Notes on Counting Tree Structures

Florian Kalinke

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Contents

1 Introduction

The idea of these notes is to introduce tree counting to computer scientists by combining extraordinary existing expositions, each focusing on a particular subtopic needed, in a consistent fashion. To do so, we let ourselves be guided by the following classical problems in combinatorics.

- Given three distinct dice, what is the probability that their eyes sum to ten?
- How many ways are there of making change for \$1?
- What is the number of necklaces that can be constructed from five beads available in three distinct colors?
- In how many ways can the corners of a square be colored?

- How many trees with a given number of nodes are there?

Indeed, by addressing these questions one by one, we build up to the Pólya enumeration theorem [Pólya, 1937], one of the most powerful results in enumerative combinatorics, and used here to enumerate the number of trees with given node degree. Along the way, we recall generating functions, some group theory, Burnside's lemma, and Otter's dissimilarity characteristic theorem.

The exposition of Pólya's enumeration theorem follows Tucker [1974]. For counting trees, we rely on Harary and Palmer [1973]. Additional helpful resources, besides the ones stated in the main text below, include Riordan [1958], Harary [1969], Shapiro [1973], Judson [2022].

2 Generating functions

Counting objects subject to different properties typically results in sequences. The most powerful way of handling sequences are generating functions. Further applications of generating functions include solving recurrence relations [Graham et al., 1994], number theory [Moser, 1962], and many more [Wilf, 2006].

Generally, an (ordinary) generating function (ogf) in the complex indeterminate z has the form

$$G(z) = g_0 + g_1 z + g_2 z^2 + \cdots = \sum_{n \geq 0} g_n z^n,$$

and we say that $G(z)$ (or G for short) generates the sequence $\langle g_n \rangle$ with (usually) $g_n \in \mathbb{Z}^+ := \{0, 1, 2, \ldots\}$. To refer to the n-th coefficient of G, we write $[z^n]G(z) := g_n$.

As an example, consider the sequence $\langle 1, 1, 1, \ldots \rangle$. Its ogf is

$$1 + z + z^2 + \ldots = \sum_{n \geq 0} z^n = \frac{1}{1-z}, \tag{1}$$

where the second equality holds for $|z| < 1$. We note that throughout these notes, we consider ogfs as formal objects, that is, we do not concern ourselves with questions of their convergence.

Let us illustrate the power of ogfs by solving two classic counting problems.

2.1 Summing dice

The first problem is: Given three distinct dice, what is the probability that their eyes sum to ten?

Let $D(z) = z + z^2 + \ldots + z^6$ be the ogf of a single die. Then,

$$[z^{10}](D(z))^3 = 27.$$

As, of the total of 6^3 possibilities, 27 result in a sum of 10, the probability is $27/6^3 = 1/8$.

Observe that, in general, for any two ogfs $A(z) = \sum_{n\geq 0} a_n z^n$ and $B(z) = \sum_{n\geq 0} b_n z^n$, one has the Cauchy product

$$A(z)B(z) = \sum_{n\geq 0} c_n z^n \text{ with } c_n = \sum_{m=0}^{n} a_m b_{n-m},$$

and it is this product rule that allows us to build complex combinatorial structures (such as the combination of three dice) from simpler structures (a single die).

2.2 Calculating change

Our next problem is: Given change of $1, 5, 10, 25$, and 50 cents, how many ways are there of making change for \$1 = 100 cents?

Notice that the p-th coefficient in $P(z) = \sum_{p\geq 0} z^p$ counts the number of ways of making change of \$$p$ with pennies. Similarly, we can count the number of ways of making change with nickels by $N(z) = \sum_{n\geq 0} z^{5n}$, with dimes by $D(z) = \sum_{d\geq 0} z^{10d}$, with quarters by $Q(z) = \sum_{q\geq 0} z^{25q}$, and with half dollars by $F(z) = \sum_{f\geq 0} z^{50f}$. The number of ways of making change for c cents using the different coins then is given by the c-th coefficient in

$$C(z) = \sum_{p\geq 0} z^p \cdots \sum_{f\geq 0} z^{50f} = \frac{1}{(1-z)(1-z^5)\ldots(1-z^{50})}, \tag{2}$$

where we used that (1) implies that $\sum_{k\geq 0} z^{nk} = 1/(1-z^n)$ for $n \in \mathbb{N} := \{1, 2, \ldots\}$. Now, the number of ways of making change for 100 cents is

$$[z^{100}]C(z) = 292,$$

obtained using Mathematica (see Appendix A).

