COUNTING TANGLEGRAMS WITH SPECIES

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Abstract. A tanglegram is a pair of binary trees with the same set of leaves. We use the theory of combinatorial species to count unlabeled tanglegrams of various kinds.

1. Introduction

A *tanglegram* is a diagram, used in biology to compare phylogenetic trees, consisting of two (usually binary) trees together with a matching of their leaves. Tanglegrams were recently counted by Billey, Konvalinka, and Matsen [4], and we refer to this paper (and their related paper [3]) for references to biological applications. We answer here several questions raised by Billey, Konvalinka, and Matsen, by giving formulas for counting three variations of tanglegrams.

We define a *binary tree* to be a rooted tree in which every vertex has either zero or two children, and in which the leaves (vertices with no children) are labeled but the interior vertices are unlabeled. (See Figure 1.) We also consider the tree with only one (labeled)

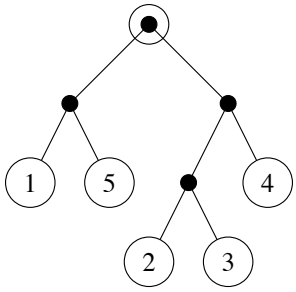

Figure 1. A binary tree

vertex to be a binary tree. The children of an interior vertex are not ordered, so, for example, there is one binary tree with label set $\{1, 2\}$. It is not hard to show that the number of binary trees with label set $[n] = \{1, 2, \ldots, n\}$ is $1 \cdot 3 \cdots (2n-3)$ for $n > 1$ (see, e.g., [12, Example 5.2.6]).

We define a *labeled tanglegram* to be an ordered pair of binary trees with the same set of leaves. Figure 2 shows a labeled tanglegram with three leaves and Figure 3 shows another way of drawing the same tanglegram. Labeled tanglegrams are easy to count: the number of labeled tanglegrams with n leaves is $(1 \cdot 3 \cdots (2n-3))^2$.

An *unlabeled tanglegram* is an isomorphism class of tanglegrams, where two tanglegrams are considered to be isomorphic if one can be obtained from the other by permutation of

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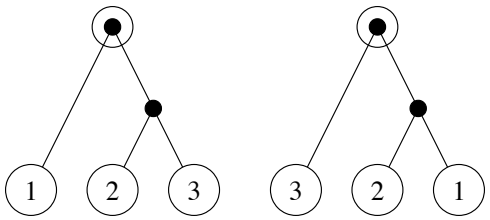

FIGURE 2. A labeled tanglegram with three leaves

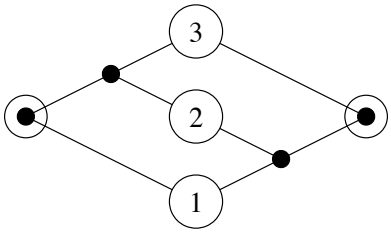

FIGURE 3. Another representation of the tanglegram of Figure 2

the labels. Billey, Konvalinka, and Matsen [4] proved a formula for the number of unlabeled tanglegrams with n leaves. They left open the problem of counting several variations of unlabeled tanglegrams: unordered tanglegrams, unrooted tanglegrams, and unordered unrooted tanglegrams. An *unordered tanglegram* is an *unordered* pair of binary trees (not necessarily distinct) with the same set of leaves and an *unrooted tanglegram* is an ordered pair of unrooted trees with the same set of leaves (vertices of degree one), in which every vertex of each tree has degree one or three, and only the leaves are labeled. (See Figure 4.)

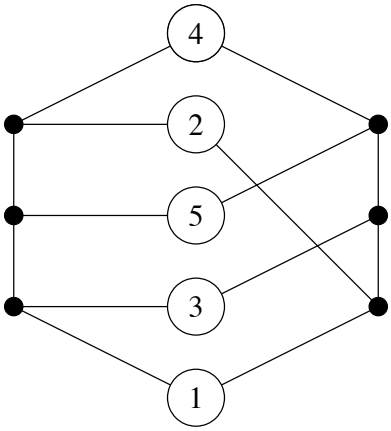

FIGURE 4. An unrooted tanglegram with five leaves

2. SPECIES

The theory of combinatorial species, initiated by André Joyal [8, 9], allows us to construct combinatorial objects in ways that enable us to count various types of tanglegrams. We give

here a very brief account of part of the theory; we refer the reader to Bergeron, Labelle, and Leroux [2] for a comprehensive exposition. A concise introduction to the theory of species can be found in [7].

