Inversion of Cycle Index Sum Relations for 2- and 3- Connected Graphs

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Abstract

Algebraic inversion of cycle index sum relations is employed to derive new algorithms for counting unlabeled graphs which are (a) 2-connected, (b) 2-connected and homeomorphically irreducible, and (c) 3-connected. The new algorithms are significantly more efficient than earlier ones, both asymptotically and for modest values of the order. Time- and space-complexity analyses of the algorithms are provided. Tables of computed results are included for the number n of nodes satisfying $n \leq 26$ in case (a) and $n \leq 25$ in cases (b) and (c). These are totals over all values of the number q of edges. Tables showing the breakdown by number of edges are included for $n \leq 16$ in case (a) and $n \leq 18$ in cases (b) and (c).

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Key Words:

graphs, unlabeled graphs, counting, enumeration, cycle index, formal power series, inversion

1 Introduction

A graph is assumed to be finite and undirected, with neither loops nor multiple edges. A graph with at least $k+1$ nodes ($k \geq 1$) is defined to be k-connected if it is connected and (for $k \geq 2$) cannot be disconnected by removing fewer than k nodes and their incident edges. The k-connectedness of smaller graphs can be defined arbitrarily, and we choose to define the smallest 1- , 2- and 3-connected graphs to be the complete graphs on 1, 2 and 4 nodes, respectively.

For enumeration purposes, an unlabelled graph is an isomorphism class of (labelled) graphs. Counting graphs with prescribed properties usually involves decomposing a graph into a core and components. For unlabelled graphs it also involves keeping track of the number of automorphisms of the core with a given cycle decomposition by means of a cycle index [2, ch. 2.2]. In the case of counting all n-node graphs, the core is the complete graph on n nodes, in which each edge is replaced by a component with 2 nodes and 0 or 1 edge to obtain the graphs to be counted; in the case of counting connected graphs, the core is a set, in which each element is replaced by a component, which is a connected graph, to obtain an arbitrary graph. In both cases, the cycle structures of the automorphisms of the core are known. Thus one can compute the sum of the cycle indices of the automorphism groups of all possible cores (cycle index sum for cores) and then use Pólya's theorem, which relates this cycle index sum and the counting series for components and compositions [2, ch. 4.1 and 4.2]. When counting graphs with up to n nodes on a computer, one stores only counting series and sums once over a cycle index sum; thus the space-complexity is polynomial in n, and the time-complexity is bounded by the number of terms in the cycle index sum (which is $p'(n)$, the number of partitions of all the numbers up to n) multiplied by a polynomial in n for the computation done on the counting series for each coefficient of the cycle index sum.

In the case of counting 2-connected graphs, the core is a set of rooted 2-connected graphs joined at the root; every other node has a rooted connected graph attached to it, to obtain another rooted connected graph. The unknown is now the cycle index sum for cores, from which the counting series can be obtained. However, this cycle index sum cannot be obtained from the counting series for components and composition; thus it was necessary to generalize Pólya's theorem to relate not counting series but cycle index sums for components and compositions to those for cores [4 and 2, ch. 8.6]. A straight-forward solution of such a relation involves storing and computing with the coefficients of cycle index sums. In that fashion, the space-complexity is bounded below by $p'(n)$ and the time-complexity by a power of $p'(n)$.

In the case of counting 2-connected graphs with no vertices of degree ≤ 2, the core is just such a graph, in which each edge is replaced by a series-parallel network to obtain an arbitrary 2-connected graph (except one which becomes a series-parallel network if an edge is deleted and its ends distinguished as poles). In the case of counting 3-connected graphs, the core is a 3-connected graph (or a polygon or a set of ≥ 3 parallel edges), in which each edge is replaced by a more general 2-pole network (a 2-connected graph with an edge removed) to obtain an arbitrary 2-connected graph. The latter decomposition is not unique, so correction terms are required. In these cases too, the unknown is the cycle index sum for cores. But now the cycle index sums which would have to be stored for a straight-forward solution contain not only node-cycles (necessary to compute the cycle index sum for 2-connected graphs) but also two types of edge-cycles: cycles which preserve the orientation of the edge and thus fix the poles of the network which replaces it, and cycles which reverse the orientation and thus exchange the poles [5]. The space and time requirements grow so explosively with n that it wasn't feasible to go much beyond 9 nodes with numerical computations.

An algebraic method of extracting counting series from systems of equations involving cycle index sums was presented in [1], where it was applied to counting 2-edge-connected graphs. The present paper presents an application of this method to counting 2-connected graphs (developed in 1978 by the first author of this paper but not published), 2-connected graphs without vertices of degree ≤ 2, and 3-connected graphs. Once the equations have been solved by hand, extracting the numbers by computer involves storing only counting series and summing $O(n)$ times over the coefficients of a cycle index sum. The time- and space-complexity of such a computation is essentially the same as for Pólya's theorem; so we were able to count the above-mentioned classes of graphs with up to 18 nodes when the number of edges is included as a parameter, and up to 25 or 26 nodes otherwise. Tables of numbers are given at the end of this article.

The cycle index sums relevant to counting unlabeled 2- and 3- connected graphs can be viewed as members of the commutative ring $Q[b_1, c_1, b_2, c_2, \ldots]$ $[[a_1, a_2, \ldots]]$, where Q is the rationals, a_i is an indeterminate representing an i-cycle of nodes for $i = 1, 2, 3, \ldots$, b_i represents an orientation-preserving i-cycle of edges for $i = 1, 2, 3, \ldots$, and c_i represents an orientation-reversing i-cycle of edges for $i = 1, 2, 3, \ldots$. The counting series which are the ultimate objective to compute (up to some given order) lie in the ring $Z[y][[x]]$ where Z is the integers, x represents a node and y represents an edge.

