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ON THE COMPUTER CALCULATION OF THE NUMBER OF NONSEPARABLE GRAPHS*

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ABSTRACT

Computation of the number b_p of unlabeled nonseparable graphs on p points has been carried out for p \leqslant 18 by one of the authors, based on equations derived by the other author. The number $b_{p,q}$ of those with q lines has similarly been obtained for p \leqslant 11. The numerical results are reported, and aspects of the computation are discussed.

The method of counting nonseparable graphs involves finding the sum of the cycle indices of the automorphism groups for all graphs, then the cycle index sum for the connected graphs and finally the cycle index sum for the non-separable graphs. Extracting the cycle index sum of the connected graphs from the cycle index sum for all graphs is based on a principle which can be applied in a number of situations. Of three methods tested for implementing this principle, the clear winner in practice was not the one with the apparent computational advantages.

* The paper was presented by the second author.

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1. INTRODUCTION

The evaluation by computer of the number of unlabeled nonseparable graphs is reported on in this paper. A graph is nonseparable if it is connected and has no point whose deletion results in an empty or disconnected graph. The nonseparable graphs other than the one with p = 2 points are just the 2-connected graphs. Nonseparable graphs have been called blocks by some graph theorists and star graphs by theoretical physicists. The graphs with which we deal are finite and undirected with no loops or multiple lines.

Calculation of the number b of unlabeled nonseparable graphs is difficult because it requires the simultaneous determination of the additional information contained in the sum of the cycle indices of the automorphism groups of the graphs being counted. Thus as we shall see b is obtained as the sum of rational numbers, one associated with each partition of p. The computation is recursive, requiring the numbers associated with the partitions less than p in order to determine those associated with the partitions of p. In addition the computation requires the analogous information for connected graphs, which in turn must be extracted from that for unrestricted graphs.

The formulas for counting unlabeled nonseparable graphs were developed in [8] and received a detailed exposition in the book by Harary and Palmer [3, Chapter 8]. The first computer implementation was carried out by L. Osterweil, who found b for p \leq 9 as reported in [8]. The values of b for p \leq 18 are presented in Section 3 after cycle index sum counting methods are introduced and the basic equations presented in Section 2. For comparison we also give the numbers c of unlabeled connected graphs and g of all unlabeled graphs on p points, for p \leq 18.

Including the number of lines as an enumeration parameter in counting nonseparable graphs is conceptually straightforward. However it expands considerably the storage required as well as the number of arithmetic operations. In Section 3 we give the numbers b of unlabeled nonseparable graphs with p points and q lines for p \leq ll. For comparison we include the corresponding numbers c and g of connected and unrestricted unlabeled graphs.

There are several alternative strategies available for solving the basic equations which determine the cycle index sum for nonseparable graphs. The choice of strategy for computer implementation is discussed in the final

section. In particular, three different ways of extracting the cycle index sum of the connected graphs from that of the unrestricted graphs were tested. The best method in practice was not the one which appeared to be most clever and efficient beforehand. The principle involved in this case can be expected to have wide application in unlabeled graph counting problems. It is in fact applied to an important part of the extraction of the cycle index sum of the nonseparable graphs from that of the connected graphs.

2. COUNTING WITH CYCLE INDEX SUMS

In this section we introduce cycle indices and cycle index sums for sets of graphs, then present the equations which are the basis for counting nonseparable graphs.

If g is any permutation on a finite set it can be expressed uniquely as a product of disjoint cyclic permutations. Let j(n;g) denote the number of these cycles which have length n. Then the cycle type of g is defined by

(1)
$$Z(g) = \prod_{n} s_n^{j(n;g)},$$

where s_1, s_2, s_3, \ldots are some set of independent commuting variables. If G is a finite permutation group then its cycle index Z(G) is the arithmetic mean of the cycle types of its elements. That is

(2)
$$Z(G) = \frac{1}{|G|} \sum_{g \in G} Z(g),$$

where |G| denotes the order of G. Often the cycle index is written $Z(G;s_1,s_2,s_3,...)$ to display the variables and to provide a convenient form for indicating substitutions for the variables.

