LABELED BIPARTITE BLOCKS

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Dedicated to Sir Edward Wright

Introduction. Graphs which are 2-connected have been called blocks in the graph theoretic literature [3] and stars in the parlance of statistical mechanics [1]. They are also called nonseparable graphs, and in this paper include the complete graph K_2 on p=2 points. The standard terminology of graphical enumeration can be found in [3].

When its points are colored using two distinct colors in such a way that adjacent points receive different colors, a graph is called *2-colored*. If the colors are considered interchangeable, such a graph is called *bicolored*. A graph which can be bicolored is called *bicolorable*. It is obvious that a connected bicolorable graph has a unique bicoloring, and so one can speak of the sizes of its color classes.

Convention. All graphs mentioned in this paper are understood to be labeled. That is, the point set of a graph on p points is labeled with the numbers $1, 2, \ldots, p$.

Bipartite blocks in which the color classes are of equal size were found by Melnyk, Rowlinson and Sawford [4] to be of interest in studying a modified penetrable sphere model of liquid-vapor equilibrium. This application is related to those considerations of statistical mechanics which led Ford and Uhlenbeck [1] to the counting of blocks. We follow the methods developed there in combination with those used originally by Read [5] to count bicolored graphs and connected bipartite graphs.

2. Generating functions. Our purpose is to establish relations satisfied by the generating function for bipartite blocks (labeled, of course, by the Convention). This will enable explicit recurrence relations to be derived and solved numerically to give tables of values up to p = 20.

The point of departure is the number M_p of 2-colored graphs on p points, which is just

(1)
$$M_p = \sum_{i=0}^p \binom{p}{i} 2^{i(p-i)}.$$

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The term $\binom{p}{i}2^{i(p-i)}$ counts the number of 2-colored graphs in which exactly i points are assigned the first color and p-i the second color. To see this in all detail, note that the binomial coefficient $\binom{p}{i}$ gives the number of ways in which the labeled points $1, 2, \ldots, p$ can be divided into two classes so that the first one contains exactly i points. As there are i(p-i) potential lines joining points of different colors, each of which may be present or absent, the factor of $2^{i(p-i)}$ gives the number of ways to fill in the lines.

The generating function which is convenient to use is the exponential one, M(x), defined by

$$M(x) = \sum_{p=0}^{\infty} M_p \frac{x^p}{p!}.$$

Exponential generating functions are well adapted to labeled counting problems because multiplication allows for the interleaving of labelings from different components automatically.

To obtain the exponential generating function for connected 2-colored graphs, one simply takes the formal logarithm. This is a special case of a well-known general principle; see [3, (1.2.6)] and Gilbert [2]. One then divides by 2 to count connected bipartite graphs. For any of these can be 2-colored in a unique way up to interchangeable color classes, and then the two classes can be assigned definite colors in just two ways. Thus, letting D_p be the number of p-point connected bipartite graphs and D(x) the corresponding exponential generating function, we see that

(2)
$$D(x) = \frac{1}{2} \log M(x)$$
.

It should be noted that for k > 2 the problem of counting labeled connected k-colored graphs with interchangeable colors is more difficult, as discussed by Read and Wright [6] and in [3, p. 17].

The relation between the exponential generating functions for blocks and connected graphs was first derived in [1]; see also [3, (1.3.3)]. Since a connected graph is bipartite if and only if all of its blocks are bipartite, the same reasoning applies without change to D(x) and the exponential generating function B(x) for the numbers B_p of labeled bipartite blocks; this gives

(3)
$$\log D'(x) = B'(xD'(x))$$

where the primes are used to denote the formal derivative of a power series with respect to x.

To handle the problem of counting bipartite blocks with equal sized color classes, we must include an additional parameter to keep track of the sizes of the color classes at each stage of the derivation. In the remainder of this section we shall restrict our attention to *specially labeled* 2-colored graphs, that is, those in which the points $1, 2, \ldots, n$ are assigned the first color and

 $n+1,\ldots,n+m$ have the second color. Then the total number of 2-colored graphs corresponding to specially labeled ones is found upon multiplying by $\binom{n+m}{n}$, which is the number of ways of distributing the n+m points among the two color classes.

To begin, let $M_{n,m}$ be the number of 2-colored graphs in which the first class contains n elements and the second contains m elements. Analogous to (1) we have

$$(4) M_{n,m} = 2^{nm}.$$

The corresponding exponential generating function is

$$M(x, y) = \sum_{n,m=0}^{\infty} M_{n,m} x^n y^m / n! m!$$

Let C(x, y) and N(x, y) be the exponential generating functions for the numbers $C_{n,m}$ and $N_{n,m}$ of connected and nonseparable labeled 2-colored graphs with color classes of sizes n and m. Then we can imitate (2) and (3) to obtain the two equations:

(5)
$$C(x, y) = \log M(x, y),$$

(6)
$$\log C_x(x, y) = N_x(xC_x(x, y), yC_y(x, y)).$$

In (5) we have not divided by 2 since we are still dealing with 2-colored graphs. In (6), C_x and C_y denote $\partial C/\partial x$ and $\partial C/\partial y$.

