Once a candidate bijection is found, it can be proved in a manner similar to Section 3.6.1. Although we do not attempt here to fully generalize that argument, the following two examples provide an indication of the issues encountered in the ‘above’ and ‘below’ cases of the general setting.

As an example of what can go wrong in the ‘above’ case, consider the replacement rule



given by the permutation 2314 on 4-leaf binary trees  $s = t_3$  and  $t = t_2$ . This rule does not induce a top-down replacement bijection from trees avoiding  $t_3$  to trees avoiding  $t_2$ . One obstruction is the mapping

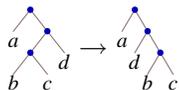


The initial tree avoids  $t_3$ . However, it contains  $t_2$ , and replacing this  $t_2$  with  $t_3$  completes another  $t_2$ . The final tree does not avoid  $t_2$ .

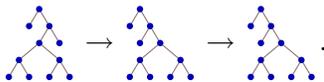
In general, for the ‘above’ case it suffices to check all trees avoiding  $s$  of a certain depth where the highest  $t$  begins at level  $\text{depth}(t) - 1$ . A bound on the depth is

possible since for a given set of replacement rules there is a maximum depth at which the structure of a subtree can affect the top  $\text{depth}(t) + 1$  levels of the image. If, after performing the top-down replacement on these trees, no  $t$  appears above level  $\text{depth}(t) - 1$ , then  $t$  can never appear above the root of the highest  $t$  in the subtree.

An example of what can go wrong in the ‘below’ case is provided by the rule



given by the permutation 1423 on 4-leaf binary trees  $s = t_1$  and  $t = t_2$ . This rule does not induce a top-down replacement bijection from trees avoiding  $t_1$  to trees avoiding  $t_2$ . (Indeed, these trees are not equivalent.) One obstruction is the mapping



The initial tree avoids  $t_1$ . However, it matches  $t_2$ , and replacing this  $t_2$  with  $t_1$  produces a copy of the intersection  $t_1 \cap t_2$  in the intermediate step. The  $t_2$  is then replaced by  $t_1$ , but this does not change the tree because  $t_1 \cap t_2$  is fixed by the rule. Therefore the final tree does not avoid  $t_2$ .

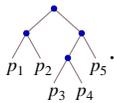
A general proof for the ‘below’ case must take into account all ways of producing, below the root of the highest  $t$  in a subtree, a copy  $t$  of that is not broken by further replacements.

We now return briefly to the replacement rule of Section 3.6.1 to mention that a minor modification produces a bijection on the full set of binary trees. Namely, take the two replacement rules

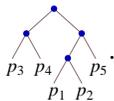


Again we perform a top-down replacement, now using both rules together. That is, if a subtree matches the left side of either rule, we restructure it according to that rule. Of course, it can happen that a particular subtree matches both replacement rules, resulting in potential ambiguity; in this case which do we apply? Well, if both rules result in the same transformation, then it does not matter, and indeed with our present example this is the case. To show this, it suffices to take the intersection  $t_2 \cap t_3$  of the

two left sides and label the leaves to represent additional branches that may be present:



Now we check that applying each of the two replacement rules to this tree produces the same labeled tree, namely



Therefore we need not concern ourselves with which rule is applied to a given subtree that matches both. Since the replacement rules agree on their intersection, the top-down replacement is again invertible and is therefore a bijection from the set of binary trees to itself. By the examination of cases in the previous section, this bijection is an extension of the bijection between binary trees avoiding  $t_2$  and binary trees avoiding  $t_3$ .

Thus we may choose from two types of bijection when searching for top-down replacement bijections that prove avoiding-equivalence. The first type is from binary trees avoiding  $s$  to binary trees avoiding  $t$ , using one rule for the top-down direction and the inverse for the bottom-up direction; these bijections in general do not extend to bijections on the full set of binary trees. The second type is a bijection on the full set of binary trees, using both rules in each direction, that induces a bijection from binary trees avoiding  $s$  to binary trees avoiding  $t$ .

Empirically, each two-rule bijection that proves avoiding-equivalence for  $s$  and  $t$  induces a one-rule bijection proving this equivalence, as in the previous example. However, not all two-rule bijections, when restricted to one rule, become bijections that prove avoiding-equivalence; the rules used to discuss the ‘above’ and ‘below’ cases in this section are two counterexamples.

One benefit to searching for two-rule bijections is that requiring the two replacement rules to agree on the leaf-labeled intersection  $s \cap t$  quickly prunes the set of candidate permutations. There is a tradeoff, however, because verifying a two-rule bijection is more complicated than verifying a one-rule bijection.