As an example, let S_3 be the symmetric group on the object set $\{1,2,3\}$. The identity permutation (1)(2)(3) has cycle type s_1^3 . The permutations (1)(23), (2)(13) and (3)(12) all have cycle type s_1s_2 . Then the cycles (123) and (132) have cycle type s_3 . Thus we have

$$Z(S_3) = \frac{1}{6}s_1^3 + \frac{1}{2}s_1s_2 + \frac{1}{3}s_3.$$

In general, let Sp denote the symmetric group of degree p and order p!.

It is well known that

$$z(s_p) = \sum_{\{(j)\}=p} \prod_{n=n}^{j_n} \prod_{n} \prod_{j=1}^{j_n} n^{j_n},$$

where the sum is over sequences

$$(j) = (j_1, j_2, ..., j_p)$$

of non-negative integers with weight

$$|(j)| = \sum_{n=1}^{p} nj_n$$

equal to p. Thus the sum of these cycle indices takes the elegant form

(3)
$$\sum_{p=0}^{\infty} Z(S_p) = \exp \sum_{1}^{\infty} S_n/n.$$

It is interesting to note that if s_n is the n^{th} power $sum \Sigma \alpha_1^n$ of variables $\alpha_1, \alpha_2, \alpha_3, \ldots$ then $Z(S_p)$ is the homogeneous product sum of order p in these variables. In this context the usual notation for $Z(S_p)$ would be h_p , and (3) expresses a familiar form of the relations between these symmetric functions [5, p.7].

Every graph has an automorphism group, which we consider to be a permutation group on the point set. For any set A of graphs we denote by Z(A) the sum of the cycle indices of the automorphism groups of the members of A. The case of the set H_3 of all four graphs on p=3 points is illustrated in Figure 1, where each graph is shown with its automorphism group. The cycle index sum is

(4)
$$Z(H_3) = 2(\frac{1}{6}s_1^3 + \frac{1}{2}s_1s_2 + \frac{1}{3}s_3) + 2(\frac{1}{2}s_1^3 + \frac{1}{2}s_1s_2)$$
$$= \frac{4}{3}s_1^3 + 2s_1s_2 + \frac{2}{3}s_3.$$

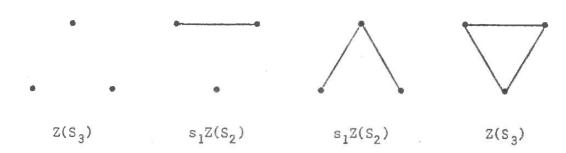


FIGURE :

The four graphs on p = 3 points.

Note that the number 4 of graphs on p = 3 points is obtained as the sum $4 = \frac{4}{3} + 2 + \frac{2}{3}$ of the coefficients of $Z(H_3)$. In general, for any set A of graphs the number with p points can always be found from Z(A) by summing the coefficients of the terms of weight p. This is because the coefficient sum in any cycle index must be 1.

Now let H_p denote the set of all graphs on p points. The cycle index sum $Z(H_p)$ can be readily computed in terms of the number c(j) of cycles of lines induced on the complete graph by a point permutation with cycle structure $(j) = (j_1, j_2, \ldots, j_p)$. The formula is

(5)
$$Z(H_{p}) = \sum_{|(j)|=p} 2^{c(j)} \prod_{n} s_{n}^{j_{n}} / \prod_{n} i_{n}^{j_{n}} n^{j_{n}}.$$

This follows from a slight generalisation of Burnside's Lemma, in the spirit of Redfield's Decomposition Theorem [7, p.445], as reported in [8, Theorem 2]. One need only observe that c(3,0,0)=3, c(1,1,0)=2 and c(0,0,1)=1 in order to evaluate formula (5) for p=3. The answer is easily seen to agree with the sum given in (4). For arbitrary (j) the number of induced line-cycles is given [3, equation 4.1.9] by

(6)
$$c(j) = \sum_{n} n\{\binom{j_n}{2} + j_{2n+1} + j_{2n}\} + \sum_{m \le n} (m,n)j_mj_n,$$

where (m,n) is the greatest common divisor of m and n.