Let us now take a different perspective. Say that we have a set S of distinct structures, and a weight function $w : S \to \mathbb{Z}^+$. Define the ogf

$$G(z) = \sum_{s\in S} z^{w(s)}.$$

Then $[z^k]G(z) = |\{s \in S : w(s) = k\}|$, that is, the coefficient of z^k yields the number of structures that have weight k.

In the context of making change, $s \in S$ is any combination of coins, and their weight is the amount they allow changing. Formally,

$$C(z) = \sum_{p,n,d,q,f\geq 0} z^{p+5n+10d+25q+50f},$$

matching (2).

3 Burnside's lemma

When counting distinct objects, we should pause a second and think about what we consider "distinct". For example, when we want to count the number of distinct necklaces possible to construct out of five beads available in three colors, the trivial answer of 5^3 overcounts if we consider two necklaces that match up to a rotation as essentially equivalent (see Figure 1). Group actions allow to formalize such symmetries, and Burnside's lemma allows to adjust our counting. We recall the underlying definitions and the result in the following.

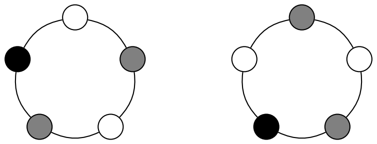

Figure 1: Two essentially equivalent necklaces but both accounted for by the trivial answer.

A group $(G, \circ)$ is a set G together with a binary operation $\circ : G \times G \to G$ such that

1. $\circ$ is associative, that is, $(f \circ g) \circ h = f \circ (g \circ h)$ for all $f, g, h \in G$,
2. there is an identity element, that is, there exists an $\mathrm{id} \in G$ such that $\mathrm{id} \circ g = g \circ \mathrm{id} = g$ for any $g \in G$, and
3. each element has an inverse, that is, for any $g \in G$ there exists a $g^{-1} \in G$ such that $g \circ g^{-1} = g^{-1} \circ g = \mathrm{id}$.

All groups that we consider in the following are assumed to be finite, that is, $|G| < \infty$.

A group $(G, \circ)$ acts on a set S if each $g \in G$ is a function $S \to S$ and

1. $(a \circ b)s = a(b(s))$ for all $a, b \in G$ and any $s \in S$,
2. $\mathrm{id}(s) = s$ for all $s \in S$, where $\mathrm{id} \in G$ is the identity in G.

Notice that if a group G acts on a set S, each $g \in G$ is a permutation of S.

Let the group G act on the set S and $s, t \in S$. If there exists $g \in G$ such that $s = gt \coloneqq g(t)$, s and t are said to be essentially equivalent, and we write $s \sim t$. The notion of "essential equivalence" is, in fact, an equivalence relation on S and thus partitions S. Any such partition of S under G is called an orbit of S under G. To count distinct structures up to essential equivalence, we are therefore interested in counting the number of orbits of S under G.

Lemma 1 (Frobenius, 1887; Burnside, 1897)**.** *Let G be a group acting on the set S and $\chi(g)$ the number of elements fixed by $g \in G$. Then*

$$\frac{1}{|G|} \sum_{g \in G} \chi(g) = \textit{the number of orbits of } S \textit{ under } G.$$

Burnside's lemma allows us to count distinct necklaces appropriately.

3.1 Counting necklaces

Our next challenge is: How many necklaces can be built from five beads having three distinct colors?

Two necklaces are considered equivalent if one can be obtained from the other by a rotation. The group G acting on the set S of 3^5 strings with beads in fixed position is illustrated in Figure 2, thought of as permutations of the labels of the beads a to d.