Searching for two-rule bijections on 4-leaf binary tree patterns, one finds only the rules given by the permutation 3124 for  $s = t_2$  and  $t = t_3$ , mentioned above, and their

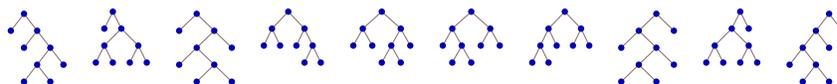
	$t_2$	$t_3$	$t_4$	$t_6$	$t_7$	$t_8$	$t_9$	$t_{11}$	$t_{12}$	$t_{13}$
$t_2$	—	14235		43125						
$t_3$		—	12534	31245					51234	
$t_4$		12453	—			41235				
$t_6$				—	12534	45123				
$t_7$				12453	—		45123			
$t_8$				34512		—	31245			
$t_9$					34512	23145	—			
$t_{11}$					13452			—	31245	
$t_{12}$		23451					12453	23145	—	
$t_{13}$							14532		13425	—

Table 3.1: Leaf permutations whose two-rule replacements prove avoiding-equivalence for pairs of trees in class 5.2.

left–right reflections, given by 1342 for  $s = t_4$  and  $t = t_3$ . (Note the asymmetry here: There is a top–down replacement bijection from trees avoiding  $t_2$  to trees avoiding  $t_3$  but not vice versa.)

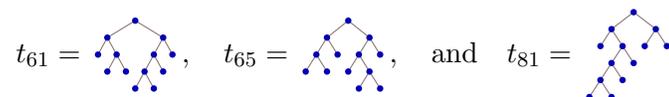
However, this does not account for all top–down replacement bijections for these patterns. The permutation 3142 for  $s = t_2$  and  $t = t_3$  and its left–right reflection 3142 for  $s = t_4$  and  $t = t_3$  provide one–rule bijections that do not extend to all binary trees.

Among equivalence classes of 5–leaf binary tree patterns, class 5.2 is the only class containing nontrivial equivalences. It consists of the ten trees  $t_2, t_3, t_4, t_6, t_7, t_8, t_9, t_{11}, t_{12}$ , and  $t_{13}$ , pictured as follows.



For each pair of trees in this class, Table 3.1 lists the leaf permutations that prove equivalence by a two–rule top–down replacement. It happens that there is at most one permutation for each pair in this class, although in general there may be more.

With this data, one might suspect that two–rule replacement bijections are sufficient to establish every equivalence class of binary tree patterns. In fact they are not. The smallest counterexample is class 7.15, which consists of the three trees



and their left–right reflections. Trees  $t_{81}$  and  $t_{61}$  are equivalent by the permutation 1456723, but no permutation of leaves produces a two-rule replacement bijection that establishes the equivalence of  $t_{65}$  to one of the others. However, the permutations 4561237 and 4571236 provide candidate one-rule bijections for  $t_{65}$  and  $t_{61}$ , and 2341675 provides a candidate bijection for  $t_{65}$  and  $t_{81}$ .

We conclude with a curious example in which two tree patterns can only be proven equivalent by a two-rule bijection that does not involve them directly. The trees

$$t_7 = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \quad \text{and} \quad t_{11} = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

in class 6.5 are avoiding-equivalent by the permutation 126345, but neither

$$t_{17} = \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

nor its left–right reflection has an equivalence-proving permutation to  $t_7$ ,  $t_{11}$ , or their left–right reflections. Thus, this equivalence cannot be established by a bijection that swaps 6-leaf tree patterns. However, it can be established by a bijection that swaps 4-leaf tree patterns: The previously mentioned bijection consisting of the two replacement rules

$$\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ a \quad b \quad c \quad d \end{array} \rightarrow \begin{array}{c} \bullet \\ / \quad \backslash \\ c \quad \bullet \\ / \quad \backslash \\ a \quad b \quad d \end{array} \quad \text{and} \quad \begin{array}{c} \bullet \\ / \quad \backslash \\ a \quad \bullet \\ / \quad \backslash \\ b \quad c \quad d \end{array} \rightarrow \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ b \quad c \quad a \quad d \end{array},$$

induces a top-down replacement bijection from trees avoiding  $t_7$  to trees avoiding  $t_{17}$ . The reason is that  $t_7$  and  $t_{17}$  are formed by two overlapping copies of the class 4.2 trees

$$\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array} \quad \text{and} \quad \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}$$

respectively, and that  $t_7$  and  $t_{17}$  are mapped to each other under this bijection.