Let H denote the set of all graphs, C the set of all connected graphs, and B the set of all nonseparable graphs. The cycle index sum Z(H) is determined by (5) and (6) as

$$Z(H) = \sum_{p=0}^{\infty} Z(H_p).$$

Of course in any actual computation there is an upper bound \overline{p} on the number of points to be considered.

To express Z(C) in terms of Z(H) we need the notion of substituting Z(C) for cycle variables. This follows the rule

(7)
$$s_n[Z(C)] = Z(C; s_n, s_{2n}, s_{3n}, ...),$$

which also applies to the substitution of any cycle index sum. The relation can now be written

(8)
$$Z(H) = \exp \sum_{i=1}^{\infty} \frac{1}{n} s_{i}[Z(C)].$$

In Section 4 we will compare three different ways of solving (8) for Z(C) in terms of Z(H). It can be seen that (8) is a generalisation of the usual relation [3, equation 4.2.3] between the ordinary generating functions $g(x) = \sum_{p=0}^{\infty} g_p x^p$ and $c(x) = \sum_{p=0}^{\infty} c_p x^p$, which follows at once from Pólya's Hauptsatz [6, p.163]. Indeed (8) follows from a direct lifting of Pólya's Hauptsatz to cycle index sums in place of ordinary generating functions [8, equation (9)].

As intermediaries in the computation of Z(B) the cycle index sums Z(C') and Z(B') of the rooted connected graphs C' and the rooted nonseparable graphs B' will be needed. A rooted graph is a graph in which one point is given the special status of root point. The root point must be left fixed by every automorphism of a rooted graph, and is omitted from consideration in the cycle index sum. It is easy to obtain Z(C') from Z(C) since

(9)
$$Z(C') = \frac{\partial Z(C)}{\partial s_1}.$$

This follows from a general result [8, Theorem 1] which was first observed by G.W. Ford, and remains true if C is replaced by B.

The relation determining Z(B') from Z(C') is

(10)
$$Z(C') = \exp \sum_{n=1}^{\infty} \frac{1}{n} s_n [Z(B')[s_1 Z(C')]].$$

Structural considerations due to R.Z. Norman are used in the proof [8, Theorem 4]. Since (9) applies with B in place of C we can integrate to obtain

(11)
$$Z(B) = \int_0^{s_1} Z(B^*) ds_1 + Z(B; 0, s_2, s_3, ...) .$$

The fixed-point-free portion of Z(B) is then determined by

(12)
$$Z(C;0,s_2,s_3,...) = Z(B;0,s_2,s_3,...)[s_1Z(C')].$$

Further consideration of the structure of a connected graph with respect to its maximal nonseparable subgraphs is required to justify this relation [8, Theorem 5].

Relations (5) through (12) serve to determine Z(B). The number b_p of unlabeled nonseparable graphs on p points is obtained from Z(B) by adding up the coefficients of all terms of weight p.

The numbers b of unlabeled nonseparable graphs with p points and q lines are counted in a parallel manner using an expanded version of the cycle index sum. For any set A of graphs, let Z(y:A) denote the sum over the graphs in A of y^q times the cycle index of the automorphism group, where q is the number of lines. Then b is obtained from Z(y:B) by summing the coefficients of the terms having the factor y^q and weight p in the point-cycle variables.