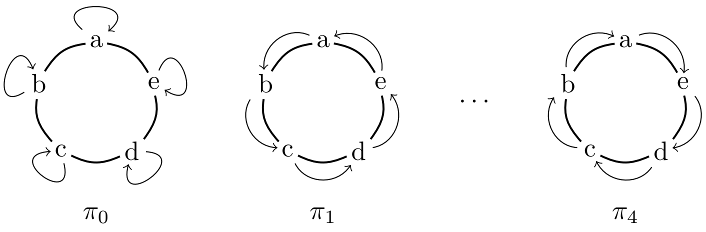

Figure 2: The rotations π_0 through π_4 that act on the necklace.

Employing cycle notation for the permutations, G consists of the motions

$$\pi_0 = \mathrm{id} \qquad \pi_1 = (abcde) \qquad \pi_2 = (acebd) \qquad \pi_3 = (adbec) \qquad \pi_4 = (aedcb),$$

where π_i indicates a counter-clock-wise rotation by i beads. To apply Burnside's lemma, we count the number of necklaces fixed by each π_i. Clearly, π_0 fixes 3^5 necklaces while π_1, π_2, π_3, and π_4 fix 3 necklaces each (those of a single color). From Burnside's lemma, we get that there are $\frac{1}{5}(3^5+3+3+3+3) = 51$ different colorings.

From a formal perspective, we omitted a key conceptual step in the argument above. Notice that, in fact, G acts on the set of beads $X = \{a, b, c, d, e\}$ and not on the set S of 3^5 possible necklaces. Also, the notion of color is missing. As a remedy, let $Y = \{$○, ◍, ●$\}$, and define a coloring of a necklace to be a function $f : X \to Y$. The set of all functions $X \to Y$ is denoted by Y^X and every $f \in Y^X$ is a coloring of a necklace, that is, $|Y^X| = |S| = 3^5$. Two colorings $f, g \in Y^X$ are essentially equivalent if there exists a $\pi \in G$ such that $f(x) = g(\pi(x))$ for all $x \in X$, that is, they are equivalent if permuting the beads by any $\pi \in G$ yields the same coloring. We are then interested in the number of orbits of Y^X under the permutation group $\tilde{G} \coloneqq \{\pi^* : \pi \in G\}$ where $\pi^* : Y^X \to Y^X$ is defined by $f \mapsto f \circ \pi$. Notice that we intuitively employed these permutations above. We return to the explicit perspective when discussing the Pólya enumeration theorem in Section 4.

3.2 Squares with colored corners

Armed with Burnside's lemma: How many 2-colorings of the corners of a square are there up to rotations and reflections?

To answer the question, we start by making the group D_4 of rotations and reflections of a square explicit. Indeed, labeling the corners of the square from a to d, rotations and reflections are described by the group D_4 of permutations

$$\begin{array}{llll} \pi_1 = (a)(b)(c)(d), & \pi_2 = (abcd), & \pi_3 = (ac)(bd), & \pi_4 = (adcb) \\ \pi_5 = (ab)(cd), & \pi_6 = (ad)(bc), & \pi_7 = (a)(c)(bd), & \pi_8 = (ac)(b)(d), \end{array}$$

as also illustrated in Figure 3. We show the set $S = \{C_1, \ldots, C_{16}\}$ of the 4^2 2-colored squares on which D_4 induces the permutation group $\tilde{D}_4$ in Figure 4.

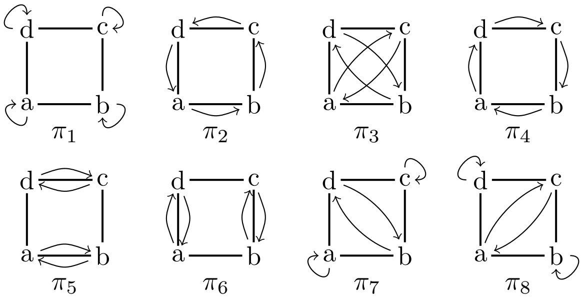

Figure 3: The rotations and reflections of a square.

