An Introduction to Combinatorial Species

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What are combinatorial species?

The theory of combinatorial species, introduced by André Joyal in 1980, is a method for counting labeled structures, such as graphs.

The main reference for the theory of combinatorial species is the book Combinatorial Species and Tree-Like Structures by François Bergeron, Gilbert Labelle, and Pierre Leroux.

If a structure has label set *A* and we have a bijection $f \colon A \to B$ then we can replace each label $a \in A$ with its image $f(b)$ in *B*.
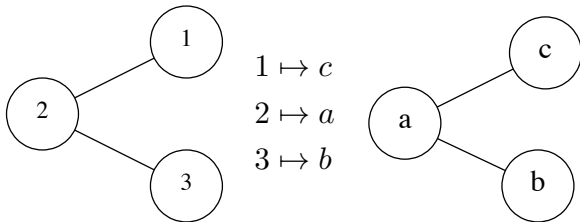
What are species good for?

The theory of species allows us to count labeled structures, using exponential generating functions.

More interestingly, it allows us to count unlabeled versions of labeled structures (unlabeled structures). If we have a bijection $A \to A$ then we also get a bijection from the set of structures with label set A to itself, so we have an action of the symmetric group on A acting on these structures. The orbits of these structures are the unlabeled structures.
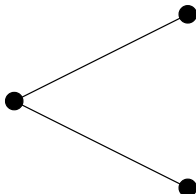
Definition of a species

A species is a functor from the category of finite sets with bijections to itself.

This means that if F is a species then for every finite set U, there is a finite set $F[U]$ (the set of F-structures on U), and for any bijection $\sigma : U \to V$ there is a bijection $F[\sigma] : F[U] \to F[V]$.

Moreover, we have the functorial properties

- If $\sigma : U \to V$ and $\tau : V \to W$ then $F[\tau \circ \sigma] = F[\tau] \circ F[\sigma]$.
- For the identity map $\text{Id}_U : U \to U$ we have $F[\text{Id}_U] = \text{Id}_{F[U]}$

Think of $F[U]$ as some sort of graph with label set U, even though there are no "labels" in the definition.

Examples of species

- The species E of sets: $E[U] = \{U\}$.
- The species E_n of n-sets:

$$E_n[U] = \begin{cases} \{U\} & \text{if } |U| = n \\ \varnothing & \text{if } |U| \neq n \end{cases}$$

- We write X for E_1, the species of singletons.
- The species Par of set partitions
- The species L of linear orders
- The species S of permutations (bijections from a set to itself).
- The species C of cyclic permutations
- the species $\mathcal{G}$ of graphs
- the species $\mathcal{G}^c$ of connected graphs

Isomorphism of species

Let F and G be species. An isomorphism α from F to G is a family of bijections $\alpha_U : F[U] \to G[U]$ for every finite set U such that for every bijection $\sigma : U \to V$, and every $s \in F[U]$ we have $G[\sigma](\alpha_U(s)) = \alpha_V(F[\sigma](\sigma))$.

In categorical terms, α is a natural isomorphism.

Notation: We write $[n]$ for $\{1, 2, \ldots, n\}$ and we write $F[n]$ instead of $F[[n]]$.

As an example, the species of subsets is isomorphic to the species of ordered partitions into two (possibly empty) blocks.

For example, the subset $\{1, 3, 4\}$ of $[5]$ corresponds to the ordered partition $(\{1, 3, 4\}, \{2, 5\})$.

A nonisomorphic example

The species S of permutations is not isomorphic to the species L of linear orders, even though for every n, $|S[n]| = |L[n]| = n!$.

Let's see what happens for $n = 2$. Here we have $|S[2]| = |L[2]| = 2$ and

$$S[2] = \{(1)(2), (1\,2)\}, \qquad L[2] = \{12, 21\}$$

There doesn't seem to be an reasonable bijection between these two sets that doesn't depend on the total ordering $1 < 2$.

What happens if apply the bijection $[2] \to [2]$ that switches 1 and 2? Both elements of $S[2]$ are fixed, but the two elements of $L[2]$ switch. So S and L can't be isomorphic.

Operations on species

There are several important operations on species.

The simplest is addition, which is just disjoint union:

$$(F + G)[U] = F[U] \sqcup G[U].$$

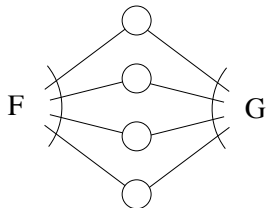So an $(F + G)$-structure is either an F-structure or a G-structure.