If J is the cycle index sum for a class of graphs, then the counting series for that class is obtained from J by substituting x^i for a_i, y^i for b_i, and y^i for c_i, for $i = 1, 2, 3, \ldots$. This set of substitutions defines a homomorphism from the cycle index sum ring to the counting series ring. The image of J under this homomorphism is denoted $J[x, y, y]$. More generally, the expression $J[\alpha(x, y), \beta(x, y), \gamma(x, y)]$ will denote the result of substituting $\alpha(x^i, y^i)$ for $a_i, \beta(x^i, y^i)$ for b_i, and $\gamma(x^i, y^i)$ for c_i, for $i = 1, 2, 3, \ldots$. In this way the triple $\alpha(x, y), \beta(x, y), \gamma(x, y)$ of series in $Q[y][[x]]$ defines a more general homomorphism from the cycle index sum ring to the counting series ring.

The defining relations for 2- and 3- connected unlabeled graphs are expressed in terms of cycle index sums. These relations are transformed by an appropriate choice of ring homomorphism so that one of them involves the desired counting series. The fundamental algebraic facts upon which this approach depends are that homomorphisms may be composed, and are associative under composition. In [1] the essential principles of this method are presented in a simpler case: only node cycles were represented in the cycle index sums. The introductory material on pages 278-81 of that paper may be found useful in supplementing this paper. We note here that only node cycles are needed to count 2-connected graphs. The relevant relations are presented and solved in greater generality here because this is needed for the other enumerations. The reader wishing a primer may want to go through Section 2 changing c_i to $b_i, \beta(x,y)$ and $\gamma(x,y)$ to y, and $\beta(x^i,y^i)$ and $\gamma(x^i,y^i)$ to y^i.

2 2-Connected Graphs

Let K, G, C and B denote the cycle index sums for the complete graphs, all graphs, the connected graphs, and the 2-connected graphs, respectively. The defining relations were derived in [4], and received a careful exposition in [2, Chapter 8]. In listing these relations below, we have used $'$ to denote $\frac{\partial}{\partial a_1}$. For any cycle index sum S, let $S_{(j)}$ denote the image of S under the homomorphism defined by substituting a_{ij} for a_i, b_{ij} for b_i and c_{ij} for $c_i, i = 1, 2, 3, \ldots$. For this section, let $[S]$ denote the homomorphism obtained by substituting $S_{(j)}$ for the node-cycle variable $a_j, j = 1, 2, 3, \ldots$, and leaving the edge-cycle variables unchanged.

The relations which define K and determine G, C, and B from K can be expressed as follows:

$$K = \sum_{\vec{\sigma}} \Lambda(\vec{\sigma}) \prod_i \frac{a_i^{\sigma_i}}{\sigma_i! i^{\sigma_i}} \tag{1}$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \cdots)$, each $\sigma_i \geq 0$,

$$\Lambda(\vec{\sigma}) = \prod_{i<j} b_{[i,j]}^{(i,j)\sigma_i\sigma_j} \prod_i b_i^{i\sigma_i(\sigma_i-1)/2+\lfloor\frac{i-1}{2}\rfloor\sigma_i} \prod_i c_i^{\sigma_{2i}},$$

$[i, j]$ is the least common multiple of i and j, and (i, j) is the greatest common divisor;

$$G = K[a_i \leftarrow a_i,\ b_i \leftarrow 1 + b_i,\ c_i \leftarrow 1 + c_i]; \tag{2}$$

$$G = \exp\left(\sum \frac{1}{i} a_i[C]\right); \tag{3}$$

$$a_1 C' = a_1 \exp\left(\sum \frac{1}{i} a_i[B'[a_1 C']]\right); \tag{4}$$

$$C = (a_1 + B - a_1 B')[a_1 C']. \tag{5}$$

The desired counting series is $B[x, y, y]$. Equation (5) contains $B[a_1 C']$, in which each a_j of B is replaced by $(a_1 C')_{(j)}$ instead of x^j; so we choose a ring homomorphism which maps $a_1 C'$ onto x. Suppose that counting series $\beta(x, y)$ and $\gamma(x, y)$ are given (for counting 2-connected graphs we can assume that they are both y) and we wish to determine a third counting series $\alpha(x, y)$ such that

$$(a_1 C')[\alpha(x, y), \beta(x, y), \gamma(x, y)] = x. \tag{6}$$

To see that such a series exists, define the <u>order</u> of a term in a cycle index sum to be the exponent of x resulting from the substitution $a_j \leftarrow x^j$; then $a_1 C' = a_1 + a_1^2 b_1 +$ (terms of higher order). Now (6) is equivalent to

$$\alpha(x, y) = x - (a_1 C' - a_1)[\alpha(x, y), \beta(x, y), \gamma(x, y)],$$

which can be seen to define $\alpha(x, y)$ iteratively in powers of x. One has $\alpha(0, y) = 0$ to start; having found $\alpha(x, y)$ through powers of x^{n-1}, substitution in the right side gives $\alpha(x, y)$ correctly through the coefficient of x^n.

The strategy now is to apply homomorphisms and simplify using associativity and the given relations in such a way that the only cycle index sum remaining in the system of equations is K. Since K is known explicitly, the need for computations within the cycle index sum ring will have been obviated.

