POLYA ENUMERATION THEOREM FROM SCRATCH

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Abstract. In this note I define Species according to the book of Bergeron, Labelle, and Leroux and present their beautiful proof of the cycle index composition theorem. The uniqueness relies on the theory of symmetric functions in infinitely many variables. No prerequisite knowledge is assumed.

1. Introduction

At the beginning, I like to recall the story from the paper "From finite sets to Feynman diagrams".

" *Long ago, when shepherds wanted to see if two herds of sheep were isomorphic, they would look for a specific isomorphism. In other words, they would line up both herds and try to match each sheep in one herd with a sheep in the other. But one day, a shepherd invented decategorification. She realized one could take each herd and 'count' it, setting up an isomorphism between it and a set of 'numbers', which were nonsense words like 'one, two, three, . . . ' specially designed for this purpose. By comparing the resulting numbers, she could show that two herds were isomorphic without explicitly establishing an isomorphism! In short, the set N of natural numbers was created by decategorifying FinSet, the category whose objects are finite sets and whose morphisms are functions between these.*

Starting with the natural numbers, the shepherds then invented the basic operations of arithmetic by decategorifying important operations on finite sets: disjoint union, Cartesian product, and so on. We describe this in detail in the next section. Later, their descendants found it useful to extend N to larger number systems with better formal properties: the integers, the rationals, the real and complex numbers, and so on. These make it easier to prove a vast range of theorems, even theorems that are just about natural numbers. But in the process, the original connection to the category of finite sets was obscured.

Now we are in the position of having an enormous body of mathematics, large parts of which are secretly the decategorified residues of deeper truths, without knowing exactly which parts these are. For example, any equation involving natural numbers may be the decategorification of an isomorphism between finite sets. In combinatorics, when people find an isomorphism explaining such an equation, they say they have found a 'bijective proof' of it. But decategorification lurks in many other places as well, and wherever we find it, we have the opportunity to understand things more deeply by going back and categorifying: working with objects directly, rather than their isomorphism classes. "

In this talk, I plan to give the basics of the theory of species. There exist intricate connections with representation theory which I don't fully understand. One of the aims of the talk is to receive some feedback from people with different background and understand, at least, partly, those connections.

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Remark. Before I start, there is one more thing that should be menioned in relationship between enumerative combinatorics and symmetric functions, but won't be discussed in this talk. As Goulden and Jackson mention, the number of d-regular graphs on n vertices equals

$$r_d(n) = [t_1^d \dots t_n^d] \prod_{i<j} (1 + t_i t_j), \tag{1}$$

and a similar formula for multigraphs also holds:

$$r'_d(n) = [t_1^d \dots t_n^d] \prod_{i<j} (1 - t_i t_j)^{-1}. \tag{2}$$

Such expansions (and also generating functions related to graphs with degree sequence constraints) are studied in the literature using modern methods of matrix integrals. In the book "Enumerative Combinatorics", they have a different viewpoint, i.e. obtain differential equations. This knowkedge is relatively new for me, though it is not related to the main topic of the talk, I just wanted to share what I've seen.

2. Preliminaries on Species

Enumerative combinatorics usually tries to answer the question "how many objects of size n are there?". In Analytic Combinatorics, people use the generating functions defined as formal power series, directly as complex-valued functions, in order to determine the asymptotics of coefficients. Theory of Species focuses on *how* to construct the equations, and tries to understand the underlying combinatorial nature of the class.

In order to give a flavour of what can be done with exponential generating functions, let us start with a simple example.

Example (Warm-up)**.** An *involution* is a mapping

$$f\colon \{1, 2, \dots, n\} \to \{1, 2, \dots, n\} \tag{3}$$

such that $f(f(x)) = x$ for each x. How many involutions on n elements there exist?

Solution. First, the question is how do we distinguish the involutions, i.e. which involutions are considered equal. Let us encode involutions by permutations such that their cycles have only lengths 1 or 2.