A *species* is a functor from the category of finite sets with bijections to itself. A species F associates to each finite set A a finite set $F[A]$, called the set of *F-structures* on A, and associates to each bijection of finite sets $\sigma : A \to B$ a bijection $F[\sigma] : F[A] \to F[B]$. In particular, any bijection $\pi : [n] \to [n]$ yields a bijection $F[\pi] : F[n] \to F[n]$, where $F[n] = F[\{1, 2, \dots, n\}]$, so the symmetric group $\mathfrak{S}_n$ acts on the set $F[n]$. The $\mathfrak{S}_n$-orbits under this action are called *unlabeled* F-structures of order n. To any species F we may associate its *cycle index series* Z_F, a symmetric function defined in terms of the *power sum symmetric functions*[1] $p_i = \sum_j x_j^i$. We define

$$Z_F = Z_F(p_1, p_2, \dots) = \sum_{n \geq 0} \frac{1}{n!} \left(\sum_{\sigma \in \mathfrak{S}_n} \operatorname{fix} F[\sigma] p_\sigma \right), \tag{1}$$

where $\operatorname{fix} F[\sigma] = |\{s \in F[n] : F[\sigma](s) = s\}|$ and $p_\sigma = p_1^{\sigma_1} p_2^{\sigma_2} \dots$, where σ_i is the number of i-cycles of σ. Since $\operatorname{fix} F[\sigma]$ depends only on the cycle type of σ, the cycle index can also be written as

$$Z_F = \sum_{n \geq 0} \left(\sum_{\lambda \vdash n} \operatorname{fix} F[\lambda] \frac{p_\lambda}{z_\lambda} \right).$$

Here the sum $\lambda \vdash n$ is over all partitions $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_k)$ of n, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 1$, $\operatorname{fix} F[\lambda]$ is the number of F-structures on $[n]$ fixed by $F[\sigma]$ where σ is a permutation of $[n]$ with cycle type λ, p_λ is the *power sum symmetric function* indexed by the partition λ of n, defined by $p_\lambda = p_{\lambda_1} p_{\lambda_2} \cdots$, and $n!/z_\lambda$ is the number of permutations in $\mathfrak{S}_n$ of cycle type λ (if λ has m_i parts equal to i for each i then $z_\lambda = 1^{m_1} m_1! \, 2^{m_2} m_2! \cdots$),

For any species F, we denote by $\widetilde{F}(x)$ the ordinary generating function for unlabeled F-structures; that is,

$$\widetilde{F}(x) = \sum_{n=0}^{\infty} f_n x^n \tag{2}$$

where f_n is the number of unlabeled F-structures of order n. Then

$$\begin{aligned} \widetilde{F}(x) &= Z_F(x, x^2, x^3, \dots) \\ &= \sum_{n \geq 0} x^n \left(\sum_{\lambda \vdash n} \frac{\operatorname{fix} F[\lambda]}{z_\lambda} \right). \end{aligned}$$

Equivalently, the number of unlabeled F-structures of order n is $\sum_{\lambda \vdash n} \operatorname{fix} F[\lambda]/z_\lambda$, as can be seen directly by Burnside's lemma (see section 3).

[1] In many accounts of cycle indices our p_i are taken simply as indeterminates. In particular, our p_i is written as x_i in [2].

We note that the sum of the terms of degree n in Z_F form the "characteristic" or "Frobenius image" of the representation of $\mathfrak{S}_n$ associated with the action of $\mathfrak{S}_n$ on $F[n]$ (see, e.g., [12, pp. 351–352 and 395–396]) and all of the operations on species that we discuss have analogues for representations of symmetric groups. This is one of the reasons why we consider cycle indices to be symmetric functions.

