

Counting components of nonisomorphic maps

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1 Counting nonisomorphic maps

In this document we will derive closed form generating functions and a set of recurrences for the number of nonisomorphic maps $F : [n] \rightarrow [n]$ and their components. Here two maps are considered isomorphic if on removing the labels from the labeled map we obtain the same directed graph or alternatively if there is a permutation acting simultaneously on domain and range which turns one into the other.

Using the notation from *Analytic Combinatorics* by Flajolet and Sedgewick [FS09] we have for the corresponding combinatorial class $\mathcal{F}$ the unlabeled specification in terms of trees and components

$$\begin{aligned}\mathcal{T} &= \mathcal{Z} \times \text{MSET}(\mathcal{T}) \\ \mathcal{C} &= \text{CYC}(\mathcal{T}) \\ \mathcal{F} &= \text{MSET}(\mathcal{C})\end{aligned}$$

Compare with the labeled specification which is in [FO89] to see the generality of the combinatorial class concept. We will thus proceed in three phases, beginning with trees, followed by components which are cycles of rooted trees and at last, maps, which are sets of these components. This material is from Theorem I.1 page 27 and page 480 of [FS09] and starting on page 4 of [FO89]. There is a directed edge between two nodes in the graph of the map when the first node is mapped to the second.

2 Rooted trees and sets

The unlabeled multiset operator is represented by the cycle index of the symmetric group which is standard and is given by

$$Z(S_m) = [w^m] \exp \left(\sum_{\ell \geq 1} a_\ell \frac{w^\ell}{\ell} \right).$$

The following recurrence can be derived from the exponential term:

$$Z(S_m) = \frac{1}{m} \sum_{k=1}^m a_k Z(S_{m-k}).$$

We thus obtain for the class of trees using the PET substitution the functional equation $T(z) = z \times \sum_{m \geq 0} Z(S_m; T(z))$ or

$$T(z) = z \exp \left(\sum_{\ell \geq 1} \frac{T(z^\ell)}{\ell} \right).$$

3 Cycles of trees

Here we join a set of trees by placing the roots on a directed cycle of some length, possibly including singletons, the fixed points of the map. As this construction is less common we derive it from the cycle index. We find for the cycle operator $\text{CYC}_{=m}$ the cycle index

$$Z(C_m) = \frac{1}{m} \sum_{d|m} \varphi(d) a_d^{m/d}.$$

Summing these cycle indices we obtain for the general cycle operator CYC applied to trees

$$\begin{aligned} C(z) &= \sum_{m \geq 1} \frac{1}{m} \sum_{d|m} \varphi(d) T(z^d)^{m/d} \\ &= \sum_{d \geq 1} \varphi(d) \sum_{j \geq 1} \frac{1}{jd} T(z^d)^j = \sum_{d \geq 1} \frac{\varphi(d)}{d} \log \frac{1}{1 - T(z^d)}. \end{aligned}$$

4 Sets of components that are cycles of trees

Following the combinatorial class specification from the introduction we thus obtain for the desired generating function of nonisomorphic maps

$$\begin{aligned} F(z) &= \exp \left(\sum_{\ell \geq 1} \frac{1}{\ell} \sum_{d \geq 1} \frac{\varphi(d)}{d} \log \frac{1}{1 - T(z^{d\ell})} \right) \\ &= \exp \left(\sum_{m \geq 1} \frac{1}{m} \log \frac{1}{1 - T(z^m)} \sum_{d|m} \varphi(d) \right) \\ &= \exp \left(\sum_{m \geq 1} \log \frac{1}{1 - T(z^m)} \right) = \prod_{m \geq 1} \frac{1}{1 - T(z^m)}. \end{aligned}$$

This form of $F(z)$ appears on page 85 of [FS09]. We now have all the data that we need to compute the required recurrence relations.