Next, we consider an *exponential generating function* (EGF) of the involutions, which is by definition,

$$I(z) := \sum_{n \geqslant 0} a_n \frac{z^n}{n!}, \tag{4}$$

where a_n equals the number of involutions on n elements. This definition is universal and very popular. Instead of a_n there can be substituted any sequence corresponding to whatever classes of objects with labelled elements. That said, an exponential generating function of the "elementary brick", i.e. of two possible cycles, of length 1 and 2, respectively, equals, by definition,

$$E(z) = z + \frac{z^2}{2!}.$$

Next, we use this elementary construction to get the whole exponential generating function for the involutions. After checking the properties of two operations, union and cartesian product, we arrive to the EGF of sets

$$e^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots$$

Next, after checking some elementary properties of the composition of exponential generating functions, we finally obtain

$$I(z) = e^{z + \frac{z^2}{2}}. \tag{5}$$

Using the convolution formula for EGF

$$\left(a_0 + \frac{a_1}{1!}z + \frac{a_2}{2!}z^2 + \dots\right)\left(b_0 + \frac{b_1}{1!}z + \frac{b_2}{2!}z^2 + \dots\right) = \sum_{n\geqslant 0} z^n \sum_{k=0}^{n} \binom{n}{k} a_k b_{n-k}, \tag{6}$$

we obtain the answer

$$I_n = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n!}{(n-2k)!2^k k!}. \tag{7}$$

If we ask a question, how many involutions are there up to an automorphism, it suddenly becomes a much more difficult question because symmetry breaking is not trivial. This is what I am going to talk about.

Remark. *Ordinary generating functions* are used to enumerate objects up to their automorphisms. Inside the definition, we don't put factorial in the denominator:

$$\widetilde{I}(z) := \sum_{n\geqslant 0} \widetilde{a_n} z^n. \tag{8}$$

Both functions $I(z)$ and $\widetilde{I}(z)$ are analytic, i.e. have a positive radius of convergence, which also means that the coefficients grow not faster than exponents. This property helps us understand which combinatorial constructions are possible within a restricted world of analytic functions.

From now on, a tilde above the function will always denote ordinary generating function.

Species contain some more information than just a combinatorial class of objects endowned with a size. Species also encode how the object behave under permutations of labels, some information about their automorphisms.

Definition (Species)**.** A *species of structures* F is a rule F which

(1) produces, for each finite set U, a finite set $F[U]$ (combinatorial class of objects, usually we take without loss of generality $U = \{1, 2, \dots, n\}$)
(2) produces, for each permutation $\sigma\colon U \to V$, a permutation

$$F[\sigma]\colon F[U] \to F[V].$$

The functions $F[\sigma]$ should satisfy two functorial properties:

(1) For all permutations $\sigma\colon U \to V, \tau\colon V \to W$,

$$F[\tau \circ \sigma] = F[\tau] \circ F[\sigma],$$

(2) For the identity permutation $\mathrm{Id}_U\colon U \to U$,

$$F[\mathrm{Id}_U] = \mathrm{Id}_{F[U]}\,.$$

Definition (Automorphisms and isomorphisms)**.** Each permutation of labels $\sigma\colon \{1, \dots, n\} \to \{1, \dots, n\}$ induces a permutation of combinatorial objects. If σ transforms object $o_1 \in F[\{1, \dots, n\}]$ into an object $o_2 \in F[\{1, \dots, n\}]$ then σ is called an *isomorphism.* An isomorphism from o_1 to o_1 is called an *automorphism.*

Definition (Cycle index series)**.** Consider a *species* F (i.e. class of combinatorial objects). A *cycle index series* is a formal power series in an infinite number of variables $x_1, x_2, \dots$ consisting of an infinite sum of monomials (each of them finite)

$$Z_F(x_1, x_2, \dots) = \sum_{n\geqslant 0} \frac{1}{n!} \left(\sum_{\sigma \in S_n} |\mathrm{Fix}\, F[\sigma]|\, x_1^{\sigma_1} x_2^{\sigma_2} \dots \right), \tag{9}$$

where $\mathrm{Fix}\, F[\sigma]$ is the set of objects in the class F left fixed under σ; σ_k is the number of cycles of length k in the permutation σ.

Example (Cycle index series of permutations)**.** Let us find the cycle indes series for the species of permutations. From the definition, we quickly compute that

$$|\mathrm{Fix}\, F[\sigma]| = 1^{\sigma_1}\sigma_1! 2^{\sigma_2}\sigma_2! \dots$$

Next, by a simple permutation of the summands in (9), we get

$$\begin{aligned} Z_F(x_1, x_2, \dots) &= \sum_{n_1+2n_2+\ldots<\infty} \mathrm{Fix}\, F[n_1, n_2, \dots] \frac{x_1^{n_1} x_2^{n_2} \dots}{1^{n_1} n_1! 2^{n_2} n_2! \dots} \\ &= \sum_{n_1}\sum_{n_2} \dots x_1^{n_1} x_2^{n_2} \dots = \frac{1}{(1-x_1)(1-x_2)\dots}. \end{aligned}$$

Theorem. Exponential and ordinary generating functions of species F satisfy, repsectively,

$$\begin{aligned} F(x) &= Z_F(x, 0, 0, \dots), \\ \widetilde{F}(x) &= Z_F(x, x^2, x^3, \dots). \end{aligned}$$

Proof. The first equality is a simple exercise. The second equality is a bit more complicated. We prove the second one, leaving the first one to reader.