We can also have infinite sums, as long as they "converge"

$$E = \sum_{n=0}^{\infty} E_n$$

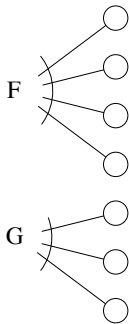Next is Cartesian product:

$$(F \times G)[U] = F[U] \times G[U]$$

So an $(F \times G)$-structure is an F-structure and a G-structure on the same set of points.

The ordinary product *FG* is more useful than the Cartesian product, but the definition is more complicated:

$$(FG)[U] = \sum_{U_1, U_2} F[U_1] \times G[U_2],$$

where the sum is over all decompositions of U into U_1 and U_2, so that $U_1 \cup U_2 = U$ and $U_1 \cap U_2 = \varnothing$.

Note that $(FG)[U]$ is not the same as $(GF)[U]$, but the species FG and GF are isomorphic. We usually identify species that are isomorphic.

We can define powers inductively, and we find that the species L_n of linear orders of n-sets is isomorphic to X^n, and
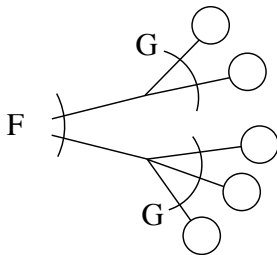
$$L = \sum_{n=0}^{\infty} X^n.$$

(Note that $X^0 = E_0$.)

Finally, we have composition or substitution of species, $F \circ G$. An element of $(F \circ G)[U]$ consists of a partition of U into (not necessarily nonempty) blocks, a G-structure on each block, and an F-structure on the set of blocks.

Formally,

$$(F \circ G)[U] = \bigcup_{\pi} \Big(F[\pi] \times \bigtimes_{V \in \pi} G[V] \Big).$$

where the union is over all partitions π of U and the Cartesian product is over all the blocks of π.

The most important special case is $F = E$, the species of sets, or $F = E_n$, the species of n-sets. Then $E \circ G$ is the species of sets of G-structures and $E_n \circ G$ is the species of n-sets of G-structures.

Since a partition is a set of nonempty sets, the species of partitions Par is $E \circ E^+$, where

$$E^+ = \sum_{n=1}^{\infty} E_n$$

is the species of nonempty sets.

Since a permutation is a set of cycles, $S = E \circ C$.

Generating functions for species

To a species *F* we may associate three generating functions.

First we have the exponential generating function

$$F(x) = \sum_{n=0}^{\infty} f_n \frac{x^n}{n!},$$

where $f_n = |F[n]|$.

The unlabeled generating function is

$$\widetilde{F}(x) = \sum_{n=0}^{\infty} \tilde{f}_n x^n,$$

where $\tilde{f}_n$ is the number of unlabeled *F*-structures on $[n]$.

These generating functions are compatible with addition and multiplication:

$$(F + G)(x) = F(x) + G(x) \qquad \widetilde{(F + G)}(x) = \widetilde{F}(x) + \widetilde{G}(x)$$
$$(FG)(x) = F(x)G(x) \qquad \widetilde{(FG)}(x) = \widetilde{F}(x)\widetilde{G}(x)$$

Also, the exponential generating function is compatible with composition:

$$(F \circ G)(x) = F(x) \circ G(x)$$

as long as $G(x)$ has no constant term; i.e., $G[\varnothing] = \varnothing$.

However, $\widetilde{(F \circ G)}(x)$ cannot be computed from $\widetilde{F}(x)$ and $\widetilde{G}(x)$.

Examples

For the species E_n of n-sets, $E_n(x) = x^n/n!$ and $\widetilde{E}_n(x) = x^n$.

For the species E of sets,

$$E(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x \quad \text{and} \quad \widetilde{E}(x) = \frac{1}{1-x}.$$

For the species C of cyclic permutations,

$$C(x) = \sum_{n=0}^{\infty} (n-1)! \frac{x^n}{n!} = \log\left(\frac{1}{1-x}\right) \quad \text{and} \quad \widetilde{C}(x) = \frac{x}{1-x}.$$

For the species $S = E \circ S$ of permutations,

$$S(x) = \exp(C(x)) = \frac{1}{1-x} = \sum_{n=0}^{\infty} n! \frac{x^n}{n!} \text{ and } \widetilde{S}(x) = \prod_{k=1}^{\infty} \frac{1}{1-x^k}$$

For the species $\mathrm{Par} = E \circ E^+$ of partitions, we have

$$\mathrm{Par}(x) = \exp(E^+(x)) = e^{e^x - 1}$$

$$\widetilde{\mathrm{Par}}(x) = \prod_{k=1}^{\infty} \frac{1}{1-x^k}$$

The cycle index series

The third important generating function associated with a species is the cycle index series, which contains the other two as special cases.