Now N(x, y) is determined by (4), (5) and (6), so we can pick out the number $N_{m,m}$ of 2-colored blocks on p = 2m points which have color classes of equal size. The corresponding number of bipartite blocks is then just $\frac{1}{2}\binom{2m}{m}N_{m,m}$.

3. Recurrence relations. In this section, recurrence relations for the coefficients in the exponential power series of equations (1)–(6) are derived. This is necessary in order to allow numerical calculation of these numbers.

A useful device for exponential or logarithmic relations, as used in [3] and other works, is to differentiate before equating coefficients. Applying this to equation (2) we obtain

$$D'(x)M(x) = \frac{1}{2}M'(x).$$

After equating coefficients and using $M_0 = 1$ as implied by (1), we find that the number of connected bipartite graphs for p > 0 is

(7)
$$D_{p} = \frac{M_{p}}{2} - \sum_{0 < i < p} D_{i} M_{p-i} \begin{pmatrix} p-1 \\ i-1 \end{pmatrix}.$$

We now reduce (3) to recurrence relations. To handle the left side of (3),

let us denote by H_p the coefficients of log D'(x), that is,

$$\sum_{p=1}^{\infty} H_p \frac{x^p}{p!} = \log D'(x).$$

Differentiating as before and equating coefficients, we find

(8)
$$H_p = D_{p+1} - \sum_{0 < i < p} H_i D_{p+1-i} \begin{pmatrix} p-1 \\ i-1 \end{pmatrix}$$
.

To express the right-hand side of (3), we require powers of D'(x). Let

$$\sum_{p=0}^{\infty} G_p^{(j)} \frac{x^p}{p!} = D'(x)^j.$$

Then the $G_p^{(k)}$ are determined by the relations

(9)
$$G_p^{(1)} = D_{p+1}, \quad G_p^{(j+1)} = \sum_{0 \le i \le p} \binom{p}{i} D_{p+1-i} G_i^{(j)}.$$

The coefficient of $x^p/p!$ on the right side of (3) can now be written

$$\sum_{0 < j \le p} \binom{p}{j} B_{j+1} G_{p-j}^{(j)}$$

since $B_0 = B_1 = 0$. Using the value $G_0^{(p)} = 1$ and equating coefficients of $x^p/p!$ in (3), we find

(10)
$$B_{p+1} = H_p - \sum_{0 \le j \le p} {p \choose j} B_{j+1} G_{p-j}^{(j)}.$$

Parallel procedures serve to transform equations (4), (5) and (6) into recurrence relations. These are more complicated, because the additional variable specifying the size of the color classes is present in each recurrence relation.

First, we know that $C_{0,1} = 1$ and $C_{0,m} = 0$ for $m \neq 1$. Differentiating (5) with respect to x and using the simple closed form 2^{nm} for $M_{n,m}$ from (4), we find

(11)
$$C_{n,m} = 2^{nm} - \sum *\binom{n-1}{a-1}\binom{m}{b} 2^{(n-a)(m-b)} C_{a,b},$$

where the asterisk on the summation indicates the rather unconventional set of conditions $1 \le a \le n$, $0 \le b \le m$, and either a < n or b < m. One can use the obvious fact that $C_{n,m} = C_{m,n}$ to reduce computation and storage in implementing (11).

To deal with the left side of (6), we let $H_{n,m}$ be the coefficients of log $C_x(x, y)$, that is,

$$\sum_{n,m\geq 0} H_{n,m} x^n y^m / n! m! = \log C_x(x, y).$$

Differentiating with respect to y, we find

(12)
$$H_{n,m} = C_{n+1,m} - \sum *\binom{n}{a}\binom{m-1}{b-1}H_{a,b}C_{n+1-a,m-b}$$

where this time the asterisk indicates the following summation conditions: $0 \le a \le n$, $1 \le b \le m$, and either b < m or a < n. It is easy to see that $H_{n,0} = 0$ for all n and that (12) determines $H_{n,m}$ recursively for all $m \ge 1$.

In order to help express the right side of (6), let $G_{n,m}^{(i,j)}$ denote the coefficient of $x^n y^m / n! m!$ in the product $\{x C_x(x, y)\}^i \{y C_y(x, y)\}^j$. These numbers are given by the recurrences

$$(13.1) \quad G_{n,m}^{(1,0)} = C_{n+1,m},$$

$$(13.2) \quad G_{n,m}^{(j+1,0)} = \sum_{\substack{0 \le a \le n \\ 0 \le b \le m}} \binom{n}{a} \binom{m}{b} G_{a,b}^{(j,0)} C_{n+1-a,m-b},$$

$$(13.3) \quad G_{n,m}^{(i,j)} = \sum_{\substack{0 \le a \le n \\ 0 \le b \le m}} \binom{n}{a} \binom{m}{b} G_{a,b}^{(i,0)} G_{m-b,n-a}^{(j,0)}$$

for all n, m, i, and j. Here we have made use of the symmetry condition

$$G_{n,m}^{(i,j)} = G_{m,n}^{(j,i)}$$

to simplify the form of these recurrences.