Two colorings C_i and C_j are essentially equivalent if there exists a permutation $\pi \in D_4$ such that $C_i = \pi^*(C_j)$. Then, to obtain the number of 2-colored squares, we want to find the number of orbits of S under $\tilde{D}_4$, that is, apply Burnside's lemma.

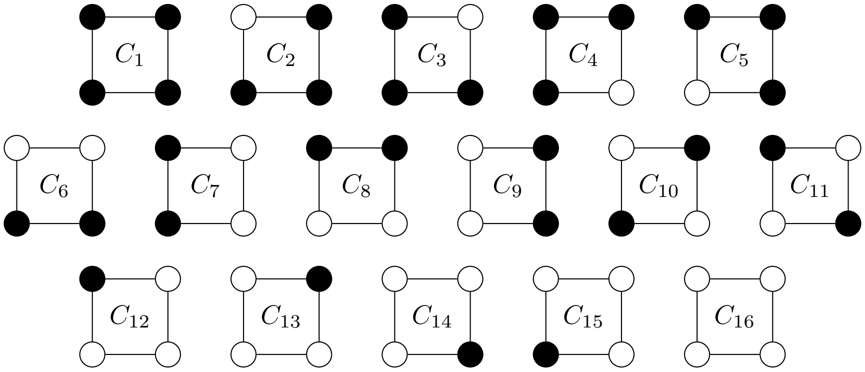

Figure 4: The different colorings of a fixed square.

While possible, obtaining the counts required for Burnside's lemma by enumerating the C_i-s is, in fact, not strictly needed. We can instead infer the number of fixed elements from the cycles of the permutations π_1 through π_8. As an example, consider first π_1, which has 4 cycles. As we can color any corner independently of the others, π_1 fixes all $2^4 = 16$ colorings. π_2 has 1 cycle and coloring any one of the corners prescribes the color of all the other corners; the permutation fixes 2^1 colorings. Similar reasoning shows that π_3, which has 2 cycles, fixes colorings where the color of a equals that of c and the color of b equals that of d; hence, we have $2^2 = 4$ fixed colorings.

We encode a permutation's cycle information in its cycle structure representation

$$z_1^{n_1} z_2^{n_2} \dots z_r^{n_r},$$

where n_i is the number of i-cycles, the number of cycles of length i. Notice that $n_1 + 2n_2 + \dots + kn_k =$ number of corners. Summing the cycle structure representations of all π_i-s, simplifying, and dividing by $|D_4| = 8$, we obtain the cycle index of the group D_4

$$Z(D_4; z_1, z_2, z_3, z_4) = \frac{1}{8}\left(z_1^4 + 2z_4^2 + 3z_2^2 + 2z_1^2 z_2^1\right),$$

and the number of 2-colorings is $Z(D_4; 2, 2, 2, 2) = 6$.[1] The cycle index of the group G also yields the number of m colorings by $Z(D_4; m, m, m, m)$.

The famous Pólya enumeration theorem permits extracting even more information from a group's cycle index.

4 Pólya's enumeration theorem

We now ask a more fine-grained question about the colorings of a square: How many colorings with a given number of black and white beads are there if we identify colorings as essentially equivalent that match up to rotations and reflections?

With our current tools, a direct answer to this question is readily obtained by considering the subsets of $S = \{C_1, \dots, C_{16}\}$ that collect colorings with a given number of white beads. Indeed, let $S_0 = \{C_1\}$, $S_1 = \{C_2, \dots, C_5\}$, $S_2 = \{C_6, \dots, C_{11}\}$, $S_3 = \{C_{12}, \dots, C_{15}\}$, and $S_4 = \{C_{16}\}$. Applying Burnside's lemma with $\tilde{D}_4$ acting on these subsets (or by inspecting Figure 4) and summing the solutions, we obtain the configuration counting series

$$b^4 + b^3 w + 2b^2 w^2 + b w^3 + w^4, \tag{3}$$

where the coefficient of $b^{4-i} w^i$ counts colorings with i white beads and $4 - i$ black beads, that is, $b^{4-i} w^i$ results from applying Burnside's lemma to S_i.