Let F be a species. For the moment, suppose that F is homogeneous of degree n; that is, $F[A] = \varnothing$ unless $|A| = n$.

For any bijection $\pi : [n] \to [n]$ there is a corresponding bijection $F[\pi] : F[n] \to F[n]$. Thus there is an action of the symmetric group $\mathfrak{S}_n$ on $F[n]$.

The cycle index Z_F of F is the characteristic of this action of $\mathfrak{S}_n$.

For each π in $\mathfrak{S}_n$, let fix $F[\pi]$ be the number of elements of $F[n]$ fixed by $F[\pi]$. Let $c_i(\pi)$ be the number of cycles of π of length i. Then we define

$$Z_F = \frac{1}{n!} \sum_{\pi \in \mathfrak{S}_n} \text{fix } F[\pi] \, p_1^{c_1(\pi)} p_2^{c_2(\pi)} \ldots,$$

where p_j is the power sum symmetric function $x_1^j + x_2^j + x_3^j + \cdots$.

Since fix $F[\pi]$ depends only on the cycle type of π, we can write this formula in another way.

Let $\lambda = (1^{m_1} 2^{m_2} \cdots)$ be a partition of n. The number of permutations in $\mathfrak{S}_n$ of cycle type λ is $n!/z_\lambda$, where

$$z_\lambda = 1^{m_1} m_1! \, 2^{m_2} m_2! \cdots.$$

Let fix $F[\lambda] = $ fix $F[\pi]$ where π is any permutation in $\mathfrak{S}_n$ of cycle type λ. Then

$$Z_F = \sum_{\lambda \vdash n} \text{fix } F[\lambda] \frac{p_\lambda}{z_\lambda}.$$

where $p_\lambda = p_1^{m_1} p_2^{m_2} \ldots$.

Examples

First let's look at $F = X = E_1$. So here $n = 1$ and $Z_{E_1} = p_1$.

Next for $F = E_2$, we have $n = 2$. Here we have $n = 2$ and $Z_{E_2} = \frac{1}{2} p_1^2 + \frac{1}{2} p_2$.

More generally, let's take $F = E_n$. Then $E_n[n]$ has only one element, $[n]$, and it's fixed by every element of $\mathfrak{S}_n$. So for every partition λ of n, we have fix $E_n[\lambda] = 1$, so

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

This is equal to the complete symmetric function

$$h_n = \sum_{i_1 \leq i_2 \leq \cdots \leq i_n} x_{i_1} x_{i_2} \cdots x_{i_n}.$$

For the species $L_n = X^n$ of linear orders of size n, only the identity element fixes anything, and it fixes all $n!$ linear orders, so

$$Z_{L_n} = \frac{1}{n!} \cdot n!\, p_1^n = p_1^n.$$

For the species C_n of n-cycles, a permutation π doesn't fix anything unless π consists of n/d d-cycles for some d dividing n. It's not too hard to show that

$$Z_{C_n} = \frac{1}{n} \sum_{d \mid n} \varphi(d) p_d^{n/d}$$

where φ is Euler's function.

For species that are not homogeneous, the cycle index is the sum of the cycle indices of the homogeneous components. So

$$Z_E = \sum_{n=0}^{\infty} Z_{E_n} = \sum_{n=0}^{\infty} h_n = \prod_{i=1}^{\infty} \frac{1}{1-x_i} = \exp\left(\sum_{j=1}^{\infty} \frac{p_j}{j}\right)$$

and

$$Z_L = \sum_{n=0}^{\infty} Z_{L^n} = \sum_{n=0}^{\infty} p_1^n = \frac{1}{1-p_1}$$

Applications of the cycle index

First we can get the exponential generating function and the unlabeled generating function from the cycle index:

$F(x)$ is obtained from Z_F by replacing p_1 with x and p_i with 0 for $i > 1$.

$\widetilde{F}(x)$ is obtained from Z_F be replacing each p_i with x^i, or equivalently, replacing x_1 with x and x_i with 0 for $i > 1$.

Species operations and the cycle index

Addition and multiplication are easy:

$$Z_{F+G} = Z_F + Z_G$$
$$Z_{FG} = Z_F Z_G$$

Corresponding to the Cartesian product of species is an operation on symmetric functions called the *Kronecker product*:

$$p_\lambda * p_\mu = z_\lambda \delta_{\lambda,\mu} p_\lambda.$$

Then

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

For composition of species, we have a corresponding operation on symmetric functions called composition or plethysm:

$$Z_{F \circ G} = Z_F \circ Z_G.$$

Plethysm can be defined in several equivalent ways. The most intuitive way to define $f \circ g$ when g has positive integer coefficients, is to write g as a sum of monic terms and substitute them for the variables of f.

