Undercover Underground

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Here I will briefly explain some mathematics related to the code in this project. We wish to count the number of connected graphs with no simple loops (i.e. no edge starts and ends at the same vertes), with N labelled verticies and K unlabelled edges. Let us denote the number of such graphs by $G(N,K)$. In the paper *Enumeration of Labelled Graphs* by E. N. Gilbert, the generating function for $G(N,K)/N!$ is given. The generating function is shown to be

$$log\left(1+\sum_{i=1}^{\infty}\frac{(1+y)^{\binom{i}{2}}x^i}{i!}\right). \tag{1}$$

We have the power series expansion

$$log(1+t)=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}t^n. \tag{2}$$

Thus taking $t=\sum_{i=1}^{\infty}\frac{(1+y)^{\binom{i}{2}}x^i}{i!}$, we have that the generating function (1) can be written as

$$\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\sum_{i=1}^{\infty}\frac{(1+y)^{\binom{i}{2}}x^i}{i!}\right)^n. \tag{3}$$

I should say that I did not use much of the algebra beyond this point in the code that I have posted with this project. I had a script that employed the final formula for the coefficient of $y^K x^N$, but the runtime for the script was quite long, and I abandoned it. We recall that the expansion of multinomials is given by the formula

$$(z_1+\cdots+z_m)^n=\sum_{k_1+k_2+\cdots+k_m=n}\binom{n}{k_1,k_2,\ldots,k_m}\prod_{1\leq t\leq m}z_t^{k_t}, \tag{4}$$

where

$$\binom{n}{k_1, k_2, \ldots, k_m} = \frac{n!}{k_1! k_2! \cdots k_m!}. \tag{5}$$

Taking $z_i = \dfrac{(1+y)^{\binom{i}{2}} x^i}{i!}$, and invoking the fact that for each n there are only finitely many sequences of length m non-negative integers that sum to n (I'm skirting around some detail here), we can write the generating function (1) as

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sum_{k_1+\cdots+k_m=n} \binom{n}{k_1, \cdots, k_m} \prod_{1\le t\le m} \left(\frac{(1+y)^{\binom{t}{2}} x^t}{t!} \right)^{k_t}. \tag{6}$$

The terms in this expression where x is raised to the power N will be those terms where the sequence of k_j satisfies the condition

$$\sum_{j=1}^{m} j k_j = N. \tag{7}$$

That is, for each n, the sum of the terms with an x^N term are

$$\sum \binom{n}{k_1, \ldots, k_m} \prod_{1\le t\le m} \left(\frac{(1+y)^{\binom{t}{2}} x^t}{t!} \right)^{k_t}, \tag{8}$$

where the sum is taken over the sequences of k_j staisfying both $\sum_{j=1}^m k_j = n$ and $\sum_{j=1}^m j k_j = N$. We note that the power of $(1+y)$ in the above expression is $\sum_{t=1}^m \binom{t}{2} k_t$. Employing the binomial theorem, we then have that the power of y^K in the above expression is

$$\binom{\sum_{t=1}^m \binom{t}{2} k_t}{K}. \tag{9}$$

Thus, for each n the coefficient of $y^K x^N$ is given by the sum

$$\sum \binom{n}{k_1, \ldots, k_m} \binom{\sum_{j=1}^m \binom{j}{2} k_j}{K} \prod_{1\le t\le m} \left(\frac{1}{t!} \right)^{k_t}, \tag{10}$$

where the sum is again taken over sequences k_j satisfying $\sum_{j=1}^m k_j = n$ and $\sum_{j=1}^m j k_j = N$. So finally, the coefficient of $y^K x^N$ in the generating function (1) can be written as

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sum_{\substack{k_1+\cdots+k_m=n \\ k_1+2k_2+\cdots+mk_m=N}} \binom{n}{k_1,\ldots,k_m} \binom{\sum_{j=1}^{m}\binom{j}{2}k_j}{K} \prod_{t=1}^{m} \left(\frac{1}{t!}\right)^{k_t}. \tag{11}$$

This is a nice closed formula, but unfortunately iterating over sequences k_j satisfying the condition in the second sum with a script is not extremely fast.