5 Recurrence for the number of trees

The functional equation yields

$$T_{n+1} = [z^n] \exp \left(\sum_{\ell \geq 1} \frac{T(z^\ell)}{\ell} \right).$$

Differentiating we find

$$\begin{aligned}
T_{n+1} &= \frac{1}{n} [z^{n-1}] \exp \left(\sum_{\ell \geq 1} \frac{T(z^\ell)}{\ell} \right) \sum_{\ell \geq 1} T'(z^\ell) z^{\ell-1} \\
&= \frac{1}{n} [z^{n-1}] \frac{T(z)}{z} \sum_{\ell \geq 1} T'(z^\ell) z^{\ell-1}.
\end{aligned}$$

We have from the Cauchy product

$$\begin{aligned}
\frac{1}{n} \sum_{k=0}^{n-1} [z^{n-1-k}] \frac{T(z)}{z} [z^k] \sum_{\ell \geq 1} T'(z^\ell) z^{\ell-1} &= \frac{1}{n} \sum_{k=0}^{n-1} T_{n-k} [z^k] \sum_{\ell \geq 1} T'(z^\ell) z^{\ell-1} \\
&= \frac{1}{n} \sum_{k=1}^n T_{n+1-k} [z^k] \sum_{\ell \geq 1} T'(z^\ell) z^\ell
\end{aligned}$$

Here we see that ℓ must divide k and find

$$\begin{aligned}
\frac{1}{n} \sum_{k=1}^n T_{n+1-k} \sum_{\ell|k} [z^k] T'(z^\ell) z^\ell &= \frac{1}{n} \sum_{k=1}^n T_{n+1-k} \sum_{\ell|k} [z^{\ell \times k/\ell}] T'(z^\ell) z^\ell \\
&= \frac{1}{n} \sum_{k=1}^n T_{n+1-k} \sum_{\ell|k} [z^{k/\ell}] T'(z) z.
\end{aligned}$$

To conclude observe that

$$[z^{k/\ell}] T'(z) z = [z^{k/\ell-1}] T'(z) = \frac{k}{\ell} T_{k/\ell}$$

which yields

$$\frac{1}{n} \sum_{k=1}^n T_{n+1-k} \sum_{\ell|k} \frac{k}{\ell} T_{k/\ell}$$

or

$$T_{n+1} = \frac{1}{n} \sum_{k=1}^n T_{n+1-k} \sum_{\ell|k} \ell T_\ell.$$

This will produce the sequence

$$\begin{aligned}
&1, 1, 2, 4, 9, 20, 48, 115, 286, 719, \\
&1842, 4766, 12486, 32973, \dots
\end{aligned}$$

which is OEIS A000081.

6 Recurrence for the number of maps

Supposing that we only need the first few values we can truncate the product in the generating function at $m = n$ and substitute the leading $\lfloor n/m \rfloor$ terms from $T(z)$. We look to turn this observation into a recurrence. Starting with

$$F_n = [z^n] \prod_{m \geq 1} \frac{1}{1 - T(z^m)} = [z^n] \prod_{m=1}^n \frac{1}{1 - T(z^m)}$$

We introduce with $q \geq 1$

$$F_{n,q} = [z^n] \prod_{m=1}^q \frac{1}{1 - T(z^m)}.$$

With the base case $F_{n,1}$ where $q = 1$ we have $\sum_{p \geq 0} F_{p,1} z^p \times (1 - T(z)) = 1$ so we get $F_{0,1} = 1$ as well as $F_{n,1} = \sum_{p=1}^n F_{n-p,1} T_p$. We find for $q \geq 2$

$$F_{n,q} = \sum_{k=0}^n [z^{n-k}] \prod_{m=1}^{q-1} \frac{1}{1 - T(z^m)} [z^k] \frac{1}{1 - T(z^q)} = \sum_{k=0}^n F_{n-k,q-1} [z^k] \frac{1}{1 - T(z^q)}$$

Here we see that k must be a multiple of q :

$$\begin{aligned} &= \sum_{k=0}^{\lfloor n/q \rfloor} F_{n-kq,q-1} [z^{kq}] \frac{1}{1 - T(z^q)} \\ &= \sum_{k=0}^{\lfloor n/q \rfloor} F_{n-kq,q-1} [z^k] \frac{1}{1 - T(z)} = \sum_{k=0}^{\lfloor n/q \rfloor} F_{n-kq,q-1} F_{k,1}. \end{aligned}$$