## Appendix. Table of equivalence classes

Here we list equivalence classes of binary trees with at most 7 leaves. Left–right reflections are omitted for compactness. For each class we provide a polynomial equation satisfied by  $f = \text{En}_{L,t}(x, y)$ ; an equation satisfied by  $\text{Av}_t(x)$  is obtained in each case by letting  $y = 0$ . These equations were computed in *Mathematica* and *Singular* using the packages `TREEPATTERNS` [27] and `SINGULAR` [18]. `TREEPATTERNS` contains additional pre-computed data extended to 8-leaf binary trees. The number of equivalence classes of  $m$ -leaf binary trees for  $m = 1, 2, 3, \dots$  is  $1, 1, 1, 2, 3, 7, 15, 44, \dots$

### Class 1.1 (1 tree)



$$xyf^2 - f + xy = 0$$

### Class 2.1 (1 tree)



$$xyf^2 - f + x = 0$$

### Class 3.1 (2 trees)



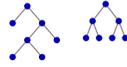
$$xyf^2 + (-x^2(y-1) - 1)f + x = 0$$

### Class 4.1 (2 trees)



$$(xy - x^3(y-1))f^2 + (-x^2(y-1) - 1)f + x = 0$$

**Class 4.2** (3 trees)



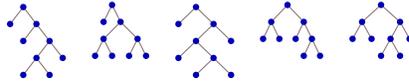
$$xyf^2 + (-2x^2(y-1) - 1)f + (x^3(y-1) + x) = 0$$

**Class 5.1** (2 trees)



$$-x^4(y-1)f^3 + (xy - x^3(y-1))f^2 + (-x^2(y-1) - 1)f + x = 0$$

**Class 5.2** (10 trees)



$$(xy - x^3(y-1))f^2 + (x^2(x^2 - 2)(y-1) - 1)f + (x^3(y-1) + x) = 0$$

**Class 5.3** (2 trees)



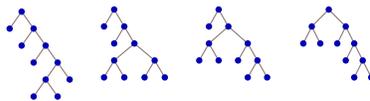
$$xyf^3 + (-3x^2(y-1) - 1)f^2 + (3x^3(y-1) + x)f - x^4(y-1) = 0$$

**Class 6.1** (2 trees)

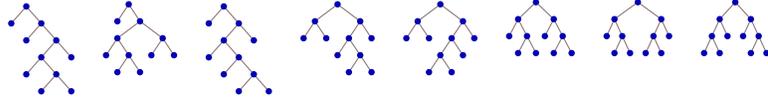


$$-x^5(y-1)f^4 - x^4(y-1)f^3 + (xy - x^3(y-1))f^2 + (-x^2(y-1) - 1)f + x = 0$$

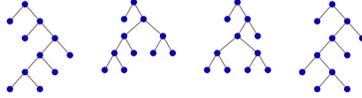
**Class 6.2** (8 trees)



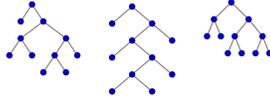
$$-x^4(y-1)f^3 + x(x^2(x^2 - 1)(y-1) + y)f^2 + (x^2(x^2 - 2)(y-1) - 1)f + (x^3(y-1) + x) = 0$$

**Class 6.3** (14 trees)

$$x(x^2(x^2-2)(y-1)+y)f^2 + (2x^2(x^2-1)(y-1)-1)f + (x^3(y-1)+x) = 0$$

**Class 6.4** (8 trees)

$$(xy - x^3(y-1))f^3 + (x^2(2x^2-3)(y-1)-1)f^2 + (-x^5(y-1) + 3x^3(y-1) + x)f - x^4(y-1) = 0$$

**Class 6.5** (6 trees)

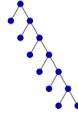
$$(xy - 2x^3(y-1))f^2 + (x^2(3x^2-2)(y-1)-1)f + (-x^5(y-1) + x^3(y-1) + x) = 0$$

**Class 6.6** (2 trees)

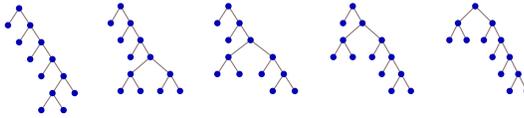
$$-xyf^4 + (4x^2(y-1)+1)f^3 + (-6x^3(y-1)-x)f^2 + 4x^4(y-1)f - x^5(y-1) = 0$$