Applying (4) over the homomorphism $[\alpha(x, y), \beta(x, y), \gamma(x, y)]$ and using (6), one has

$$\alpha(x, y) = x \exp(-\sum \frac{1}{i} B'[x^i, \beta(x^i, y^i), \gamma(x^i, y^i)]).$$

Taking the natural logarithm and applying Möbius inversion [2, p.183], one has

$$B'[x, \beta(x,y), \gamma(x,y)] = -\sum \frac{\mu(k)}{k} ln(\alpha(x^k, y^k)/x^k)$$

If we denote $G[\alpha(x,y), \beta(x,y), \gamma(x,y)]$ by $f(x,y)$ then (3) can be solved in the same way to obtain

$$C[\alpha(x,y), \beta(x,y), \gamma(x,y)] = \sum \frac{\mu(k)}{k} lnf(x^k, y^k).$$

One can then apply (5) over the homomorphism $[\alpha(x,y), \beta(x,y), \gamma(x,y)]$ to find

$$B[x, \beta(x,y), \gamma(x,y)] = -x + \sum \frac{\mu(k)}{k} \left\{ lnf(x^k, y^k) - xln(\alpha(x^k, y^k)/x^k) \right\}. \tag{7}$$

Finally, operating on (3) with $a_1 \frac{\partial}{\partial a_1}$ gives

$$a_1 G' = G \cdot a_1 C'.$$

Composed over $[\alpha(x,y), \beta(x,y), \gamma(x,y)]$, expressed in terms of K using (2), and simplified using (6), this gives

$$(a_1 K')[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)] = xK[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)]. \tag{8}$$

From (1) it is immediate that $a_1 K'$ can be directly calculated (add a factor of σ_1 inside the sum). Thus (8) can be applied to calculate $\alpha(x,y)$ iteratively to any desired order in x. Note that the right side of (8) is $xf(x,y)$, so that $f(x,y)$ is determined at the same time. Then (7) completes the determination of $B[x, \beta(x,y), \gamma(x,y)]$ with the help of formal logarithms.

For the sake of completeness, note that in general, if $F(0,y) = 0$ and $L(x,y) = ln(1 + F(x,y))$ then $L(0,y) = 0$ and differentiation with respect to x gives

$$F'(x,y) = L'(x,y) + L'(x,y)F(x,y).$$

For $n \geq 1$ a comparison of coefficients of $x^{n-1}y^k$ then leads to

$$L_{n,k} = F_{n,k} - \frac{1}{n} \sum_{m=1}^{n-1} \sum_{i=0}^{k} m L_{m,i} F_{n-m,k-i}.$$

The latter shows how to calculate the logarithms needed in (7); see [2, p.9] for a fuller exposition of the general method.

The counting series for unlabeled 2-connected graphs in terms of nodes and edges is $B[x, y, y]$, so one can apply (7) and (8) with $\beta(x, y) = \gamma(x, y) = y$. The resulting equations were used to calculate the numbers through 16 nodes, with all the different numbers of edges (see Table IV). If only the total by nodes is desired, the calculation is much faster. The equations obtained from (7) and (8) by setting $\beta(x, y) = \gamma(x, y) = 1$ only require calculation in the single variable using $Q[[x]]$. In this way the totals through 26 nodes were computed (see Table I).

3 2-Connected Graphs without Nodes of Degree Two

Let B denote the cycle index sum for all 2-connected graphs (as in §2), and let I denote the cycle index sum for those with no nodes of degree two (homeomorphically irreducible) except for the single edge. Auxilliary cycle index sums which will be needed to determine I from B are as follows: R for series-parallel graphs; D^+ and D^- for all 2-pole series-parallel networks; S^+ and S^- for series-union networks; P^+ and P^- for parallel-union networks, including the single edge; and K^+, K^- for all networks with non-adjacent poles. Here the superscripts + and − represent pole-preserving and pole-reversing automorphisms, respectively. The following relations were derived in [5] in essentially this form, but with a few typographical errors corrected:

$$I[a_1, D^+, D^-] = B - R; \tag{9}$$

$$S^+ = a_1 D^+ P^+; \tag{10}$$

$$S^- = P^+_{(2)} \cdot (a_1 + a_2 D^-); \tag{11}$$

$$K^+ = \exp\left(\sum \frac{1}{k} S^+_{(k)}\right); \tag{12}$$

$$K^- = \exp\left(\sum_{k\ odd} \frac{1}{k} S^-_{(k)} + \sum_{k\ even} \frac{1}{k} S^+_{(k)}\right); \tag{13}$$

$$D^+ = (1 + b_1)K^+ - 1; \tag{14}$$

$$
\begin{aligned}
D^- &= (1+c_1)K^- - 1; && (15)\\
P^+ &= D^+ - S^+; && (16)\\
P^- &= D^- - S^-; && (17)\\
R &= -\frac{1}{2}a_1P^+ - \frac{1}{4}a_1^2(P^+)^2 - \frac{1}{4}a_2P^+_{(2)} && (18)\\
&+ \frac{1}{2}\sum \frac{\phi(d)}{d}(-ln(1-a_dP^+_{(d)}))\\
&+ (1-a_2P^+_{(2)})^{-1}P^+_{(2)}\left(\frac{1}{2}a_1a_2P^- + \frac{1}{4}a_2^2(P^-)^2 + \frac{1}{4}a_1^2a_2P^+_{(2)}\right)\\
&+ \frac{1}{2}a_1^2P^+ + \frac{1}{2}a_2P^- - \frac{1}{4}(a_1^2+a_2)S^+_{(2)}\\
&- \frac{1}{4}a_1^2S^+(D^++P^+) - \frac{1}{4}a_2S^-(D^-+P^-),
\end{aligned}
$$

where $\phi(d)$ is the Euler totient function.