We always have $F_{0,q} = 1$. We obtain the sequence given by $F_n = F_{n,n}$

$$1, 3, 7, 19, 47, 130, 343, 951, 2615, 7318, 20491, 57903, \dots$$

which is OEIS A001372. These recurrences will enable us to replicate and extend the data on line at the OEIS. For example, showing only the most significant digits, the sequence at $n = 1024$ to $n = 1032$ will produce

$$\begin{aligned} &1.279991183 \times 10^{480}, 3.781507078 \times 10^{480}, 1.117179773 \times 10^{481}, \\ &3.300512766 \times 10^{481}, 9.750793870 \times 10^{481}, 2.880704692 \times 10^{482}, \\ &8.510551606 \times 10^{482}, 2.514298775 \times 10^{483}, 7.428074700 \times 10^{483}, \\ &\dots \end{aligned}$$

7 The number of components

We can now ask about the average number Q_n of components in a random nonisomorphic map. This is done by introducing a secondary variable u to get the bivariate GF with components marked

$$Q(z, u) = \exp \left(\sum_{m \geq 1} \frac{1}{m} \log \frac{1}{1 - T(z^m)} \sum_{d|m} \varphi(d) u^{m/d} \right)$$

This is the combinatorial class $\text{MSET}(\mathcal{U} \times \mathcal{C})$. We then have for the average number of components,

$$Q_n = \frac{[z^n] \frac{\partial}{\partial u} Q(z, u) \big|_{u=1}}{[z^n] F(z)}.$$

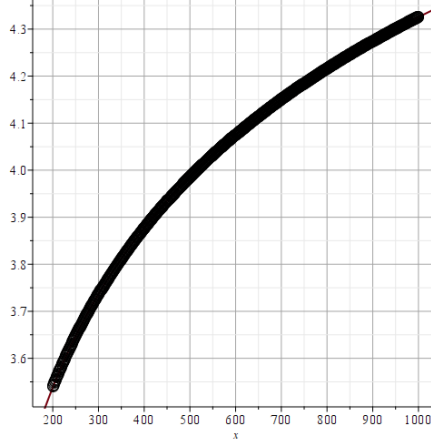


Figure 1: Average number of components.

We find for the numerator which counts the number of components summed over all maps

$$\begin{aligned}
 R_n &= [z^n] \prod_{m \geq 1} \frac{1}{1 - T(z^m)} \sum_{m \geq 1} \frac{1}{m} \log \frac{1}{1 - T(z^m)} \sum_{d|m} \varphi(d) \frac{m}{d} \\
 &= \sum_{k=0}^n F_{n-k} [z^k] \sum_{m \geq 1} \left(\sum_{d|m} \frac{\varphi(d)}{d} \right) \log \frac{1}{1 - T(z^m)}
 \end{aligned}$$

Introducing $\nu(m) = \sum_{d|m} \frac{\varphi(d)}{d}$

$$\begin{aligned}
 &= \sum_{k=1}^n \frac{F_{n-k}}{k} [z^{k-1}] \sum_{m \geq 1} \nu(m) \frac{m z^{m-1} T'(z^m)}{1 - T(z^m)} \\
 &= \sum_{k=1}^n \frac{F_{n-k}}{k} [z^k] \sum_{m \geq 1} \nu(m) \frac{m z^m T'(z^m)}{1 - T(z^m)}
 \end{aligned}$$

We must have m a divisor of k :

$$\begin{aligned}
 &= \sum_{k=1}^n \frac{F_{n-k}}{k} \sum_{m|k} \nu(m) [z^{k/m \times m}] \frac{m z^m T'(z^m)}{1 - T(z^m)} \\
 &= \sum_{k=1}^n \frac{F_{n-k}}{k} \sum_{m|k} \nu(m) [z^{k/m}] \frac{m z T'(z)}{1 - T(z)} \\
 &= \sum_{k=1}^n F_{n-k} \sum_{m|k} \frac{1}{m} \nu(k/m) [z^m] \frac{z T'(z)}{1 - T(z)} \\
 &= \sum_{k=1}^n F_{n-k} \sum_{m|k} \frac{1}{m} \nu(k/m) \sum_{j=0}^{m-1} (j+1) T_{j+1} F_{m-1-j,1}
 \end{aligned}$$

Observe that the coefficients on F_{n-k} only depend on k so they too can be memorized. This gives the sequence

$$1, 4, 11, 33, 88, 254, 697, 1984, 5585, 15938, 45424, \\ 130381, 374450, 1079361, 3115291, 9010177, \dots$$

which is OEIS A217860. With the recurrences in place we can compute Q_n for large n . For example the value at $n = 1024$ is $5.5524155141249376050 \times 10^{480}$ (only the most significant digits shown, the recurrences are exact).

