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COUNTING DISCONNECTED  
STRUCTURES

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# Counting Disconnected Structures

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## Abstract

When counting isomers with a given number of atoms one usually assumes that we want to count (connected) molecules. In this note we present a method that can be used for counting disconnected structures if counts of connected structures are given. The method can be used also in the reverse direction. If the numbers of all structures are known, the number of connected structures can be readily determined.

## 1 Introduction

We assume that the reader is familiar with graph-theoretic language; for a reference, see [8]. In order to present the problem addressed in this paper, we ask the following simple question. What is the number of regular graphs of valence 1 on  $n$  vertices? Let  $b_n$  denote the number of such graphs. Clearly, the only connected regular graph of valence 1 is  $K_2$ , the complete graph on two vertices that consists of a single edge. If we let  $a_n$  denote the number of connected regular graphs of valence 1 on  $n$  vertices, then we have the following table:

$n$	0	1	2	3	4	5	6	7	8	9	10	...
$a_n$	0	0	1	0	0	0	0	0	0	0	0	...

It is not hard to see that the only regular 1-valent graphs are disjoint unions of some number of  $K_2$ -s. Hence

$n$	0	1	2	3	4	5	6	7	8	9	10	...
$b_n$	1	0	1	0	1	0	1	0	1	0	1	...

Instead of writing the sequence  $a_n$  we can provide its generating function:

$$F(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \dots$$

Similarly, we can define:

$$G(x) = b_0 + b_1x + b_2x^2 + b_3x^3 + \dots$$

In our particular example we have

$$F(x) = x^2$$

and

$$G(x) = 1 + x^2 + x^4 + x^6 + \dots = 1/(1 - x^2).$$

There is a similar question for regular 2-valent graphs. The only connected ones are the cycles. Hence:

$$\begin{array}{c|cccccccccccc} n & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \dots \\ a_n & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \dots \end{array}$$

and

$$F(x) = x^3 + x^4 + x^5 + \dots = x^3/(1-x).$$

One has to think a bit before we can compile the table of **all** regular 2-valent graphs.

$$\begin{array}{c|cccccccccccc} n & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \dots \\ b_n & 1 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 3 & 4 & 5 & \dots \end{array}$$

It is not at all obvious what should the corresponding generating function  $G(x)$  look like. In this paper we will show how to apply the theory of combinatorial species for answering this question. The formula relating  $F(x)$  to  $G(x)$  is general and gives a method of calculating  $b_n$  if  $a_n$  is known and vice versa.

Long time ago we extended our computer system Vega [9] to handle similar problems. We will present examples that will show how our method can be used to obtain new enumeration results.

## 2 The Method

If  $F(x)$  is the generating function of the counting sequence of connected structures, then the corresponding generating function  $G(x)$  of the counting sequence of all structures is given by

$$G(x) = \exp \sum_{k \geq 1} \frac{F(x^k)}{k} \quad (1)$$

(cf. [1, Eqn. 1.4.20]). Applying a variant of Möbius inversion to this formula it is also possible to express  $F(x)$  in terms of  $G(x)$ :

$$F(x) = \sum_{k \geq 1} \frac{\mu(k)}{k} \log G(x^k) \quad (2)$$

where  $\mu$  denotes the well-known Möbius function (cf. [1, Eqn. 1.4.60]).

Now we give some examples.

**Example 1** Let  $a_n$  be the number of connected regular 1-valent graphs on  $n$  vertices and  $b_n$  the number of all regular 1-valent graphs on  $n$  vertices. Then  $F(x) = x^2$  and

$$G(x) = \exp \sum_{k \geq 1} \frac{x^{2k}}{k} = \exp(-\log(1-x^2)) = \frac{1}{1-x^2},$$

in agreement with our observation above.