Enumerating the necessary subsets of S and repeatedly applying Burnside's lemma is cumbersome and we now obtain a more efficient solution. Again encoding by $w^i b^{4-i}$ the number of white and black beads, we associate to each $\pi \in D_4$ the colorings that it fixes. As an example, π_2 fixes C_1 and C_{16}, which we encode as $b^4 + w^4$. π_3 fixes C_1 (encoded as b^4), C_{10} and C_{11} (encoded as $2b^2 w^2$), and C_{16} (encoded as w^4). Adding these up, the fixed configurations of π_3 are summarized by $b^4 + 2b^2 w^2 + w^4$.

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[1] The 'Z' comes from *Zyklenzeiger*, the German word for cycle index.

$\pi \in D_4$	Cyc. rep.	Fixed configurations
π_1	z_1^4	$(b+w)^4 = b^4 + 4b^3w + 6b^2w^2 + 4bw^3 + w^4$
π_2	z_4^1	$(b^4+w^4)^1 = b^4 + w^4$
π_3	z_2^2	$(b^2+w^2)^2 = b^4 + 2b^2w^2 + w^4$
π_4	z_4^1	$(b^4+w^4)^1 = b^4 + w^4$
π_5	z_2^2	$(b^2+w^2)^2 = b^4 + 2b^2w^2 + w^4$
π_6	z_2^2	$(b^2+w^2)^2 = b^4 + 2b^2w^2 + w^4$
π_7	$z_1^2z_2^1$	$(b+w)^2(b^2+w^2)^1 = b^4 + 2b^3w + 2b^2w^2 + 2bw^3 + w^4$
π_8	$z_1^2z_2^1$	$(b+w)^2(b^2+w^2)^1 = b^4 + 2b^3w + 2b^2w^2 + 2bw^3 + w^4$

Table 1: Cycle structure representation and fixed configurations of any permutation $\pi \in D_4$.

Table 1 collects, for all $\pi \in D_4$, the cycle structure representation and the fixed configurations. We make two observations. First, summing up all fixed configurations and dividing by 8, we again obtain (3). Second, the cycle index of any permutation corresponds to its fixed configurations upon setting z_j to $b^j + w^j$. Accordingly, we obtain the configuration counting series (3) using

$$Z(D_4; b+w, b^2+w^2, b^3+w^3, b^4+w^4) = b^4 + b^3w + 2b^2w^2 + bw^3 + w^4.$$

For counting the different configurations of a square using three colors, say, black, white, and green, we substitute $z_j = b^j + w^j + g^j$ into Z. Pólya's enumeration theorem answers the general case. We state its simplified version, which suffices for our purposes, after collecting a few notations.

Let $X = \{1, 2, \ldots, n\}$, Y a countable object set with at least two elements, G a group acting on X, and $w : Y \to \mathbb{Z}^+$ a weight function satisfying $|w^{-1}(k)| < \infty$ for all $k \in \mathbb{Z}^+$. Write $c_k = |w^{-1}(k)|$ for the number of "figures" having weight k. The figure counting series is

$$c(z) := \sum_{k=0}^{\infty} c_k z^k$$

and enumerates the elements of Y by weight. The weight of a function $f \in Y^X$ is

$$w(f) := \sum_{x \in X} w(f(x))$$

and functions in the same orbit of $\tilde{G}$ have the same weight. The weight of an orbit F of $\tilde{G}$ is the weight of any $f \in F$. Let C_k be the number of orbits of weight k. The configuration counting series is

$$C(z) := \sum_{k=0}^{\infty} C_k z^k.$$

We are ready to state the main result, which relates $C(z)$ to $c(z)$.