The authors write at the cited location in *Analytic Combinatorics* that the number of components should be $\frac{1}{2} \log n$. Computing the values up to $n = 1000$ we get an approximate fit of $Q_n \approx 0.94660 + 0.4891 \log n$ as expected, shown in the graph above.

For this document a second version was tested with no fractions appearing in the recurrences, which had comparable resource usage.

8 Addendum, counting by the number of components

P. Luschny (OEIS) suggests to also count the number of mappings with k components. This is $\text{MSET}_{=k}(\mathcal{C})$. We get from the corresponding cycle index the form $Z(S_k; C(z))$ so we first require the coefficients on $C(z)$ which counts connected maps. We find

$$\begin{aligned} K_n &= [z^n]C(z) = [z^n] \sum_{d \geq 1} \frac{\varphi(d)}{d} \log \frac{1}{1 - T(z^d)} \\ &= \sum_{d|n} [z^{d \times n/d}] \frac{\varphi(d)}{d} \log \frac{1}{1 - T(z^d)} = \sum_{d|n} [z^{n/d}] \frac{\varphi(d)}{d} \log \frac{1}{1 - T(z)} \\ &= \frac{1}{n} \sum_{d|n} [z^{n/d-1}] \varphi(d) \frac{T'(z)}{1 - T(z)} = \frac{1}{n} \sum_{d|n} [z^{d-1}] \varphi(n/d) \frac{T'(z)}{1 - T(z)} \\ &= \frac{1}{n} \sum_{d|n} \varphi(n/d) \sum_{j=0}^{d-1} (j+1) T_{j+1} F_{d-1-j,1}. \end{aligned}$$

Here we have $K_0 = 0$. This gives the sequence

$$1, 2, 4, 9, 20, 51, 125, 329, 862, 2311, 6217, 16949, 46350, 127714, \dots$$

which is OEIS A002861. The cycle index recurrence yields

$$Z(S_k; C(z)) = \frac{1}{k} \sum_{p=1}^k C(z^p) Z(S_{k-p}; C(z))$$

Extracting coefficients

$$K_{n,k} = [z^n]Z(S_k; C(z)) = [z^n] \frac{1}{k} \sum_{p=1}^k C(z^p) Z(S_{k-p}; C(z))$$

where $K_{n,k} = 0$ when $k > n$ and $K_{n,1} = K_n$ as well as $K_{n,0} = [[n = 0]]$. Continuing

$$= \frac{1}{k} \sum_{p=1}^k \sum_{q=1}^n [z^q]C(z^p) [z^{n-q}]Z(S_{k-p}; C(z))$$

$$\begin{aligned}
&= \frac{1}{k} \sum_{q=1}^n \sum_{p|q, p \leq k} [z^q] C(z^p) [z^{n-q}] Z(S_{k-p}; C(z)) \\
&= \frac{1}{k} \sum_{q=1}^n \sum_{p|q, p \leq k} [z^{q/p \times p}] C(z^p) K_{n-q, k-p} \\
&= \frac{1}{k} \sum_{q=1}^n \sum_{p|q, p \leq k} [z^{q/p}] C(z) K_{n-q, k-p} = \frac{1}{k} \sum_{q=1}^n \sum_{p|q, p \leq k} K_{q/p} K_{n-q, k-p}.
\end{aligned}$$

We can then verify that

$$R_n = \sum_{k=1}^n K_{n,k} \times k.$$

If R_n only is desired it should be calculated from the recurrence that was established earlier. We obtain the following data for the initial ten rows:

1	0	0	0	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
4	2	1	0	0	0	0	0	0	0
9	7	2	1	0	0	0	0	0	0
20	17	7	2	1	0	0	0	0	0
51	48	21	7	2	1	0	0	0	0
125	127	60	21	7	2	1	0	0	0
329	352	174	65	21	7	2	1	0	0
862	963	504	190	65	21	7	2	1	0
2311	2689	1456	570	196	65	21	7	2	1

Note that OEIS A127136 points out that when $k > n/2$ there must be at least one singleton i.e. fixed point in the map, we cannot have all components of size at least two because there are only n nodes and $2k > n$. Subtracting a singleton which is in its own component with no edges to the rest of the map we have the property that in this case $K_{n,k} = K_{n-1, k-1}$.