**Example 2** Let  $a_n$  be the number of connected regular 2-valent graphs on  $n$  vertices and  $b_n$  the number of all regular 2-valent graphs on  $n$  vertices. Then  $F(x) = x^3/(1-x)$  and

$$G(x) = \exp \sum_{k \geq 1} \frac{x^{3k}}{k(1-x^k)} = 1 + x^3 + x^4 + x^5 + 2x^6 + 2x^7 + 3x^8 + 4x^9 + 5x^{10} + \dots$$

**Example 3** Let  $a_n$  be the number of connected graphs on  $n$  vertices and  $b_n$  the number of all graphs on  $n$  vertices. Then

$$F(x) = x + x^2 + 2x^3 + 6x^4 + 21x^5 + 112x^6 + 853x^7 \\ + 11117x^8 + 261080x^9 + 11716571x^{10} + \dots$$

(cf. [7, sequence A001349]) and

$$G(x) = \exp \sum_{k \geq 1} F(x^k)/k \\ = 1 + x + 2x^2 + 4x^3 + 11x^4 + 34x^5 + 156x^6 + 1044x^7 \\ + 12346x^8 + 274668x^9 + 12005168x^{10} + \dots$$

(cf. [7, sequence A000088]).

**Example 4** The number of fullerene isomers is well known (cf. [7, sequence A007894]). There is one on 20 atoms, none on 22 atoms, one on 24 atoms, etc. The values of  $a_{20}, a_{22}, a_{24}, \dots, a_{60}$  are

$$1, 0, 1, 1, 2, 3, 6, 6, 15, 17, 40, 45, 89, 116, 199, 271, 437, 580, 924, 1205, 1812, \dots$$

Thus there are 1812 non-isomorphic fullerenes on 60 atoms, one being the renowned buckminsterfullerene. Using our method we can easily compute  $b_{60} = 1892$ .

It is now a simple matter to apply the method to a number of sequences that were produced for connected structures. For instance, in [8] the initial numbers of chemical trees

$$1, 1, 1, 1, 2, 3, 5, 9, 18, 35, 75, 159, 355, 802, 1858, 4347, 10359, 24894, \dots$$

are presented (cf. [7, sequence A000602]). The corresponding numbers of chemical forests on  $n$  carbon atoms are easily computed using the same procedure.

Generically,  $b_n$  is a polynomial in  $a_1, a_2, \dots, a_n$  and vice versa. Expanding the right-hand side of (1) into power series we obtain the explicit formula

$$b_n = \sum_{j=0}^n \frac{1}{j!} \sum_{i_1 k_1 + \dots + i_j k_j = n} \frac{a_{i_1} \dots a_{i_j}}{k_1 \dots k_j}$$

where the inner sum is taken over all  $j$ -tuples  $(i_1, \dots, i_j)$  and  $(k_1, \dots, k_j)$  of positive integers whose dot product equals  $n$ . If we first differentiate (1) w.r.t.  $x$ , then expand both sides into power series we obtain the recursive formula

$$b_n = \frac{1}{n} \sum_{k=1}^n b_{n-k} \sum_{j|k} j a_j \quad \text{for } n \geq 1. \quad (3)$$

Here we list the first five  $b$ 's as polynomials in the  $a$ 's:

$$\begin{aligned} b_0 &= 1, \\ b_1 &= a_1, \\ b_2 &= (a_1 + a_1^2)/2 + a_2, \\ b_3 &= (2a_1 + 3a_1^2 + a_1^3)/6 + a_1 a_2 + a_3, \\ b_4 &= (6a_1 + 11a_1^2 + 6a_1^3 + a_1^4)/24 + (a_2 + a_1 a_2 + a_1^2 a_2 + a_2^2)/2 + a_1 a_3 + a_4. \end{aligned}$$

In general, we always have  $b_n = a_n + B_n(a_1, a_2, \dots, a_{n-1})$ . All the coefficients of  $B_n$  are non-negative, and the products  $a_p^q a_r^s \dots$  have the property that  $pq + rs + \dots \leq n$ .