The expanded cycle index sum Z(y:B) is determined from Z(y:H) and Z(y:C) by modified forms of equations (6) and (8) through (12). The modification is simply to replace Z() by Z(y:) at every occurrence. To compute Z(y:H) initially one modifies equation (5) by replacing $2^{C(j)}$ with the polynomial

(13)
$$\prod_{n} (1+y^{n})^{j} 2n^{+\left[\frac{n-1}{2}\right]} j_{n}^{+n} {j \choose 2} \prod_{m < n} (1+y^{[m,n]})^{(m,n)} j_{m}^{-j} j_{n}^{-1}.$$

Here [m,n] is the least common multiple of m and n, and $[\frac{n-1}{2}]$ is the greatest integer less than or equal to $\frac{n-1}{2}$. This corresponds [8, equation (7)] to a factor of $(1+y^n)$ for each induced line-cycle of length n. The only other change needed is to generalise equation (7) to

(14)
$$s_n[Z(y:A)] = Z(y^n:A;s_n,s_{2n},s_{3n},...).$$

3. NUMERICAL RESULTS

The numbers b_{D} of unlabeled nonseparable graphs on p points computed on the basis of equations (5) through (12) for p < 18 are presented in Table 1. Development of the programs was the work of the first author. Some of the experimentation concerning choice of methods for solving the equations is reported in the next section. The calculation was performed on a PDP 11/45 with a 56 kilobyte parity core memory and a twin RKO5 fixed disk system for secondary storage. The programs were written in FORTRAN with the exception of some sections of the multiple precision integer arithmetic routines, which were written in the assembly language. They were compiled and run using the DOS/BATCH operating system. Because the disks provide essentially permanent storage of results, it was possible to compute Z(H), Z(C), and Z(B) in order, each through terms of weight p = 18. Approximate times for these runs are 1/4 hour, 3 hours and 21 hours respectively, with an additional 1/4 hour for printing out all of the 1596 different terms needed for Z(B). Storage requirements were met with a single disk, having 2.4 megabytes total capacity including .5 megabytes taken up with the operating system.

Also provided in Table 1 for purposes of comparison are the numbers g_p and c_p of unlabeled unrestricted and connected graphs, respectively. C. King had computed g_p for $p \le 25$ as reported in [3, Table A3]. Stein and Stein [9] had computed c_p for $p \le 18$, from which one can obtain c_p by summing q from 0 to $\binom{p}{2}$. Our own computations confirm the values of g_p and c_p reported in Table 1. It will be seen that our results for p are in agreement with those of L. Osterwiel for $p \le 9$, as reported in [3, Table A3].

It is shown in [3, Section 9.4] that b $_p$ $_p$ $_p$ $_p$ From Table 1 it appears that c $_p$ /g approaches 1 much more rapidly than b $_p$ /c.

The numbers $b_{p,q}$ of unlabeled nonseparable graphs with p points and q lines computed on the basis of equations (5) through (12) modified by (13) and (14) for $p \le 11$ are presented in Tables 2, 3 and 4. Program development and implementation for the determination of Z(y:H), Z(y:C) and Z(y:B) through terms of point weight p = 11 followed the same pattern as for Z(B). The additional line parameter increased storage and time demands so much that in spite of the reduction of p = 11 form 18 to 11, two disks were required for storage and the total running time rose from 27 hours to 60 hours.

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TABLE 1

The numbers of unlabeled graphs, connected graphs and nonseparable graphs on p $\leqslant 18$ points.

Again, Tables 2, 3 and 4 are supplied with the numbers $c_{p,q}$ and $g_{p,q}$ of unlabeled connected and unrestricted graphs with p points and q lines for $p \le 11$ for purposes of comparison. These numbers were calculated by computer for $p \le 18$ by Stein and Stein [9], in what seems to have been the first major graphical enumeration project undertaken on a computer. Our own results serve to verify the accuracy of theirs for $p \le 11$. In computing $g_{p,q}$, it is necessary to compute every term of Z(y:H) in the process; however, these can be summed in running totals for each $p \le p$ and $q \le \binom{p}{2}$. Since only the totals $g_{p,q}$ need to be kept in order for the $c_{p,q}$ to be determined, the requirements for storage space and consequent retrieval time are much less than for our procedure, which used all of Z(y:H) to determine all of Z(y:C) for $p \le p$. The latter was necessary for obtaining Z(y:B) and indeed all terms of Z(y:B) for p < p were needed in order to compute those terms of the highest order p = p.