Theorem 1 (Pólya, 1937). *The configuration counting series* $C(z)$ *is determined by substituting for each variable* z_j *in* $Z(G; z_1, z_2, \ldots)$ *the figure counting series* $c(z^j)$*. Symbolically,*

$$C(z) = Z\big(G; c(z), c(z^2), \ldots\big) =: Z(G; c(z)).$$

As an example application, we count again the 2-colorings of a square up to permutations in D_4. Let $X = \{1, 2, 3, 4\}$, $Y = \{\bigcirc, \bullet\}$, $w(\bigcirc) = 0$, and $w(\bullet) = 1$. Then the figure counting series is $c(z) = 1 + z$ and a function $f \in X^Y$ of weight i is a coloring of a square having $4 - i$ white corners and i black corners. Two functions should be identified when they are in the same orbit of $\tilde{D}_4$.[2] Applying Pólya's enumeration theorem, we obtain the configuration counting series

$$C(z) = Z(D_4, 1 + z) = 1 + z + 2z^2 + z^3 + z^4,$$

where the coefficient of z^i gives the number of different configurations having i black corners.

5 Counting trees

We are ready to take on the final question: How many trees with a given number of nodes are there?

Let us first make two types of trees explicit. A free or unrooted tree is a connected undirected acyclic graph with indistinguishable nodes (also called points). A rooted tree is a free tree in which one node is designated as root. Figure 5 illustrates both types.

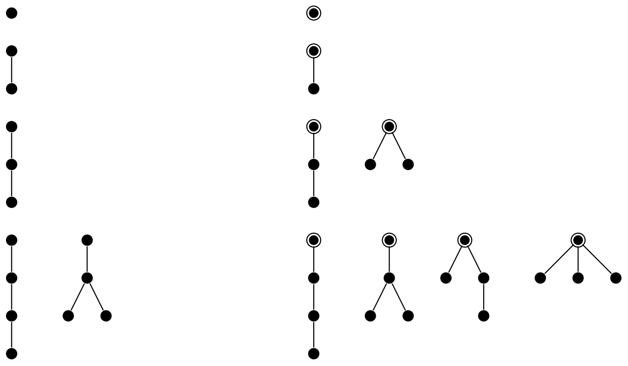

Figure 5: Free trees (left) and rooted trees (right) ordered by node count.

It seems that to count free trees, which is what one intuitively wishes, one must first count rooted trees. The number of rooted trees can then be related to the number of free trees by using Otter's dissimilarity characteristic theorem. We follow this approach in the following.

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[2] Recall that two colorings, which are actually two functions, are essentially equivalent if there exists a permutation in $\tilde{D}_4$ mapping one to the other.

5.1 Rooted trees

To count the number of rooted trees, we first relate the number of rooted trees with root degree d to the number of rooted trees of all root degrees. Indeed, denote by

$$T^d(z) = \sum_{p \geq 1} T_p^d z^p$$

the counting series of rooted trees with root degree d, and by

$$T(z) = \sum_{p \geq 1} T_p z^p$$

the counting series of rooted trees. In other words, the coefficients T_p^d and T_p count the rooted trees of root degree d and rooted trees, respectively.

Figure 6: Combining four rooted trees to a rooted tree with root degree four.

To relate one to the other, notice that as illustrated in Figure 6, every rooted tree of root degree d can be constructed by combining d rooted trees in any order. To count the number of combinations while ignoring the order, let $X = \{1, \ldots, d\}$ and Y the set of all rooted trees. A rooted tree with root degree d is then a function $f \in Y^X$, and two trees are essentially equivalent if there is any permutation π acting on X such that π^* maps one tree to the other. The group of all permutations on X is the symmetric group S_d. Hence, by Pólya's enumeration theorem, we obtain that the coefficient of z^p in

$$T^d(z) = Z(S_d; T(z))$$

is the number of rooted trees with root degree d and $p+1$ points. Multiplying by z corrects this offset and by summing over all T^d-s, we obtain $T(z)$. Formally,

$$T(z) = z \sum_{d \geq 0} Z(S_d; T(z)).$$

Using the identity

$$\sum_{d \geq 0} Z(S_d; f(z)) = \exp\left\{ \sum_{k \geq 1} f\left(z^k\right)/k \right\},$$

we have proved the following result.