From (2) we obtain similarly

$$a_n = \sum_{k|n} \frac{\mu(k)}{k} \sum_{(i_1+\dots+i_j)k=n} \frac{(-1)^{j+1}}{j} b_{i_1} \cdots b_{i_j}$$

where the inner sum is taken over all  $j$ -tuples  $(i_1, \dots, i_j)$  of positive integers whose sum equals  $n/k$ . From (3) we also obtain the recursive formula

$$a_n = b_n - \frac{1}{n} \left( \sum_{\substack{j|n \\ j \neq n}} j a_j + \sum_{k=1}^{n-1} b_{n-k} \sum_{j|k} j a_j \right) \quad \text{for } n \geq 1.$$

Here we list the first six  $a$ 's as polynomials in the  $b$ 's:

$$\begin{aligned} a_0 &= 0, \\ a_1 &= b_1, \\ a_2 &= b_2 - (b_1 + b_1^2)/2, \\ a_3 &= b_3 - b_1 b_2 - (b_1 - b_1^3)/3, \\ a_4 &= b_4 - b_1 b_3 + b_1^2 b_2 - (b_2 + b_2^2)/2 + (b_1^2 - b_1^4)/4, \\ a_5 &= b_5 - b_1 b_4 + b_1^2 b_3 + b_1 b_2^2 - b_1^3 b_2 - b_2 b_3 + (b_1^5 - b_1)/5. \end{aligned}$$

Again we have  $a_n = b_n - A_n(b_1, b_2, \dots, b_{n-1})$ , and the products  $a_p^q a_r^s \cdots$  in  $A_n$  have the property that  $pq + rs + \cdots \leq n$ .

### 3 A Related Problem

Finally, let us turn to another problem. Let us start with a sequence  $a_n$  counting connected objects of certain type on  $n$  elements. Assume that a disconnected object on  $n$  elements can be formed by selecting  $k$  identical connected objects with  $m$  elements where  $m \cdot k = n$ . Let  $b_n$  count the total number of elements. Then  $b_n = \sum_{k|n} a_k$  and, by Möbius inversion,  $a_n = \sum_{k|n} \mu(n/k) b_k$ .

**Example 5** Let  $a_n$  be the number of connected vertex-transitive graphs on  $n$  vertices. Then  $b_n$  is the total number of vertex-transitive graphs on  $n$  vertices.

**Example 6** The generalized Petersen graph  $G(n, k)$  is a graph with vertex set

$$V(G(n, k)) = \{u_0, u_1, \dots, u_{n-1}, v_0, v_1, \dots, v_{n-1}\}$$

and edge set

$$E(G(n, k)) = \{u_i u_{i+1}, u_i v_i, v_i v_{i+k} : i = 0, \dots, n-1\}.$$

Here subscripts are to be read modulo  $n$ . Note that  $G(n, k)$  is isomorphic to  $G(n, n-k)$ , and  $G(n, n/2)$  is not simple. Therefore, for  $n \geq 3$ , we consider only graphs  $G(n, k)$  where  $k < n/2$ .

Generalized Petersen graphs constitute a standard family of graphs which represents a generalization of the renowned Petersen graph  $G(5, 2)$ . This important and well-known family of graphs introduced in 1969 by Mark Watkins [10] possesses a number of interesting properties. For example,  $G(n, r)$  is vertex transitive if and only if  $n = 10$ ,  $r = 2$  or  $r^2 \equiv \pm 1 \pmod{n}$ . It is a Cayley graph if and only if  $r^2 \equiv 1 \pmod{n}$ . It is arc-transitive only in the following seven cases:  $(n, r) = (4, 1), (5, 2), (8, 3), (10, 2), (10, 3), (12, 5), (24, 5)$ . The family contains some very important