But if f and g expressed in terms of the p_i, a more efficient procedure is to first define $p_j \circ g$ to be the result of replacing each p_i in g with p_{ij}, and then replacing each p_j in f with $p_j \circ g$.

Pólya's theorem and the coefficients of the cycle index

There is a simple and sometimes useful interpretation for the coefficients of the cycle index. We know that the coefficient of x_1^n in Z_F is the number of unlabeled F-structures on n points.

More generally, the coefficient of $x_1^{n_1} x_2^{n_2} \cdots$ in Z_F is the number of "F-structures labeled with the multiset $\{1^{n_1}, 2^{n_2}, \dots\}$."

Example: One of the structures counted by the coefficient of $x_1^2 x_2^3$ in Z_{C_5} is
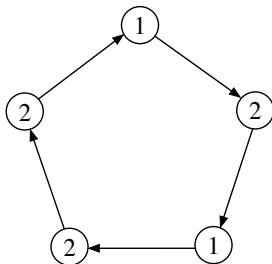
Indirect decompositions

We have seen that the species of set partitions can be expressed as a composition $E \circ E^+$. There are other cases, where we can't easily construct a species directly, but we can find an equation that it satisfies.

For example, consider the species $\mathcal{G}^c$ of connected graphs. Every graph may be viewed as a set of connected graphs, so the species $\mathcal{G}$ of graphs and the species $\mathcal{G}^c$ of connected graphs are related by $\mathcal{G} = E \circ \mathcal{G}^c$ and so $Z_{\mathcal{G}} = Z_E \circ Z_{\mathcal{G}^c}$. This formula can be inverted to compute $Z_{\mathcal{G}^c}$ and thereby count labeled and unlabeled connected graphs.

Trees

Indirect decompositions also arise in counting trees of various types. For now, I will talk about leaf-labeled (unordered) rooted binary trees, which I'll call simply binary trees.
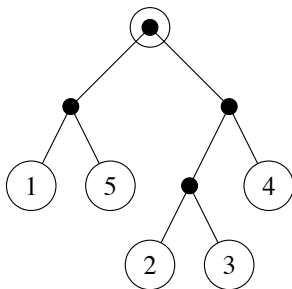
A binary tree is either a single labeled vertex or an unordered pair of binary trees. So the species R of binary trees satisfies

$$R = X + E_2 \circ R$$

and therefore the cycle index satisfies

$$Z_R = p_1 + h_2 \circ Z_R.$$

For the exponential generating function this reduces to

$$R(x) = x + R(x)^2/2,$$

which can easily be solved to give

$$R(x) = 1 - \sqrt{1 - 2x} = \sum_{n=1}^{\infty} 1 \cdot 3 \cdots (2n-3) \frac{x^n}{n!}$$

For the cycle index, there is a surprisingly simple formula discovered recently by Sara Billey, Matjaž Konvalinka, and Frederick A. Matsen IV:

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

where r_λ is zero if λ is not a binary partition (a partition in which every part is a power of 2), and if λ is a binary partition, $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_k)$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 1$ then

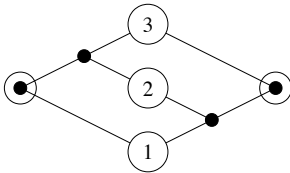$$r_\lambda = \prod_{i=2}^{k} \big(2(\lambda_i + \cdots + \lambda_k) - 1\big),$$

So the number of unlabeled binary trees with n leaves is

$$\sum_{\lambda \vdash n} r_\lambda / z_\lambda.$$

Billey, Konvalinka, and Matsen were interested in tanglegrams, which are ordered pairs of binary trees that share the same leaves. They wanted to count unlabeled tanglegrams. Here's a tanglegram
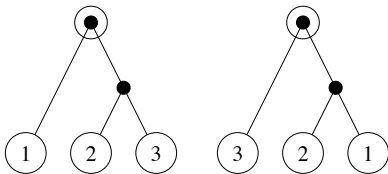
which we can also draw as

Since a tanglegram is an ordered pair of trees, the species of tanglegrams is the Cartesian product $R \times R$, so the cycle index for tanglegrams is

$$Z_{R \times R} = Z_R * Z_R = \sum_\lambda r_\lambda^2 \frac{p_\lambda}{z_\lambda}.$$

and therefore the number of unlabeled tanglegrams with n leaves is

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