One of the most important species is the species E_n of n-sets, defined by

$$E_n[A] = \begin{cases} \{A\}, & \text{if } |A| = n \\ \varnothing, & \text{otherwise.} \end{cases}$$

The cycle index of E_n is the *complete symmetric function* h_n, defined by

$$h_n = \sum_{i_1 \le i_2 \le \cdots \le i_n} x_{i_1} x_{i_2} \cdots x_{i_n},$$

and also given by the formula

$$h_n = \sum_{\lambda \vdash n} \frac{p_\lambda}{z_\lambda}.$$

The special case E_1, the species of *singleton sets*, is denoted by X. It has cycle index $Z_X = p_1$.

Given species F and G we can combine them to get the *sum* $F + G$, the *product* FG, the *composition* $F(G)$ (also denoted $F \circ G$), and the *Cartesian product* $F \times G$, and these operations on species translate into operations on cycle indices. We refer the reader to [2, pp. 1–58] for details about these operations.

For the sum, $(F + G)[A]$ is the disjoint union of $F[A]$ and $G[A]$. An FG-structure on the set A is obtained by partitioning A into disjoint subsets B and C (possibly empty) and taking an F-structure on B and a G-structure on C.

An $F(G)$-structure on the set A is an F-structure of G-structures; more precisely, $F(G)[A]$ is the set of triples (π, α, β), where π is a partition of the set A, α is an F-structure on π, and β is a set of G-structures on the blocks of π. In particular, an $E_n(G)$-structure on A is a partition of A into n blocks, together with a G-structure on each block.

The Cartesian product is defined by $(F \times G)[A] = F[A] \times G[A]$; thus an $F \times G$-structure is a pair of structures on the same set.

The corresponding operations for cycle indices are simple for the sum and product: $Z_{F+G} = Z_F + Z_G$ and $Z_{FG} = Z_F Z_G$. The cycle index operation for composition of species is an operation on symmetric functions called *composition* or *plethysm* (see, e.g., [12, p. 447]). The composition of f and g, denoted by $f[g]$ or $f \circ g$, may be defined by

$$f[g] = f(g(p_1, p_2, p_3, \dots,), g(p_2, p_4, p_6, \dots), \dots);$$

i.e., $f[g]$ is obtained from f by replacing each p_i with $p_i[g] = g(p_i, p_{2i}, p_{3i}, \dots)$. Then $Z_{F(G)} = Z_F[Z_G]$. In particular, since $Z_{E_2} = h_2 = \frac{1}{2}(p_1^2 + p_2)$, we have $Z_{E_2}[g] = \frac{1}{2}(g^2 + p_2[g])$. The cycle index operation corresponding to the Cartesian product on species is an operation on symmetric functions called the *Kronecker product*, *internal product*, or *inner product*. The Kronecker product, denoted by $*$, is defined by $p_\lambda * p_\mu = z_\lambda \delta_{\mu\lambda} p_\lambda$ and linearity, or equivalently,

$$\sum_\lambda a_\lambda \frac{p_\lambda}{z_\lambda} * \sum_\lambda b_\lambda \frac{p_\lambda}{z_\lambda} = \sum_\lambda a_\lambda b_\lambda \frac{p_\lambda}{z_\lambda}.$$

Then $Z_{F \times G} = Z_F * Z_G$.

As is customary in discussing species we will consider isomorphic species to be equal; for example, in equation (3) below the two sides are really isomorphic rather than equal.

3. Tanglegrams

Let R be the species of (rooted) binary trees with labeled leaves and unlabeled internal vertices. A binary tree is either a single labeled vertex or an unlabeled root together with an unordered pair of binary trees. Thus R satisfies the equation

$$R = X + E_2(R), \tag{3}$$

so the cycle index Z_R satisfies

$$Z_R = p_1 + h_2[Z_R]. \tag{4}$$

Terms of Z_R can be computed fairly easily by successive substitution in (4), though there are other ways to compute them that are more efficient. (See, e.g., [10, Corollary D1] and Section 6.) The first few terms of Z_R are

$$p_1 + \left(\frac{1}{2}p_1^2 + \frac{1}{2}p_2\right) + \left(\frac{1}{2}p_1p_2 + \frac{1}{2}p_1^3\right) + \left(\frac{5}{8}p_1^4 + \frac{3}{8}p_2^2 + \frac{3}{4}p_1^2p_2 + \frac{1}{4}p_4\right) + \cdots$$

It is easy to see from (4) that for evey power sum p_n that occurs in Z_R, n is a power of 2. From (4) we can also easily derive the well-known functional equation for the ordinary generating function $\widetilde{R}(x)$ (see [1, A001190])

$$\widetilde{R}(x) = x + \frac{1}{2}(\widetilde{R}(x)^2 + \widetilde{R}(x^2)),$$

but to count tanglegrams, we need the full cycle index.