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TABLE 2

The numbers of (p,q)-graphs which are nonseparable, connected, and unrestricted for p < 8.

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TABLE 3

The number of (p,q)-graphs which are nonseparable, connected and unrestricted, for p = 9 and 10.

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NUMERICAL METHODS

The polynomials Z(H), Z(C), Z(B) of Section 2 are specified by an array of coefficients and an array of partitions. In calculating Table 1 an array of the 1596 partitions of the numbers < 18 is required. All the polynomials in the calculation are referenced through this partition array so it was held in core throughout. The rational coefficients, however, were held as direct access disk files since the fractions had quite large numerators and several separate arrays were required.

The partitions were precalculated in lexicographic order and were stored so that if the partition of p being considered was $p = \Sigma p_i n_i$, where $p_i, n_i > 0$, then p_i and n_i were packed into one word. An array of pointers marked the beginning and end of each partition. Another array of pointers marked the beginning and end of the terms for each value of p. For the enumeration by lines shown in Tables 2, 3 and 4 the only difference in the storage arrangments was that arrays of fractions were held instead of single fractions.

Three methods were considered for the calculation of Z(C) from Z(H) solving equation (8). These were tested for p \leq 15 which required 684 terms. The best of these methods was chosen for the enumeration up to \overline{p} = 18, which required 1596 terms. Immediately from (8) we have

$$\sum_{k=1}^{\infty} \frac{1}{k} s_k[Z(C)] = \log Z(H).$$

This can be solved using a method suggested by Cadogan [1] based on Möbius inversion, giving

(15)
$$Z(C) = \sum_{k=1}^{\infty} \frac{\mu(k)}{k} s_k [\log Z(H)].$$

This equation is the point of departure for the first and third of our methods. In the first, or "dumb", method log Z(H) was replaced by

$$\sum_{i=1}^{\infty} \frac{(-1)^{i+1}}{i} (Z(H) - 1)^{i}.$$

The time taken for this method was $5\frac{1}{2}$ hours up to $\overline{p}=15$.

The second method was described in [8, p.339] and seemed attractive enough to be dubbed the "clever" method initially. Let $H^{(i)}$ be the set of graphs with all components having order at least i and let C_j be the set of connected graphs on j points. Then $Z(H^{(1)}) = Z(H)$, and Z(C) can be read off by selecting the terms of weight 1. Next, $Z(H^{(2)})$ is calculated from the relation

$$Z(H^{(2)}) = Z(H^{(1)}) \exp{-\sum_{k=1}^{\infty} \frac{1}{k} s_{k}[Z(C_{1})]}.$$

Now we can read off $Z(C_2)+Z(C_3)$, denoted for brevity by $Z(C_{2-3})$, since the smallest nonempty disconnected graph with components all of order at least 2 must itself have order at least 4. In similar fashion

$$Z(H^{(4)}) = Z(H^{(2)}) \exp{-\sum_{j=1}^{\infty} \frac{1}{k} s_{k}[Z(C_{2-3})]}$$

from which one can read off $Z(C_{4-7})$. Finally

$$Z(H^{(8)}) = Z(H^{(4)}) \exp{-\sum_{1}^{\infty} \frac{1}{k} s_{k}[Z(C_{4-7})]}$$

giving $Z(C_{8-15})$. In this process the exponentiation was computed by the recursive scheme described for the third method below. Extensive use was made of an additional array of flags to indicate whether a number in a disk held array was zero or not; the point was to save disk access time where possible. The time taken for calculation up to $\overline{p}=15$ was $3\frac{1}{2}$ hours.