According to Burnside's lemma, for any group G acting on a finite set X, ,the number of equivalence classes ω can be obtained from the formula

$$\omega = \frac{1}{|G|} \sum_{g \in G} |X^g|, \tag{10}$$

where X^g is the subset of X fixed by g. We consider only a simple case of S_n acting on $F[\{1, \dots, n\}]$. Substituting the right-hand side into the definition of cycle index series, we obtain

$$Z_F(x, x^2, \dots) = \sum_{n \geqslant 0} \left(\frac{1}{n!} \sum_{\sigma \in S_n} |\mathrm{Fix}\, F[\sigma]| \right) x^n = \sum_{n \geqslant 0} \omega_n x^n \ , \tag{11}$$

where ω_n denotes the number of object of size n up to equivalence. □

3. Notion of Composition

First, let us return back to a very simple example without cycle indices and exponential generating functions.

Example (Wrong intuition)**.** Consider the class of binary strings of arbitrary length $\mathcal{S} = \{0, 1\}^* = \{\varepsilon, 0, 1, 00, 01, 10, 11, \dots\}$. It is clear that OGF equals

$$S(x) = \sum_{n \geqslant 0} 2^n x^n = \frac{1}{1-2x}.$$

Let us consider another representation of binary strings: each string consists of a block of consecutive ones and zeros. We consider strings that don't have two consecutive ones or zeros:

$$\mathcal{A} = \{\varepsilon, 0, 1, 01, 10, 010, 101, \dots\}$$

which has OGF $A(x) = 1 + 2\dfrac{x}{1-x}$. After substituting for each symbol a sequence of symbols, we obtain

$$A\left(\frac{x}{1-x}\right) = 1 + \frac{2\dfrac{x}{1-x}}{1 - \dfrac{x}{1-x}} = 1 + \frac{2x}{1-2x} = \frac{1}{1-2x}. \tag{12}$$

Usually such lucky elegant formulas don't hold for unlabelled classes, and in order to understand the OGF of composition of the two classes, we need to understand their corresponding cycle index series.

Example (Powerset construction)**.** If $A(x)$ is ordinary generating function of species $\mathcal{A}$ then the species of *sets* of objects from $\mathcal{A}$ has ordinary generating function

$$E(x) = \exp\left(A(x) - \frac{A(x^2)}{2} + \frac{A(x^3)}{3} - \dots\right). \tag{13}$$

This can be proven by a simple manipulation with logarithms and log-exp transform of another representation

$$A(x) = \prod_{n\geqslant 0}(1 + x^{a_n}), \tag{14}$$

where $a_n = [x^n]A(x)$.

This powerset construction is a part of more general framework. We are going to formally define the composition species below, but first we present the formulation of the composition theorem.

Theorem (Cycle index composition theorem)**.** If F and G are species such that there are no objects of size 0 in the species G, then for their cycle index series it holds

$$Z_{F\circ G} = Z_F(Z_G(x_1, x_2, \dots), Z_G(x_2, x_4, \dots), Z_G(x_3, x_6, \dots), \dots). \tag{15}$$

However, before we can have the proof, we need to understand a more general concept.

4. Weighted Structures

Example. Consider the species of rooted plane trees $\mathcal{A}$, and to each rooted plane tree $\alpha \in \mathcal{A}$ assign a *weight* equal

$$w(\alpha) = t^{f(\alpha)},$$

where t is a formal variable. The weighted number of trees is defined as a sum of weights

$$|\mathcal{A}[U]|_w = \sum_{\alpha\in\mathcal{A}[U]} w(\alpha).$$

After regrouping the summands we obtain a part of bivariate generating function

$$|\mathcal{A}[U]|_w = \sum_{k=0}^{n} a_{n,k}t^k,$$

where $a_{n,k}$ is the number of trees with n vertices and k leaves. If we put $t = 1$, we obtain $|A[U]| = n^{n-1}$.

Note that weight can be a multivariate product, with each variable marking a separate parameter.