Now let T be the species of (labeled) tanglegrams. Since a tanglegram is a pair of binary trees with the same set of labels, T is the Cartesian product $R \times R$, so $Z_T = Z_{R\times R} = Z_R * Z_R$. Thus if

$$Z_R = \sum_\lambda r_\lambda \frac{p_\lambda}{z_\lambda}, \tag{5}$$

where the sum is over all partitions λ, then $Z_T = \sum_\lambda r_\lambda^2 p_\lambda / z_\lambda$, and the number of unlabeled tanglegrams with n leaves is

$$\sum_{\lambda\vdash n} \frac{r_\lambda^2}{z_\lambda}. \tag{6}$$

A formula equivalent to (6) was given by Billey, Konvalinka, and Matsen [4, Theorem 1]; we will discuss their result further in Section 6.

A *tangled chain of length* k is a k-tuple of binary trees sharing the same set of leaves. It is clear that the species of tangled chains is the kth Cartesian power of R, so the number of unlabeled tangled chains of length k is

$$\sum_{\lambda\vdash n} \frac{r_\lambda^k}{z_\lambda}, \tag{7}$$

as also shown by Billey, Konvalinka, and Matsen [4, Theorem 3].

It may be noted that (7) is an easy consequences of Burnside's lemma: if a group G acts on a finite set S then the number of orbits is

$$\frac{1}{|G|}\sum_{g\in G} \operatorname{fix} g. \tag{8}$$

To derive (6) from Burnside's lemma, we consider the action of $\mathfrak{S}_n$ on k-tuples of labeled binary trees with leaf set $[n]$. A k-tuple is fixed by a permutation if and only if all its entries are fixed, so the $n!/z_\lambda$ permutations of cycle type λ contribute $(n!/z_\lambda)r_\lambda^k$ to the sum (8). Thus the number of orbits is

$$\frac{1}{n!}\sum_{\lambda\vdash n}\frac{n!}{z_\lambda}r_\lambda^k = \sum_{\lambda\vdash n}\frac{r_\lambda^k}{z_\lambda}.$$

4. Unordered tanglegrams

To count unordered tanglegrams with species, we need another operation on species, *inner plethysm*, that is not as well known as the other operations. Inner plethysm is a kind of composition of species that bears the same relation to the Cartesian product that ordinary composition bears to the ordinary product. It is also closely related to the operation of functorial composition of species introduced in [5] and discussed further in [2, Section 2.2]. The term "inner plethysm" was introduced by D. E. Littlewood [11] for the corresponding operation on symmetric functions, and the species operation was introduced by L. Travis in his Ph. D. thesis [15], and we refer to his thesis for results about inner plethysm not proved here.

There is no standard notation for inner plethysm, so we will introduce the notation $F\{G\}$ for the inner plethysm of species, with the same notation for inner plethysm of symmetric functions. We will define here only the inner plethysm $E_n\{G\}$, which is the only case that we will need: for any finite set A, $E_n\{G\}[A]$ is the set of multisets of size n of elements of $G[A]$. We can define $E_n\{G\}$ in another way: The symmetric group $\mathfrak{S}_n$ acts on the elements of the nth Cartesian power $G^{\times n}[A]$ by permuting the coordinates, and the elements of $E_n\{G\}[A]$ are the orbits under this action. (The functorial composition of species is defined similarly, but with a *set*, rather than a multiset of elements of $G[A]$.)