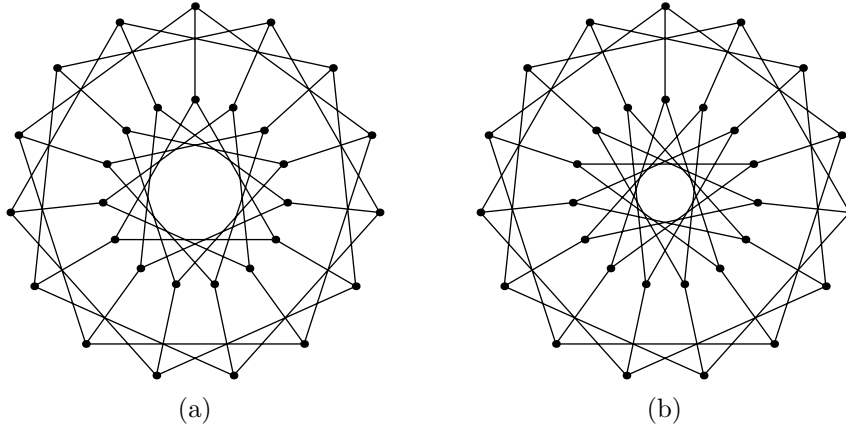


Figure 1: I-graphs  $I(15, 3, 5)$  (a) and  $I(15, 3, 6)$  (b). The former is connected and the latter is not.

graphs, such as the  $n$ -prism  $G(n, 1)$ , the Dürer graph  $G(6, 2)$ , the Möbius-Kantor graph  $G(8, 3)$ , the dodecahedron  $G(10, 2)$ , the Desargues graph  $G(10, 3)$ , etc.

The generalized Petersen graphs form a special case of the so-called I-graphs, see [6]. The *I-graph*  $I(n, j, k)$  is a graph with vertex set

$$V(I(n, j, k)) = \{u_0, u_1, \dots, u_{n-1}, v_0, v_1, \dots, v_{n-1}\}$$

and edge set

$$E(I(n, j, k)) = \{u_i u_{i+j}, u_i v_i, v_i v_{i+k} : i = 0, \dots, n-1\}.$$

Since  $I(n, j, k) = I(n, k, j)$  we usually assume that  $j \leq k$ . Clearly  $G(n, k) = I(n, 1, k)$ . Following the usual representation of these graphs where we draw vertices  $u_i$  on one circle and vertices  $v_i$  on another concentric circle (with smaller radius), we call  $u_i$  and  $v_i$  the *vertices on the outer rim* and the *vertices on the inner rim*, respectively. The edges between the two rims are called *spokes*. The class of graphs  $I(n, j, k)$  contains the class  $G(n, k)$ . The I-graphs  $I(15, 3, 5)$  and  $I(15, 3, 6)$  are depicted in Figure 1.

If  $a_n$  counts connected I-graphs then  $b_n$  counts all I-graphs.

**Example 7** There are only 7 arc-transitive I-graphs. They are the generalized Petersen graphs  $G(4, 1)$ ,  $G(5, 2)$ ,  $G(8, 3)$ ,  $G(10, 2)$ ,  $G(10, 3)$ ,  $G(12, 5)$ ,  $G(24, 5)$ . Hence

$$\begin{array}{c|cccccccccccc} n & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \dots \\ a_n & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 2 & \dots \end{array}$$

There are infinitely many arc-transitive I-graphs if we drop the condition of connectivity.

$$\begin{array}{c|cccccccccccc} n & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \dots \\ b_n & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 2 & 0 & 3 & \dots \end{array}$$

If we think of  $a$  and  $b$  as infinite column vectors  $a = (a_1, a_2, \dots)^T$  etc., then there is an infinite triangular 0-1 matrix  $M$  such that  $b = Ma$ .

Clearly  $(M)_{nk} = 1$  if and only if  $k | n$ , and we have

$$\begin{aligned} b_1 &= a_1, \\ b_2 &= a_1 + a_2, \\ b_3 &= a_1 + a_3, \\ b_4 &= a_1 + a_2 + a_4, \quad \text{etc.} \end{aligned}$$

Let  $N$  be the inverse of  $M$ . Matrices  $M$  and  $N$  do not depend on  $a$  (or  $b$ ). By Möbius inversion,  $(N)_{nk} = \mu(n/k)$  if  $k | n$ , otherwise 0. Hence

$$\begin{aligned} a_1 &= b_1, \\ a_2 &= -b_1 + b_2, \\ a_3 &= -b_1 + b_3, \\ a_4 &= -b_2 + b_4, \quad \text{etc.} \end{aligned}$$

## 4 Conclusion

The method explained in this paper has numerous applications not only in mathematics and computer science but also in chemistry. A possible application would be to find connected particles from a mass spectrogram that presents also some particle combinations.

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