For species equipped with weights, there can also be defined ordinary and exponential generating functions, cycle index series:

$$F_w(x) = \sum_{n\geqslant 0} |F[n]|_w \frac{x^n}{n!},$$

$$\widetilde{F}_w(x) = \sum_{n\geqslant 0} \left|\frac{F[n]}{\sim}\right|_w x^n,$$

$$Z_{F_w} = \sum_{n\geqslant 0} \frac{1}{n!}\left(\sum_{\sigma\in S_n} |\operatorname{Fix} F[\sigma]|_w x_1^{\sigma_1} x_2^{\sigma_2}\dots\right),$$

where $|\operatorname{Fix} F[\sigma]|_w$ is the weight of the set consisting of the fixed objects under action of σ. It still holds

$$F_w(x) = Z_{F_w}(x, 0, 0, \dots),$$

$$\widetilde{F}_w(x) = Z_{F_w}(x, x^2, x^3, \dots).$$

Example (Hermite Polynomials)**.** Consider weighted class of involutions equiped with two weight variables. To each involution assign a weight

$$w(\varphi) = t^{\varphi_1}(-1)^{\varphi_2}, \tag{16}$$

where φ_1, φ_2 denote, respectively, the number of fixed points and the number of cycles of length 2 of the involution φ. If you believe me that composition of exponential generating functions "works the same way", then

$$\operatorname{Inv}_w(x) = \exp\left(tx - \frac{1}{2}x^2\right) = \sum_{n\geqslant 0} He_n(t)\frac{x^n}{n!}, \tag{17}$$

where suddenly, $He_n(t)$ appear to be Hermite polynomials defined by

$$He_n(t) = (-1)^n e^{t^2/2}\frac{d^n}{dt^n}e^{-t^2/2}.$$

Definition (Composition of weighted species)**.** Consider species equipped with weight F_w, G_v, such that $G_v \neq 0$, $G_v(0) = 0$. Then, their composition consists of objects of type

$$(U, \theta), \quad \theta = (\pi, f, (\gamma_p)_{p\in\pi})$$

where π is a partition of U; $f \in F_w[\pi]$; $\gamma_p \in G_v[p]$ for each p.

The weight of the structure is defined as a product of all internal weights

$$w(\theta) = w(f)\prod_{p\in\pi} v(\gamma_p).$$

With a little notation abuse, to each weighted species $F = F_w$ we can put into correspondence another weighted species $\widetilde{F} = \widetilde{F_w}$ wuch that EGF of $\widetilde{F}$ coincides with and OGF of F. In other words, intuitively speaking, objects from $\widetilde{F}$ are additionally endowned with an automorphism.

5. Proof of Composition Theorem

We start with a meta-argument that the theorem about the composition of ordinary generating functions is equivalent to the theorem of composition of cycle indices.

Proposition. Suppose the validity of two following propositions.

(1) For any weighted species F_w and H_u it holds

$$\widetilde{F_w \circ H_u} = Z_{F_w}(\widetilde{H}_u(x), \widetilde{H}_{u^2}(x^2), \widetilde{H}_{u^3}(x^3), \dots),$$

(2) If some formal power series $f(h_1, h_2, \ldots)$ satisfies for any class H_u
$$\widetilde{F_w \circ H_u} = f(\widetilde{H}_u(x), \widetilde{H}_{u^2}(x^2), \widetilde{H}_{u^3}(x^3), \ldots),$$
then f coincides with Z_{F_w}.

Then, weighted cycle index composition theorem holds:
$$Z_{F_w \circ G_v} = Z_{F_w}(Z_{G_v}(x_1, x_2, \ldots), Z_{G_{v^2}}(x_2, x_4, \ldots), Z_{G_{v^3}}(x_3, x_6, \ldots), \ldots).$$

Proof. In a rather shameless manner, we use that the composition of species is associative with respect to the operation of taking ordinary generating function (why?).

It implies
$$\begin{aligned}
&\widetilde{(F_w \circ G_v) \circ H_u}(x) = \widetilde{F_w \circ (G_v \circ H_u)}(x) \\
&= Z_{F_w}\left(\widetilde{G_v \circ H_u}(x), \widetilde{G_{v^2} \circ H_{u^2}}(x^2), \ldots\right) \\
&= Z_{F_w}\left(Z_{G_v}\left(\widetilde{H}_u(x), \widetilde{H}_{u^2}(x^2), \ldots\right), Z_{G_{v^2}}\left(\widetilde{H}_{u^2}(x^2), \widetilde{H}_{u^4}(x^4), \ldots\right), \ldots\right) \\
&= (Z_{F_w} \circ Z_{G_v})\left(\widetilde{H}_u(x), \widetilde{H}_{u^2}(x^2), \ldots\right).
\end{aligned}$$

□

Lemma. The first proposition holds.