For this section and the next, $[U, V, W]$ for cycle index sums U, V, W denotes the ring homomorphism which maps a_i to $U_{(i)}$, b_i to $V_{(i)}$ and c_i to $W_{(i)}$ for $i = 1, 2, 3, \ldots$. The notation is used in equation (9). When u, v, and w are counting series the corresponding notation $[u(x,y), v(x,y), w(x,y)]$ denotes the ring homomorphism which maps a_i to $u(x^i, y^i)$, b_i to $v(x^i, y^i)$, and c_i to $w(x^i, y^i)$ for $i = 1, 2, 3, \ldots$. Notice the compatibility of these notations. In particular, the "inflation" from U to $U_{(j)}$ can be delayed in composing over power series, because

$$U_{(j)}[\alpha(x,y), \beta(x,y), \gamma(x,y)] = U[\alpha(x^j, y^j), \beta(x^j, y^j), \gamma(x^j, y^j)].$$

This general fact, along with the associativity of composition for homomorphisms, is relied on frequently and without specific mention in performing algebraic simplifications in what follows.

To extract $I[x, y, y]$ from equation (9), which involves $I[a_1, D^+, D^-]$, let $\beta(x, y)$ and $\gamma(x, y)$ denote for the remainder of this section power series satisfying

$$D^+[x, \beta(x,y), \gamma(x,y)] = y, \qquad (19)$$

$$D^-[x, \beta(x,y), \gamma(x,y)] = y. \qquad (20)$$

To see that $\beta(x,y)$ and $\gamma(x,y)$ exist and are unique, note that

$$D^{+} = b_1 + a_1 b_1^2 + a_1 b_1^3 + \cdots,$$

$$D^{-} = c_1 + a_1 b_2 + a_1 b_2 c_1 + \cdots.$$

where the remaining terms are of higher order in the node-cycle variables. Thus the conditions to be satisfied can be expressed in the form

$$\beta(x,y) = y - x\beta(x,y)^2 - x\beta(x,y)^3 \mp \cdots,$$

$$\gamma(x,y) = y - x\beta(x^2,y^2) - x\beta(x^2,y^2)\gamma(x,y) \mp \cdots.$$

From these we have first

$$\beta(x,y) = y \mp \cdots,$$

$$\gamma(x,y) = y \mp \cdots,$$

then substituting on the right side we have

$$\beta(x,y) = y - x(y^2 + y^3) \mp \cdots,$$

$$\gamma(x,y) = y - x(y^2 + y^3) \mp \cdots.$$

Each iteration increases by one the power of x to which the approximation is correct. In this way one sees by induction simultaneously for $\beta(x,y)$ and $\gamma(x,y)$ that existence and uniqueness are guaranteed through the terms in x^n, for $n = 0, 1, 2, \ldots$.

We can now proceed to determine $\beta(x,y)$, $\gamma(x,y)$, and $R[x,\beta(x,y),\gamma(x,y)]$ by combining equations (10) through (20). To shorten the notation, let $\tilde{R}$ denote $R[x,\beta(x,y),\gamma(x,y)]$ and likewise for other cycle index sums. From (10), (11), (19), and (20)

$$\tilde{S}^{+} = xy\tilde{P}^{+} \text{ and } \tilde{S}^{-} = (x + x^2 y)\tilde{P}^{+}_{(2)},$$

while from (16) and (17) with (19) and (20)

$$y = \tilde{P}^{+} + \tilde{S}^{+} \text{ and } y = \tilde{P}^{-} + \tilde{S}^{-}.$$

Combining, we have

$$y = \tilde{P}^{+} + xy\tilde{P}^{+}$$

and so

$$\tilde{P}^{+} = y(1+xy)^{-1} \text{ and } \tilde{S}^{+} = xy^2(1+xy)^{-1}.$$

In turn,

$$\tilde{S}^{-} = (x + x^2y)\cdot y^2(1+x^2y^2)^{-1} = xy^2(1+xy)(1+x^2y^2)^{-1},$$

$$\tilde{P}^{-} = y - xy^2(1+xy)(1+x^2y^2)^{-1} = y(1-xy)(1+x^2y^2)^{-1}.$$

Now

$$\begin{aligned}
\tilde{S}^{+} &= \sum_{i=1}^{\infty}(-1)^{i-1}x^iy^{i+1}, \\
\sum_{k=1}^{\infty}\frac{1}{k}\tilde{S}^{+}_{(k)} &= \sum_{k=1}^{\infty}\frac{1}{k}\sum_{i=1}^{\infty}(-1)^{i-1}x^{ik}y^{ik+k} \\
&= \sum_{i=1}^{\infty}(-1)^{i-1}\sum_{k=1}^{\infty}\frac{(x^iy^{i+1})^k}{k} \\
&= \sum_{i=1}^{\infty}(-1)^{i-1}(-ln(1-x^iy^{i+1})) \\
&= \sum_{i=1}^{\infty}(-1)^{i}ln(1-x^iy^{i+1}),
\end{aligned}$$

so from (12) we find

$$\begin{aligned}
\tilde{K}^{+} &= \prod_{i=1}^{\infty}(1-x^iy^{i+1})^{(-1)^i} = (1-xy^2)^{-1}(1-x^2y^3)(1-x^3y^4)^{-1}\cdots. \\
&= \prod_{j=1}^{\infty}(1-x^{2j-1}y^{2j})^{-1}(1-x^{2j}y^{2j+1}).
\end{aligned}$$