Theorem 2. *The configuration counting series $T(z)$ for rooted trees satisfies*

$$T(z) = z \exp\left\{\sum_{k=1}^{\infty} T\left(z^k\right)/k\right\}.$$

The first few terms of $T(z)$ are given by

$$T(z) = z + z^2 + 2z^3 + 4z^4 + \cdots .$$

The coefficients match the counts on the r.h.s. of Figure 5.

We are ready to relate rooted trees to unrooted trees.

5.2 Unrooted trees

To state the key theorems needed to obtain our final result, let us recall a few definitions.

An automorphism of a tree is an isomorphism of a tree with itself. Two points a and b of a tree are similar if there is an automorphism sending a to b; similarity of two lines is defined analogously. The set of all automorphisms of a tree is a permutation group and hence similarity is an equivalence relation. The number of dissimilar points p^* or lines q^* is the number of equivalence classes of points or lines, respectively. A symmetry line s joins two similar points and it is clear that every tree has either no or one symmetry line. We illustrate these definitions in Figure 7.

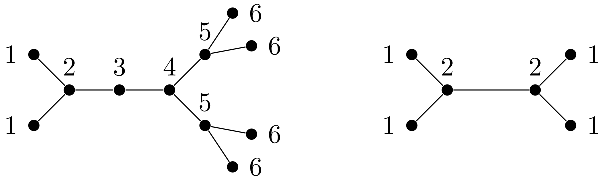

Figure 7: Two trees and the equivalence classes of their points. The left tree has no symmetry line while the right tree has a symmetry line.

The following result relates those quantities.

Theorem 3 (Otter, 1948)**.** *The number s of symmetry lines of any tree is* 0 *or* 1 *and*

$$p^* - (q^* - s) = 1. \tag{4}$$

We also require another result of Pólya, counting one-to-one functions.

Theorem 4 (Pólya 1937)**.** *The generating function $C(z)$ that enumerates one-to-one functions from n indistinguishable elements into a collection of objects with figure counting series $c(z)$ is given by*

$$C(z) = Z(A_n; c(z)) - Z(S_n; c(z)) =: Z(A_n - S_n; c(z)),$$

where A_n is the alternating and S_n the symmetric group.

With the preliminaries established, we are ready to derive the counting series

$$t(z) = \sum_{p \geq 1} t_p z^p$$

of the number t_p of unrooted trees with p points.

Indeed, summing (4) over all (unrooted) trees with p points, we obtain

$$\sum 1 = \sum p^* - \sum (q^* - s).$$

Notice that $\sum 1 = t_p$ is the number of trees with p points. Similarly, $\sum p^* = T_p$, as one can root every given tree in p^* ways. Now, write $L_p \coloneqq \sum (q^* - s)$, which is the number of trees with p points rooted at a line which is not a symmetry line. In other words, we have $t_p = T_p - L_p$. Let $L(z) = \sum_{p \geq 1} L_p z^p$. Multiplying the previous equation by z^p and summing over $p \geq 1$, we obtain

$$t(z) = T(z) - L(z).$$

Figure 8: Two rooted trees and the corresponding line-rooted tree.

It remains to express $L(z)$ in terms of $T(z)$. As illustrated in Figure 8, any two different trees can be used to build a tree rooted at a non-symmetry line. Using Theorem 4, we therefore have

$$L(z) = Z(A_2 - S_2; T(z)).$$

The combination of (5.2) and (5.2) yields the following result.

Theorem 5. *The counting series $t(z)$ for unrooted trees is expressed in terms of the counting series of rooted trees $T(z)$ as*

$$t(z) = T(z) - \frac{1}{2}\Big(T^2(z) - T(z^2)\Big).$$

The series $t(z)$ takes the form

$$t(z) = z + z^2 + z^3 + 2z^4 + \cdots,$$

as we anticipated from Figure 5.

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A Mathematica code

To find the ways of making change for $1, we use the following code.

```
Series[1/((1-z)(1-z^5)(1-z^10)(1-z^25)(1-z^50)), {z, 0, 100}]
Coefficient[%, z, 100]
```