Inner plethysm of symmetric functions is determined by the following:

(1) for fixed g, the map $f \mapsto f\{g\}$ is a homomorphism from the ring of symmetric functions with the usual product to the ring of symmetric functions with the Kronecker product
(2) For a partition λ of n and an integer k, let λ^k denote the cycle type of the kth power of a permutation with cycle type λ. Then

$$p_k\left\{\sum_{\lambda\vdash n} a_\lambda \frac{p_\lambda}{z_\lambda}\right\} = \sum_{\lambda\vdash n} a_{\lambda^k}\frac{p_\lambda}{z_\lambda}.$$

Travis [15, Theorem 2.12] showed that for any species F and G, we have $Z_{F\{G\}} = Z_F\{Z_G\}$.

It is clear that the species of unordered tanglegrams is $E_2\{R\}$, where R is the species of binary trees. So the cycle index for unordered tanglegrams is $h_2\{Z_R\} = \frac{1}{2}(p_1^2 + p_2)\{Z_R\}$. Thus if $Z_R = \sum_\lambda r_\lambda p_\lambda/z_\lambda$ then the cycle index for unordered tanglegrams is

$$\frac{1}{2}\left(\sum_\lambda r_\lambda^2\frac{p_\lambda}{z_\lambda}\right) + \frac{1}{2}\left(\sum_\lambda r_{\lambda^2}\frac{p_\lambda}{z_\lambda}\right),$$

and we obtain the number of unordered tanglegrams with n leaves by setting each p_λ to 1 in the sum of the terms of degree n. This formula for unordered tanglegrams can also be

derived directly from Burnside's lemma, using the action of $\mathfrak{S}_n \times \mathfrak{S}_2$ on labeled tanglegrams, where $\mathfrak{S}_2$ acts by permuting the entries.

Here are the first few values of the number a_n of unordered tanglegrams with n leaves (see [1, A259114]):

n	1	2	3	4	5	6	7	8	9	10	11
a_n	1	1	2	10	69	807	13048	269221	6660455	191411477	6257905519

Symmetric function computations were done with the help of John Stembridge's Maple package for symmetric functions [13, 14].

Similarly, $E_k\{R\}$ is the species of unordered tangled chains of length k.

5. Unrooted tanglegrams

To find the cycle index for unrooted trees, we use a *dissymmetry theorem*, which reduces the enumeration of unrooted to the enumeration of several types of rooted trees, which can usually be counted by decomposing them. The basic dissymmetry theorem says that if A is a species of unrooted trees of some type, $A^\bullet$ is the species of A-trees rooted at a vertex[2], A^- is the species of A-trees rooted at an edge, and $A^{\bullet-}$ is the species of A-trees rooted at a vertex and incident edge (or equivalently, at a directed edge), then

$$A + A^{\bullet-} = A^\bullet + A^-. \tag{9}$$

We give here a brief sketch of the proof of (9), referring the reader to [2, Section 4.1] for a more detailed discussion. Every tree has a unique "center", which is a vertex or edge that is fixed by every automorphism of the tree. An unrooted tree may be identified with a tree rooted at its center. To prove (9), we describe a bijection, equivariant with respect to the automorphism group of the tree, from the non-center vertices and edges of a tree to pairs consisting of a vertex and an incident edge. If v is a non-center vertex, we pair it with the first edge on the unique path from v to the center (this edge may be the center), and if e is a non-center edge, we pair it with the first vertex on the unique path from e to the center (this vertex may be the center). From the bijection just described, we get a bijection from A-trees rooted at a vertex or edge to A-trees rooted at a center vertex or edge (equivalent to unrooted A-trees) or at a vertex and incident edge.

Now let U be the species of "unrooted binary trees"; that is, unrooted trees in which every vertex has degree one or three, the leaves (vertices of degree one) are labeled, and the internal vertices (of degree three) are unlabeled. (We are not including the tree with one vertex.) First we consider U-trees rooted at an edge e. Removing the edge e and rooting the remaining two trees at the vertices incident with e gives two rooted binary trees. Thus $U^- = E_2(R) = R - X$. Similarly, we can remove the root edge from a U-tree rooted at a vertex and incident edge to obtain a pair of rooted trees, but in this case the rooted trees are ordered, so $U^{\bullet-} = R^2$. Finally, the U-trees rooted at a vertex may be rooted at either an internal vertex or a leaf. The species of U-trees rooted at an internal vertex is $E_3(R)$ and