9 Addendum II, size of the largest component

We can also compute the expectation of the size of the maximum component. This requires the OGF of cycles of trees on at most m nodes, which is

$$C_m(z) = \sum_{n=1}^m z^n [w^n] C(w) = \sum_{n=1}^m K_n z^n.$$

We then have for the number of maps $X_{n,m}$ on n nodes with component size at most m (these maps are multisets of the latter) that it is given by

$$X_{n,m} = [z^n] \exp \left(\sum_{\ell=1}^n \frac{1}{\ell} C_m(z^\ell) \right).$$

We have by inspection that $X_{0,m} = 1$ and $X_{n,0} = 0$ and by differentiation

$$X_{n,m} = \frac{1}{n} [z^{n-1}] \exp \left(\sum_{\ell=1}^n \frac{1}{\ell} C_m(z^\ell) \right) \sum_{\ell=1}^n C'_m(z^\ell) z^{\ell-1}.$$

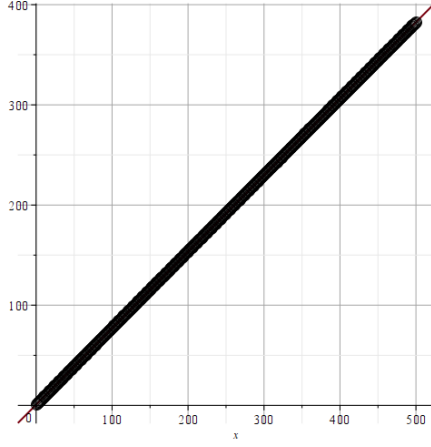


Figure 2: Average of maximum component size over all maps.

This yields

$$\begin{aligned}
X_{n,m} &= \frac{1}{n} \sum_{q=0}^{n-1} X_{n-1-q,m} [z^q] \sum_{\ell=1}^n C'_m(z^\ell) z^{\ell-1} \\
&= \frac{1}{n} \sum_{q=1}^n X_{n-q,m} [z^{q-1}] \sum_{\ell=1}^n C'_m(z^\ell) z^{\ell-1} \\
&= \frac{1}{n} \sum_{q=1}^n X_{n-q,m} [z^q] \sum_{\ell=1}^n C'_m(z^\ell) z^\ell.
\end{aligned}$$

Here we see that ℓ must divide q and we obtain for the remaining extractor (the upper range n is enforced by q)

$$\begin{aligned}
\sum_{\ell|q} [z^q] C'_m(z^\ell) z^\ell &= \sum_{\ell|q} [z^{q/\ell}] C'_m(z) z \\
&= \sum_{\ell|q} [z^{q/\ell-1}] C'_m(z) = \sum_{\substack{\ell|q, \\ q/\ell \leq m}} (q/\ell) K_{q/\ell} = \sum_{\substack{\ell|q, \\ \ell \leq m}} \ell K_\ell
\end{aligned}$$

This finally gives the recurrence

$$X_{n,m} = \frac{1}{n} \sum_{q=1}^n X_{n-q,m} \sum_{\substack{\ell|q, \\ \ell \leq m}} \ell K_\ell.$$

We then have for the maximum component size summed over all maps on n nodes that it is given by

$$M_n = \sum_{m=1}^n m(X_{n,m} - X_{n,m-1}).$$

This yields starting at $n = 1$ the sequence

1, 5, 17, 59, 183, 599, 1854, 5856, 18184, 56546, 174577, 538288, ...

The average size of the maximum component is then obtained from M_n/F_n which gives the values

1,	1.666666667,	2.428571429,	3.105263158,
3.893617021,	4.607692308,	5.405247813	6.157728707,
6.953728489,	7.726974583,	8.519691572,	9.296374972,
...			

Here we encounter a remarkably close linear fit of about $0.76 \times n$ which is shown in Figure 2, where we have computed the first 500 values.

References

- [FO89] Philippe Flajolet and Andrew Odlyzko. Random mapping statistics. Research Report 1114, Institut National de Recherche en Informatique et en Automatique, 1989.
- [FS09] Philippe Flajolet and Robert Sedgewick. *Analytic Combinatorics*. Cambridge University Press, 2009.