**Class 6.7** (2 trees)

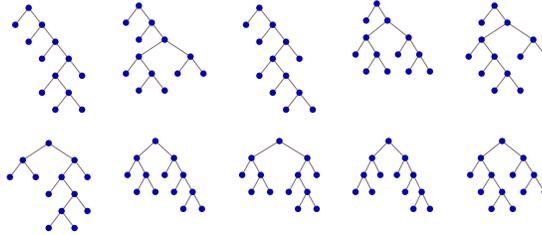
$$x^4(x^2(y-1)-y)(y-1)f^3 + (-2x^7(y-1)^2 + x^5(y-1)(3y-2) - x^3(y-1) + xy)f^2 + (x^2(x^6(y-1) - 3x^4(y-1) + x^2 - 2)(y-1) - 1)f + (x^7(y-1)^2 + x^3(y-1) + x) = 0$$

**Class 7.1** (2 trees)

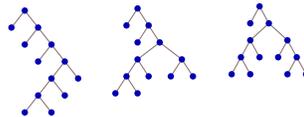
$$-x^6(y-1)f^5 - x^5(y-1)f^4 - x^4(y-1)f^3 + (xy - x^3(y-1))f^2 + (-x^2(y-1) - 1)f + x = 0$$

**Class 7.2** (10 trees)

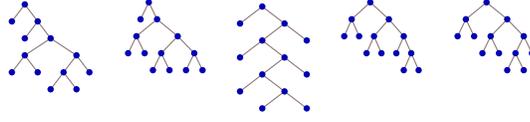
$$-x^5(y-1)f^4 + x^4(x^2-1)(y-1)f^3 + x((x^2-1)x^2(y-1) + y)f^2 + (x^2(x^2-2)(y-1) - 1)f + (x^3(y-1) + x) = 0$$

**Class 7.3** (20 trees)

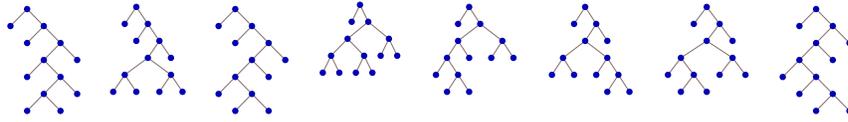
$$x^4(x^2-1)(y-1)f^3 + x(2(x^2-1)x^2(y-1) + y)f^2 + (2x^2(x^2-1)(y-1) - 1)f + (x^3(y-1) + x) = 0$$

**Class 7.4** (6 trees)

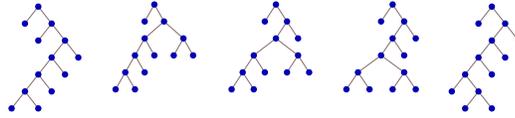
$$-x^4(y-1)f^4 + x((2x^2-1)x^2(y-1) + y)f^3 + (-x^4 - 2x^2 + 3)x^2(y-1) - 1)f^2 + (-x^5(y-1) + 3x^3(y-1) + x)f - x^4(y-1) = 0$$

**Class 7.5** (10 trees)

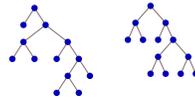
$$\begin{aligned}
 & -x^4(y-1)f^3 + x(2(x^2-1)x^2(y-1)+y)f^2 \\
 & + (-x^4-3x^2+2)x^2(y-1)-1)f + (-x^5(y-1)+x^3(y-1)+x) = 0
 \end{aligned}$$

**Class 7.6** (16 trees)

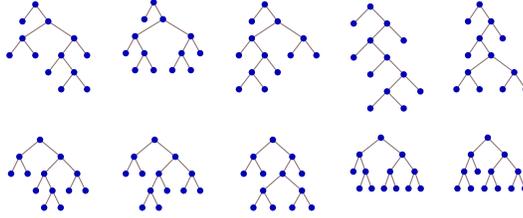
$$\begin{aligned}
 & x((x^2-2)x^2(y-1)+y)f^3 + (-x^4-4x^2+3)x^2(y-1)-1)f^2 \\
 & + (-2x^5(y-1)+3x^3(y-1)+x)f - x^4(y-1) = 0
 \end{aligned}$$

**Class 7.7** (10 trees)

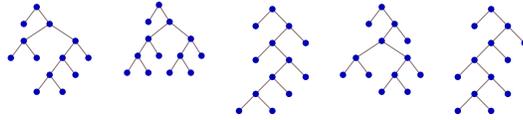
$$\begin{aligned}
 & (x^3(y-1)-xy)f^4 + (1-x^2(3x^2-4)(y-1))f^3 \\
 & + x(3x^2(x^2-2)(y-1)-1)f^2 - x^4(x^2-4)(y-1)f - x^5(y-1) = 0
 \end{aligned}$$