[2]A tree rooted at a vertex is formally an ordered pair (T, v), where T is a tree and v is a vertex of T. Trees rooted at edges etc. are defined similarly.

the species of U-trees rooted at a leaf is XR, so $U^\bullet = E_3(R) + XR$. Thus (9) gives

$$U + R^2 = E_3(R) + XR + R - X,$$

and we obtain a formula for the cycle index of U,

$$Z_U = h_3[Z_R] + p_1 Z_R + Z_R - Z_R^2 - p_1$$

The first few terms of Z_U are

$$\left(\frac{1}{2}p_1^2 + \frac{1}{2}p_2\right) + \left(\frac{1}{2}p_1p_2 + \frac{1}{6}p_1^3 + \frac{1}{3}p_3\right) + \left(\frac{1}{4}p_1^2p_2 + \frac{1}{8}p_1^4 + \frac{3}{8}p_2^2 + \frac{1}{4}p_4\right) + \cdots$$

Then the species of unrooted tanglegrams is the Cartesian product $U \times U$, with cycle index $Z_U * Z_U$ and the species of unrooted unordered tanglegrams is $E_2\{U\}$, with cycle index $h_2\{Z_U\}$. The numbers b_n of unrooted tanglegrams and c_n of unrooted unordered tanglegrams for small values of n are as follows:

n	2	3	4	5	6	7	8	9	10	11	12
b_n	1	1	2	4	31	243	3532	62810	1390718	36080361	1076477512

n	2	3	4	5	6	7	8	9	10	11	12
c_n	1	1	2	4	22	145	1875	31929	698183	18056523	538340256

The sequence b_n is [1, A259115] and the sequence c_n is [1, A259116].

6. The formula of Billey, Konvalinka, and Matsen

Billey, Konvalinka, and Matsen [4, Proposition 4] proved (though they did not state it this way) that if λ is a binary partition of n (a partition in which every part is a power of 2) then the coefficient r_λ of p_λ/z_λ in Z_R is given by the simple explicit formula

$$r_\lambda = \prod_{i=2}^{l(\lambda)} \big(2(\lambda_i + \cdots + \lambda_{l(\lambda)}) - 1\big), \tag{10}$$

where $l(\lambda)$ is the number of parts of λ. (If λ is not a binary partition then $r_\lambda = 0$.) They proved (10) by showing that the right side satisfies the recurrence corresponding to (4).

It would be nice to place (10) in a larger context, but I do not know how to do this. One possible approach is Lagrange inversion. If we let $r(z)$ be the result of setting $p_1 = z$ and $p_i = 0$ for $i > 1$ in Z_R then, as noted in [4], $r(z)$ is the exponential generating function for labeled binary trees, and (4) yields

$$r(z) = z + r(z)^2/2, \tag{11}$$

which can be solved by Lagrange inversion to give

$$r(z) = \sum_{n=1}^{\infty} \frac{1}{2^{n-1}n}\binom{2n-2}{n-1} z^n = \sum_{n=1}^{\infty} 1 \cdot 3 \cdot 5 \cdots (2n-3)\frac{z^n}{n!}, \tag{12}$$

which is what (10) gives for $\lambda = (1^n)$. (Equation (12) can also be obtained directly by solving (11) to get $r(z) = 1 - \sqrt{1-2z}$, and then applying the binomial theorem.) So we might hope that some generalization of Lagrange inversion might yield (10). There is a

Lagrange inversion formula for composition of symmetric functions, due to Labelle [10] (see also [6]), and Labelle applies it, in his Corollary B, to (4), obtaining

$$Z_R = \sum_{k_1,k_2,\ldots=0}^{\infty} \frac{\partial^{k_1+k_2+\cdots}}{\partial p_1^{k_1}\partial p_2^{k_2}\cdots} \cdots p_1 \prod_{i=1}^{\infty}(1-p_i) \cdot \prod_{i=1}^{\infty} \frac{(p_i^2+p_{2i})^{k_i}}{2^{k_i}k_i!}. \tag{13}$$

However, it is not clear that (10) can be derived from (13); it is not even obvious from (13) that the only nonzero terms in Z_R correspond to binary partitions.

Another possible approach to deriving the formula for r_λ is that of Wagner [16], but I was not able to get it to work.

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