The third or "best" method differed from the first in that log Z(H) was calculated recursively. The recurrence is obtained from the following general relation by replacing v_i with $Z(C_i)$ and E_i with the terms of weight i in Z(H). If

$$\sum_{i=0}^{\infty} E_{i} x^{i} = \exp \sum_{i=1}^{\infty} v_{i} x^{i},$$

then $E_0 = 1$, and

$$E_n = v_n + \frac{1}{n} \sum_{k=1}^{n-1} E_k v_{n-k} (n-k)$$

for n>0. In the theory of symmetric functions this is equivalent to the well-known recurrence relation between the s_i and the h_j [4, p.83] which can be

derived from (3) by differentiation. The idea has been used in counting labeled connected graphs by Gilbert [2], and in counting unlabeled connected graphs by Stein and Stein [9, p.9] and Cadogan [1, p.195].

Clearly the recursion will serve to calculate either exponentials or logarithms. The time taken to calculate Z(C) up to $\overline{p}=15$ was $1\frac{1}{4}$ hours, so that the third method was by far the quickest. It was used to extend the results up to $\overline{p}=18$, and took some 3 hours for the calculation.

The calculation of Z(B) from Z(C) falls naturally into two parts as described in Section 2; the calculation of Z(B') using relation (10) and the calculation of $Z(B;0,s_2,s_3,\ldots)$ using (12). It is relatively trivial to find Z(C') by differentiating Z(C) as indicated in (9). Then $Z(B')[s_1Z(C')]$ is obtained from Z(C') in exactly the same way that Z(C) was obtained from Z(H), using of course the third method for the computation. From this Z(B') is extracted recursively. One keeps a running total of the contributions by the terms of Z(B') obtained from composing over $s_1Z(C')$ up to, say, weight i. Subtraction of this total from $Z(B')[s_1Z(C')]$ leaves just the terms of weight i+1 in Z(B'), which are used to update the running total so that the process can be continued.

It is worth pointing out here that the composition $Z(B')[s_1Z(C')]$ involves the substitution, for each factor s_i in each term of Z(B'), of the polynomial $s_1Z(C')$ with all the subscripts multiplied by i, that is, inflated by i. The consequences of this are that for $p \le 18$, up to 18 inflated forms of $s_1Z(C')$ will be required, raised to powers up to 18. Varying combinations of these polynomials are then multiplied together (up to 5 factors in all for $p \le 18$) to complete the substitution. The very great deal of computation here was economised by precomputing all the inflated powers, saving only nonzero coefficients, and setting up an array of pointers. The total disk space required for $p \le 18$ was only 4 times that required to store just $s_1Z(C')$. The multiplication together of the polynomials was performed by nested loops. Extracting $Z(B;0,s_2,s_3,\ldots)$ from $Z(C;0,s_2,s_3,\ldots)$ using equation (12) follows exactly the same recursive method, but is much less demanding of time since the number of nonzero terms is relatively small. The final step of integrating Z(B') and adding $Z(B;0,s_2,s_3,\ldots)$ to obtain Z(B) is quite straightforward.

Times taken for the various calculations up to $\overline{p} = 18$ were:

(a) 3 hours for determining Z(B')[s,Z(C')],

- (b) 7 hours for precomputation of the inflated powers of $s_1Z(C')$,
- (c) 21 hours for extracting Z(B'),
- (d) $l_{\overline{4}}^{1}$ hours for extracting $Z(B;0,s_{2},s_{3},...)$,
- (e) $\frac{1}{2}$ hour for the integration of $\mathbb{Z}(B')$ and its collation with $\mathbb{Z}(B;0,s_2,s_3,...)$.

Calculation of Z(y:B) followed the same pattern as used for Z(B), but did require considerable modification of the programs. Extension was necessary to deal with the fact that the coefficients of the partition arrays are now polynomials in y, rather than simple fractions. This means for instance that computing up to $\overline{p}=11$ requires up to 55 fractional coefficients for each partition. The longest single step in the computation was the analogue of step (c) above, which took 50 hours up to $\overline{p}=11$. The whole of the free space on two 2.4 megabyte disks was required for working storage.

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