Thus (14) can be solved explicitly for $\beta(x,y)$;

$$\beta(x,y) = -1 + (1+y)\prod_{j=1}^{\infty}(1-x^{2j-1}y^{2j})(1-x^{2j}y^{2j+1})^{-1}. \tag{21}$$

In much the same way, our explicit expressions for $\tilde{S}^{+}$ and $\tilde{S}^{-}$ can be combined with (13) and (15) to deduce that

$$\gamma(x,y) = -1 + (1+y)\prod_{i=1}^{\infty}\frac{(1-x^{4i-3}y^{4i-2})(1+x^{4i-1}y^{4i})}{(1+x^{4i-2}y^{4i-1})(1-x^{4i}y^{4i+1})}. \tag{22}$$

We are now in a position to evaluate each term on the right side of (18) explicitly. There is considerable cancellation, and for simplifying the sum containing Euler's totient function it is helpful to observe the identity

$$\sum_{i|k}(-1)^{i-1}\phi\left(\frac{k}{i}\right) = \begin{cases} k & if \quad k \quad is \quad odd, \\ 0 & if \quad k \quad is \quad even. \end{cases}$$

The net result is

$$\tilde{R} = -x^2y^2 + xy(x + xy(1-x))(1 - x^4y^4)^{-1}.$$

From (9), (19), and (20) we thus have

$$I[x,y,y] = \tilde{B} + x^2y^2 - xy(x + xy(1-x))(1 - x^4y^4)^{-1}. \tag{23}$$

This is the counting series for unlabeled homeomorphically irreducible 2-connected graphs by number of nodes and edges. To complete the evaluation, treat

$$\tilde{B} = B[x, \beta(x,y), \gamma(x,y)]$$

as described in the previous section. That is, with $\beta(x,y)$ and $\gamma(x,y)$ as given in (21) and (22), apply (8) to determine corresponding series $\alpha(x,y)$ and $f(x,y)$ in iterative fashion. Then (7) can be used to calculate $\tilde{B}$ from $\alpha(x,y)$ and $f(x,y)$. In this way homeomorphically irreducible 2-connected graphs were counted by nodes and edges up to 18 nodes (see Table V) and by nodes alone up to 25 nodes (see Table II).

4 3-Connected Graphs

Let F denote the cycle index sum for all 3-connected graphs, and (as in previous sections) let B denote the cycle index sum for all 2-connected graphs. Auxilliary cycle index sums needed to determine F from B are the following: D^+ and D^- for all (nonempty) 2-pole networks; K^+ and K^- for 2-pole networks with non-adjacent poles; P^+ and P^- for parallel networks (including the single edge); S^+ and S^- for series networks; Q^+ and Q^- for non-series networks; and H^+ for h-networks (non-series and non-parallel). As in the previous section the superscripts $+$ and $-$ refer to pole-preserving and pole-reversing automorphisms, respectively. The following relations were derived in [5]:

$$
\begin{aligned}
F[a_1, D^+, D^-] &= B - (\frac{1}{2}a_1^2 P^+ + \frac{1}{2}a_2 P^-) \\
&+ \frac{1}{2}a_1 Q^+ + \frac{1}{4}a_2 Q^+_{(2)} \\
&+ \frac{1}{2}\sum \frac{\phi(d)}{d} ln(1 - a_d Q^+_{(d)}) \\
&- Q^+_{(2)}(1 - a_2 Q^+_{(2)})^{-1}\left(\frac{1}{2}a_1 a_2 Q^- + \frac{1}{4}a_2^2 (Q^-)^2 + \frac{1}{4}a_1^2 a_2 Q^+_{(2)}\right) \\
&+ \frac{1}{4}(a_1^2 + a_2) S^+_{(2)} + \frac{1}{4}a_1^2 D^+(D^+ + 2H^+) \\
&+ \frac{1}{2}a_2 D^-(D^- - P^-) - \frac{1}{4}a_2 (S^-)^2;
\end{aligned}
\tag{24}
$$

$$K^+ = \exp \sum \frac{1}{k}(D^+_{(k)} - P^+_{(k)}); \tag{25}$$

$$K^- = \exp \left\{ \sum_{k\ odd} \frac{1}{k}(D^-_{(k)} - P^-_{(k)}) + \sum_{k\ even} \frac{1}{k}(D^+_{(k)} - P^+_{(k)}) \right\}; \tag{26}$$

$$S^+ = a_1 D^+(D^+ - S^+); \tag{27}$$

$$S^- = (a_1 + a_2 D^-)(D^+_{(2)} - S^+_{(2)}); \tag{28}$$

$$Q^+ = D^+ - S^+; \tag{29}$$

$$Q^- = D^- - S^-; \tag{30}$$

$$H^+ = Q^+ - P^+; \tag{31}$$

$$D^+ = (1 + b_1)K^+ - 1; \tag{32}$$

$$D^- = (1 + c_1)K^- - 1; \tag{33}$$

$$K^+ = \frac{2}{a_1^2}\frac{\partial B}{\partial b_1}; \tag{34}$$

$$K^- = \frac{2}{a_2}\frac{\partial B}{\partial c_1}. \tag{35}$$

In order to invert (24) we will need counting series $\beta(x, y)$ and $\gamma(x, y)$ satisfying

$$D^+[x, \beta(x, y), \gamma(x, y)] = y, \tag{36}$$

$$D^{-}[x, \beta(x,y), \gamma(x,y)] = y. \tag{37}$$

By (32), (33), (34) and (35), these are equivalent to

$$(1 + \beta(x,y)) \frac{2}{x^2} \frac{\partial B}{\partial b_1}[x, \beta(x,y), \gamma(x,y)] = 1 + y, \tag{38}$$

$$(1 + \gamma(x,y)) \frac{2}{x^2} \frac{\partial B}{\partial c_1}[x, \beta(x,y), \gamma(x,y)] = 1 + y. \tag{39}$$