Proof. This statement is at the core of the proof and it is the most technical part. Recall the structure of the composition species. Since we consider only automorphisms, we restrict ourselves only to permutations that have the following specific structure: it induces the permutation of the partition, and within each partition it induces a separate permutation.

Let's prove that EGF of corresponding species $\widetilde{F \circ G}$ can be expressed as the right-hand side $Z_{F_w}(\widetilde{H}_u(x), \widetilde{H}_{u^2}(x^2), \widetilde{H}_{u^3}(x^3), \ldots)$.

Suppose that σ_π has cycle type N. Clearly, the species $\widetilde{F \circ G}$ can be decomposed into subspecies over all possible cycle types
$$\widetilde{F \circ G} = \sum_N (\widetilde{F \circ G})_N.$$

Each object from $(\widetilde{F \circ G})_N$ is a set of necklaces of objects from G and its EGF can be computed as
$$(\widetilde{F \circ G})_N(x) = |\mathrm{Fix}\, F[N]|_w \frac{(CYC_1(G)(x))^{n_1}}{n_1!} \frac{(CYC_2(G)(x))^{n_2}}{n_2!} \ldots, \tag{18}$$
where $CYC_k(G)(x) = \frac{1}{k}\widetilde{G}_{v^m}(x^m)$.

This immediately implies
$$\begin{aligned}
&\widetilde{F_w \circ G_v}(x) = \sum_N (\widetilde{F_w \circ G_v})_N(x) \\
&= \sum_{n_1, n_2, \ldots} |\mathrm{Fix}\, F[n_1, n_2, \ldots]|_w \frac{(\widetilde{G}_v(x))^{n_1}}{1^{n_1} n_1!} \frac{(\widetilde{G}_{v^2}(x^2))^{n_2}}{2^{n_2} n_2!} \ldots \\
&= Z_{F_w}(\widetilde{G}_v(x), \widetilde{G}_{v^2}(x^2), \ldots).
\end{aligned}$$

□

Lemma. The second proposition holds.

Proof. Consider

$$H_u = X_{t_1} + X_{t_2} + X_{t_3} + \dots$$

For the class H_u it holds

$$\widetilde{H}_{u^k}(x^k) = S_k x^k := (t_1^k + t_2^k + t_3^k + \dots)x^k.$$

We show that if for all $\vec{t}, x$ it holds

$$f(S_1 x, S_2 x^2, S_3 x^3, \dots) = 0$$

then for all $\vec{x}$ it holds

$$f(x_1, x_2, \dots) = 0.$$

By considering the differences, it would be enough for the theorem. Suppose that $f(x_1, x_2, \dots) = \sum_{n_1, n_2, \dots} a_{n_1, n_2, \dots} x_1^{n_1} x_2^{n_2} \dots$. Set

$$f_n(x_1, x_2, x_3, \dots) = \sum_{n_1 + 2n_2 + \dots = n} a_{n_1, n_2, \dots} x_1^{n_1} x_2^{n_2} \dots$$

Then, each f_n is a polynomial of degree n and $f(S_1 x, S_2 x, \dots) = 0$ implies

$$\sum_{n \geqslant 0} f_n(S_1, S_2, \dots) x^n = 0$$

which implies coefficientwise the desired equality.

□

6. Conclusion

I will summarise some key ideas of the proof.

- Near the end, we discovered that OGF can be considered as an EGF of a richer structure which simplifies the analysis from an algebraic viewpoint and complexifies the combinatorial counterpart.
- It is useful to know cycle index of the considered species but equations are far from trivial, because they involve infinite sums. However, the methods for asymptotic analysis have been developed.
- We were not able to prove the composition theorem directly, rather we had to use the full generality of the composition theorem in an essential way. The weights played their role when we used the uniqueness which was one of the key ingredient.
- Bergeron, Labelle and Leroux point out that cycle index series correspond to characters of permutation representations of the symmetric group. Moreover, the substitution formula gives a direct link between the composition of species and operation of plethysm on symmetric functions. I cannot fully appreciate this statement yet, but hope to understand it in the course of the discussion.
- Assymetry index series is a tool for studying objects like unrooted trees, whose stabilizer is reduced to the identity permutation:

  $$\overline{F_w \circ G_v}(x) = \Gamma_{F_w}(\overline{G_v}(x), \overline{G_{v^2}}(x^2), \dots)$$

  which also satisfies

  $$\Gamma_{F_w \circ G_v} = \Gamma_{F_w} \circ \Gamma_{G_v}.$$

  The negative signs in the assymetry index series make it difficult to sample unrooted object (but sometimes it is enough to unroot a randomly generated rooted object).