**Class 7.8** (4 trees)

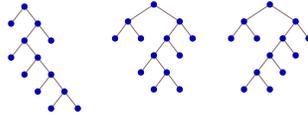
$$\begin{aligned}
 & x^4(y-1)(2x^2(y-1)-y-1)f^3 + (-5x^7(y-1)^2+3x^5(y-1)y-x^3(y-1)+xy)f^2 \\
 & + (x^2(y-1)(4x^6(y-1)+x^4(2-3y)+x^2-2)-1)f \\
 & - x(x^4(y-1)+1)(x^2(x^2-1)(y-1)-1) = 0
 \end{aligned}$$

**Class 7.9** (20 trees)

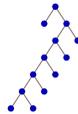
$$x((2x^2 - 3)x^2(y - 1) + y)f^2 + (-x^4 - 4x^2 + 2)x^2(y - 1) - 1)f + (-x^5(y - 1) + x^3(y - 1) + x) = 0$$

**Class 7.10** (10 trees)

$$(xy - 2x^3(y - 1))f^3 + (x^2(5x^2 - 3)(y - 1) - 1)f^2 + (-4x^5(y - 1) + 3x^3(y - 1) + x)f + x^4(x^2 - 1)(y - 1) = 0$$

**Class 7.11** (6 trees)

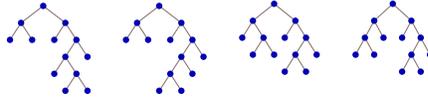
$$(x(x^2 - 1)^3 y - x^3(x^4 - 3x^2 + 3))f^3 + (x^2(3(x^2 - 2)x^2(y - 1) + 3y - 2) + 1)f^2 + x(3x^2(x^2 - 1)(y - 1) - 2)f + (x^4(y - 1) + x^2) = 0$$

**Class 7.12** (2 trees)

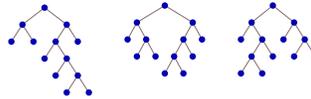
$$xyf^5 + (-5x^2(y - 1) - 1)f^4 + (10x^3(y - 1) + x)f^3 - 10x^4(y - 1)f^2 + 5x^5(y - 1)f - x^6(y - 1) = 0$$

**Class 7.13** (2 trees)

$$\begin{aligned}
& -x^{10}(y-1)^3(x^2(y-1)-y)f^5 + x^5(y-1)(4x^8(y-1)^3 - x^6(y-1)^2(5y-2) + x^2(y-1)(2y-1) - y^2)f^4 \\
& \quad - x^4(y-1)(6x^{10}(y-1)^3 - x^8(y-1)^2(10y-7) + x^4(y-1)(7y-5) + x^2(3-4y)y - y + 1)f^3 \\
& + x(x^2(y-1)(x^2(y-1)(x^2(x^2(x^4(y-1)(4x^2(y-1)-10y+9) + 9y-8) - 6y+2) - 3) - 2) + y)f^2 \\
& \quad + (-x^2(y-1)(x^2(x^2(y-1)(x^2(x^2(y-1)((x^2-5)x^4(y-1)+5) - 4y+3) - 3) - 3) + 2) - 1)f \\
& \quad - x(x^2(y-1)(x^{12}(y-1)^3 - x^8(y-1)^2 + x^6(y-1)^2 + x^4(y-1) + x^2 - 1) - 1) = 0
\end{aligned}$$

**Class 7.14** (8 trees)

$$\begin{aligned}
& (x-1)x^4(x+1)(y-1)((x^2-2)x^2(y-1)+y)f^3 \\
& \quad + x((x-1)(x+1)x^2(y-1)(3(x^2-1)x^2(y-1)+2)+y)f^2 \\
& \quad + ((x-1)x^2(x+1)(y-1)(3x^4(y-1)+2)-1)f + (x^7(y-1)^2 + x^3(y-1) + x) = 0
\end{aligned}$$

**Class 7.15** (6 trees)

$$\begin{aligned}
& x^6(y-1)f^3 + x((x^2-3)x^2(y-1)+y)f^2 \\
& \quad + (2x^2(2x^2-1)(y-1)-1)f + (-x^5(y-1) + x^3(y-1) + x) = 0
\end{aligned}$$

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## Vita

### Eric Rowland

- 2009** Ph.D. in Mathematics, Rutgers University
- 2003** B.A. in Mathematics, University of California Santa Cruz
- 2000** Graduated from Clark High School, Las Vegas, NV.
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- 2009** Graduate assistant, Department of Mathematics, Rutgers University
- 2005–2008** Teaching assistant, Department of Mathematics, Rutgers University
- 2003–2005** Henry C. Torrey graduate assistant, Department of Mathematics, Rutgers University