To rewrite these relations in terms of the connected graph cycle index sum C (and ultimately, the complete graph cycle index sum K), we use

$$\frac{\partial B}{\partial b_1}[a_1 C', b_1, c_1] = \frac{\partial C}{\partial b_1}, \tag{40}$$

$$\frac{\partial B}{\partial c_1}[a_1 C', b_1, c_1] = \frac{\partial C}{\partial c_1}. \tag{41}$$

These latter can be seen directly from the decomposition of an edge-rooted connected graph into an edge-rooted block along with node-rooted connected branches at the nodes of the block (a block is a 2-connected graph). Alternatively, they can be derived from equations (4) and (5) of Section 2 by appropriate differentiation and simplification.

In any case, a third power series $\alpha(x,y)$ is needed to proceed with the inversion, such that

$$(a_1 C')[\alpha(x,y), \beta(x,y), \gamma(x,y)] = x. \tag{42}$$

Then (40) can be combined with (38) and (41) with (39), giving

$$(1 + \beta(x,y)) \frac{2}{x^2} \frac{\partial C}{\partial b_1}[\alpha(x,y), \beta(x,y), \gamma(x,y)] = 1 + y, \tag{43}$$

$$(1 + \gamma(x,y)) \frac{2}{x^2} \frac{\partial C}{\partial c_1}[\alpha(x,y), \beta(x,y), \gamma(x,y)] = 1 + y. \tag{44}$$

Next, equations (2) and (3) can be differentiated to yield

$$a_1 C' K[a_1, 1 + b_1, 1 + c_1] = a_1 K'[a_1, 1 + b_1, 1 + c_1], \tag{45}$$

$$\frac{\partial C}{\partial b_1}K[a_1, 1+b_1, 1+c_1] = \frac{\partial K}{\partial b_1}[a_1, 1+b_1, 1+c_1], \tag{46}$$

$$\frac{\partial C}{\partial c_1}K[a_1, 1+b_1, 1+c_1] = \frac{\partial K}{\partial c_1}[a_1, 1+b_1, 1+c_1]. \tag{47}$$

Then (42) can be combined with (45), (43) with (46), and (44) with (47) to deduce

$$xK[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)] = (a_1K')[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)], \tag{48}$$

$$x^2(1+y)K[a(x,y), 1+\beta(x,y), 1+\gamma(x,y)] = \left(2b_1\frac{\partial K}{\partial b_1}\right)[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)], \tag{49}$$

$$x^2(1+y)K[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)] = \left(2c_1\frac{\partial K}{\partial c_1}\right)[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)]. \tag{50}$$

To see how (48), (49) and (50) determine the three unknown counting series uniquely, note that

$$\begin{aligned}
K &= 1 + a_1 + \frac{1}{2}a_1^2b_1 + \frac{1}{2}a_2c_1 + \frac{1}{6}a_1^3b_1^3 + \frac{1}{2}a_1a_2b_2c_1 + \frac{1}{3}a_3b_3 + \cdots \\
a_1K' &= a_1 + a_1^2b_1 + \cdots, \\
2b_1\frac{\partial K}{\partial b_1} &= a_1^2b_1 + a_1^3b_1^3 + \cdots, \\
2c_1\frac{\partial K}{\partial c_1} &= a_2c_1 + a_1a_2c_1b_2 + \cdots.
\end{aligned}$$

Thus, to start with $\alpha(x,y) = x + \cdots$, $\beta(x,y) = 1 + y + \cdots$, and $\gamma(x,y) = 1 + y + \cdots$. Substitution into (48) gives the left side correctly through terms of order x^2, and likewise on the right for all terms except for $\alpha(x,y)$ which comes from the a_1 term of a_1K'. This allows us to solve for the order x^2 terms of $\alpha(x,y)$. Similarly, substitution into (49) and (50) with attention to the terms arising from $\alpha_1^2b_1$ and α_2c_1 will show that the order x terms of $\beta(x,y)$ and $\gamma(x,y)$ are also uniquely determined. Since K and its derivatives can be computed term-wise rather than stored, the determination of the series $\alpha(x,y)$, $\beta(x,y)$, and $\gamma(x,y)$ can be carried out simultaneously in an iterative fashion, with only the currently known initial terms of the series needing to be kept in memory.

In the process of solving (48) - (50) for $\alpha(x,y)$ to order $\leq n+1$ in powers of x, and for $\beta(x,y)$ and $\gamma(x,y)$ to order $\leq n$, it is no extra effort to keep track of the series

$$f(x,y) = K[\alpha(x,y), 1+\beta(x,y), 1+\gamma(x,y)]$$

which is determined to order $\leq n$ as part of the computation. Then equation (7) of Section 2 evaluates $B[x, \beta(x,y), \gamma(x,y)]$.

For any cycle index sum U let $\tilde{U}(x,y) = U[x, \beta(x,y), \gamma(x,y)]$. Then $\tilde{D}^{+} = \tilde{D}^{-} = y$ by (36) and (37), so applying this homomorphism to $F[a_1, D^{+}, D^{-}]$ yields $F[x,y,y]$, the counting series for 3-connected graphs. Thus equation (24) can be seen as expressing the counting series $F(x,y)$ for 3-connected graphs in terms of $\tilde{B}, \tilde{P}^{+}, \tilde{P}^{-}, \tilde{Q}^{+}, \tilde{Q}^{-}, \tilde{S}^{+}, \tilde{S}^{-}$, and $\tilde{H}^{+}$. We have already observed that $\tilde{B}$ can be calculated by equation (7), so the next step is to determine the contributions of the other terms obtained from the right side of equation (24).

From (32) and (25) we have

$$(1+D^{+})\mathrm{exp} \sum \frac{1}{k}(P^{+}_{(k)} - D^{+}_{(k)}) = 1 + b_1.$$

Applying to this the homomorphism $[x, \beta(x,y), \gamma(x,y)]$ we obtain

$$(1+y)\ \mathrm{exp}\ \sum \frac{1}{k}(\tilde{P}^{+}_{(k)} - y^k) = 1 + \beta(x,y).$$

Since $1+y = \ \mathrm{exp} \sum \frac{1}{k}(-1)^{k-1}y^k = \ \mathrm{exp} \sum \frac{1}{k}(y^k - y^{2k})$, the relation simplifies to

$$\mathrm{exp}\ \sum \frac{1}{k}(\tilde{P}^{+}_{(k)} - y^{2k}) = 1 + \beta(x,y).$$

By Möbius inversion one then obtains

$$\tilde{P}^{+} = y^2 + \sum_{i=1}^{\infty} \frac{\mu(i)}{i} ln(1 + \beta(x^i, y^i)). \tag{51}$$

Similarly, from (33) and (26) we have

$$(1+D^-)\text{exp}\left\{\sum_{k\ odd}\frac{1}{k}(P^-_{(k)}-D^-_{(k)})+\sum_{k\ even}\frac{1}{k}(P^+_{(k)}-D^+_{(k)})\right\}=1+c_1.$$

Applying to this the homomorphism $[x,\beta(x,y),\gamma(x,y)]$ we obtain

$$(1+y)\exp\left\{\sum_{k\ odd}\frac{1}{k}(\tilde{P}^-_{(k)}-y^k)+\sum_{k\ even}\frac{1}{k}(\tilde{P}^+_{(k)}-y^k)\right\}=1+\gamma(x,y),$$

which simplifies to

$$\exp\left\{\sum_{k\ odd}\frac{1}{k}(\tilde{P}^-_{(k)}-y^{2k})+\sum_{k\ even}\frac{1}{k}(\tilde{P}^+_{(k)}-y^{2k})\right\}=1+\gamma(x,y),$$

and hence

$$\sum_{k\ odd}\frac{1}{k}(\tilde{P}^-_{(k)}-y^{2k})+\sum_{k\ even}\frac{1}{k}(\tilde{P}^+_{(k)}-y^{2k})=ln(1+\gamma(x,y)).$$

Möbius inversion now gives

$$\tilde{P}^-=y^2+\sum_{i\ odd}\frac{\mu(i)}{i}ln(1+\gamma(x^i,y^i))+\sum_{i\ odd}\frac{\mu(i)}{i}\sum_{k\ even}\frac{1}{k}(y^{2ki}-\tilde{P}^+_{(ki)}).$$

Using the identity

$$\sum_{2|j|m}\mu(j)=\begin{cases}1 & \text{if } m=2^{1+e}, \text{ for } e\geq 0\\ 0 & \text{otherwise}\end{cases}$$

the rightmost sum simplifies to

$$\sum_{m=2^{1+e}}\frac{1}{m}(y^{2m}-\tilde{P}^+_{(m)})$$

so that

$$\tilde{P}^-=y^2+\sum_{i\ odd}\frac{\mu(i)}{i}ln(1+\gamma(x^i,y^i))+\sum_{m=2^{1+e}}\frac{1}{m}(y^{2m}-\tilde{P}^+_{(m)}).\qquad(52)$$

From (27) it is immediate that

$$\tilde{S}^+ = \frac{xy^2}{1+xy}. \tag{53}$$

This can be combined with (28) to find

$$\tilde{S}^- = \frac{xy^2(1+xy)}{1+x^2y^2}. \tag{54}$$

From (29) and (30) one then has

$$\tilde{Q}^+ = \frac{y}{1+xy}, \tag{55}$$

$$\tilde{Q}^- = \frac{y(1-xy)}{1+x^2y^2}. \tag{56}$$

Using the identity

$$\sum_{d|m} \phi(d)(-1)^{\frac{m}{d}} = \begin{cases} 0 & \text{if m is even,} \\ -m & \text{if m is odd.} \end{cases}$$

and the expression (55) for $\tilde{Q}^+$, we find that

$$\frac{1}{2}\sum \frac{\phi(d)}{d} ln(1 - x^d \tilde{Q}^+_{(d)}) = \frac{\frac{-1}{2}xy}{1-x^2y^2}. \tag{57}$$

Finally, from (31) and (55) we have

$$\tilde{H}^+ = \frac{y}{1+xy} - \tilde{P}^+. \tag{58}$$

Using $\tilde{D}^+ = \tilde{D}^- = y$ and equations (53) - (58), the image of the right side of (24) under the homomorphism $[x, \beta(x,y), \gamma(x,y)]$ can be expressed explicitly in terms of $\tilde{B}, \tilde{P}^+$ and $\tilde{P}^-$. There is considerable cancellation of terms in the process, which results in the formula

$$F(x,y) = \tilde{B}(x,y) - \frac{x^2}{2}(1+y)(\tilde{P}^+(x,y) + \tilde{P}^-(x,y)) + x^2y^2 - \frac{x^3y^3}{1-x^4y^4}. \tag{59}$$

To summarize the algorithm for calculating $F(x,y)$; one starts with (48) - (50) to find $\alpha(x,y), \beta(x,y), \gamma(x,y)$, and $f(x,y)$; then (7) is applied to determine $\tilde{B}(x,y)$; next $\tilde{P}^{+}(x,y)$ is found from (51); then $\tilde{P}^{-}(x,y)$ can be calculated from (52); finally, $F(x,y)$ is given very simply in (59) in terms of $\tilde{B}(x,y), \tilde{P}^{+}(x,y)$ and $\tilde{P}^{-}(x,y)$. In this manner 3-connected graphs were counted by nodes and edges up to 18 nodes (see Table VI) and by nodes alone up to 25 nodes (see Table III).

5 Example and Complexity Analysis

To illustrate the method, we compute $B[x,y,y]$ up to order 3. The two sides of formula (8) are

$$xf(x,y) = xK[\alpha(x,y),1+y,1+y] = x\{1+\alpha(x,y)+\frac{1}{2}(\alpha^2(x,y)(1+y)+\alpha(x^2,y^2)(1+y))$$

$$+\frac{1}{6}(\alpha^3(x,y)(1+3y+3y^2+y^3)+3\alpha(x,y)\alpha(x^2,y^2)(1+y+y^2+y^3)+2\alpha(x^3,y^3)(1+y^3))+\cdots\}$$

and

$$\alpha_1 k'[\alpha(x,y),1+y,1+y] = \alpha(x,y)+\alpha^2(x,y)(1+y)$$

$$+\frac{1}{2}(\alpha^3(x,y)(1+3y+3y^2+y^3)+\alpha(x,y)\alpha(x^2,y^2)(1+y+y^2+y^3))+\cdots.$$

Equating coefficients of x^0 we find that $\alpha(x,y)$ has no term independent of x. Equating coefficients of x^1 we find that $\alpha(x,y) = x+\cdots$ and $f(x,y) = 1+\cdots$. Equating coefficients of x^2 we find that $\alpha(x,y) = x+x^2(-y)$ and $f(x,y) = 1+x+\cdots$. Equating coefficients of x^3 we find that $\alpha(x,y) = x+x^2(-y)+x^3(-y^3)$ and $f(x,y) = 1+x+x^2+\cdots$. The coefficient of x^4 in $xf(x,y)$ turns out to be 1 too; so

$$f(x,y) = 1+x+x^2+x^3+\cdots$$

(the next term is not x^4!),

$$lnf(x,y) = x+\frac{1}{2}x^2+\frac{1}{3}x^3+\cdots,$$

$$\sum_{k=1}^{\infty}\frac{\mu(k)}{k}lnf(x^k,y^k) = x+0x^2+0x^3+\cdots.$$

Returning to $\alpha(x, y)$, we have

$$\alpha(x, y)/x = 1 + x(-y) + x^2(-y^3) + \cdots,$$

$$ln(\alpha(x, y)/x) = x(-y) + x^2(-\frac{1}{2}y^2 - y^3) + \cdots,$$

$$x \sum \frac{\mu(k)}{k} ln(\alpha(x^k, y^k)/x^k) = x^2(-y) + x^3(-y^3) + \cdots.$$

Thus by (7) $B[x, y, y] = x^2y + x^3y^3 + \cdots$, which is correct since the two smallest 2-connected graphs are the single edge and the triangle.

The cost of computing $B[x, y, y]$ up to order n is dominated by that of computing $\alpha(x, y)$. For each i up to n, one has to sum through all the partitions of the numbers up to i and compute the coefficient of x^{i-k} in the corresponding monomial

$$\prod_{j \leq k} (\alpha(x^j, y^j)/x^j)^{a_j} = \exp \sum_{j \leq k} a_j log(\alpha(x^j, y^j)/x^j).$$

Since the necessary terms of $log(\alpha(x, y)/x)$ have already been computed and stored, and can always be "inflated" by j, the cost of this computation is dominated by that of evaluating exp which is $O(n^2)$ multiplications. We do this at most n times for each partition of each number up to n; so the total cost is $O(n^3p'(n))$. An idea of the growth rate of $p'(n)$ can be obtained from the asymptotic formula for $p(n)$, the number of partitions of n: $p(n) \sim \frac{c^{\sqrt{n}}}{4n\sqrt{3}}$, where $c = e^{\pi\sqrt{2/3}} \approx 13.001954..$ [3]; so $p'(n) \leq np(n) = O(c^{\sqrt{n}})$.

If we are counting by nodes only and using fixed precision, each multiplication is an elementary operation and so $O(n^3p'(n))$ is an accurate estimate of the time-complexity. If we are counting by edges too, each coefficient is a polynomial in y of degree $O(n^2)$. It takes $O(n^4)$ elementary operations to multiply two such polynomials; so the complexity is $O(n^7p'(n))$. If we are using multiple-precision arithmetic, the numbers are bounded by the number of labelled n-vertex graphs, $2^{n(n-1)/2}$, which has $O(n^2)$ bits. Multiplying two such numbers by brute force (in base 10000) takes $O(n^4)$ operations, which increases the time-complexity to $O(n^7p'(n))$ if one counts by nodes alone, and to $O(n^{11}p'(n))$ if one counts by edges too (in fact we used REAL*32 to count by edges too, which guarantees the accuracy of the numbers up to 18 nodes).

The space complexity is the cost of storing a constant number of counting series: $O(n)$ if we count by nodes alone in fixed precision, $O(n^5)$ if we count by edges too in multiple precision, and $O(n^3)$ in the other two cases.

The analysis of the computation of $I(x, y, y)$ and $F(x, y, y)$ is similar and gives the same time- and space-complexities to within a constant factor.

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