We can now equate coefficients of $x^n y^m / n! m!$ in (6). Using the fact that $G_{0,0}^{(n,m)} = 1$, this gives

(14)
$$N_{n+1,m} = H_{n,m} - \sum_{i=1}^{n} {m \choose i} N_{i+1,j} G_{n-i,m-j}^{(i,j)},$$

where the asterisk means that $3 \le i \le n$, $0 \le j \le m$, and either i < n or j < m. This serves to determine $N_{n+1,m}$ recursively for $n \ge 0$. Of course $N_{0,m} = 0$ for all m.

Finally, the number $B_{n,m}$ of bipartite blocks with n points of one color class and m of the other is just

(15)
$$B_{n,m} = \begin{cases} \binom{n+m}{n} N_{n,m} & \text{if } n \neq m, \\ \frac{1}{2} \binom{2m}{m} N_{m,m} & \text{if } n = m. \end{cases}$$

For if the sizes of the color classes are equal, the $\binom{2m}{m}$ ways to distribute the labels over the color classes overcounts by a factor of two since it assumes distinct colors.

4. Numerical results. In Table 1 we display the numbers $M_p/2$, D_p and B_p for p up to 20. These were calculated on the basis of equations (1), (7), (8), (9) and (10). These are comparable because they represent the number of

Table 1. Bicolored labeled graphs

$M_p/2$		D_{p}				B_p				
	1				1				0	1
	3				1				1	2
	13				3				0	3
	81				19				3	4
	721				195				10	5
9	153			3	031				355	6
	5 313				263			6	986	7
4 24			2	086					619	8
154 732				224			15	077		9
8 005 686		5		054		1		452		10
587 435 099		426						799		11
001 100 00.	61	120	000	020	47	111	100	100	15	
116 916 98		982	981	969		350	524	923		12
	011				507	30-			875	
561 121 23		894	696			055	248	515		13
1 885	2 834		1	641	072			738	416	
327 457 349	9 633	554	263	066	471	821	509	929	731	14
557 25'	7 804		502	596	525		260	316	039	1.7
202 631 21	7 153	992	239	961	103	943	139	322	858	15
233 610 650	6002	216	218	525	837		_	202		16
563 147 03	8 721	808	950	623	459	042	630	866	787	10
	138				130				84	
681 207 65				385				550		17
645 785 55		881	114	006		212	558	332		
238 610 10	3 575 e 50e	010	769	111 166	653	417	416	78 749	847	10
799 428 16				636				926		18
138 732		000		349		003		857		
504 824 44		458				313		871		19
466 218 40		622						293		10
233 733 370		228						380		
912 993 60		548	646	520	045			129		20
463 554 293	3 761	389	483	662	539	674	727	445	419	

bicolored labeled graphs with interchangeable colors. The total number of these graphs on p points is given by $M_p/2$, while the number which are connected is D_p and the number which are blocks is B_p . Of course D_p and B_p also counts bipartite graphs, since every connected bipartite graph has a unique bicoloring.

The numbers 2^{m^2} , $C_{m,m}$ and $N_{m,m}$ are displayed in Table 2 for m up to 12. These are the numbers of specially labeled 2-colored graphs with the color classes of equal size m. To be compared with the bicolored graphs of Table 1

2^{m^2}	$C_{m,m}$				$N_{m,m}$				m	
	2				1				1	1
	16				5				1	2
	512				205				34	3
65	536			36	317			7	037	4
33 554	432		23	679	901		6	317	926	5
68 719 476	736	56	294	206	205	21	073	662	977	6
	562				502				251	_
949 953 421	312	757	743	028	605	973	418	941	994	7
18 446	744		17	309	316		10	878	710	0
073 709 551	616	971	673	776	957	974	408	306	717	8
	2				2				1	
417 851 639	229			400		727	230	695	707	9
258 349 412	352	646	874	734	621	098	000	548	430	
1 267	650		1	243	000		1	028	983	
600 228 229				173				641		10
496 703 205	376	659	593	056	765	604	161	840	065	
	2				2				2	
658 455 991				962				062	-	11
831 745 807				413				492		
120 560 689		363		293		616		549		
22 300				170				683		
198 530 623				058				841		12
535 718 272				804				707		
361 505 980	416	596	601	690	557	751	484	424	893	

Table 2. Specially labeled 2-colored graphs with equal color classes

these numbers should be multipled by $\frac{1}{2} \binom{2m}{m}$. They were calculated on the basis of equations (11), (12), (13) and (14).

To enable a direct comparison of the number B_{2m} of labeled bipartite blocks and the number $B_{m,m}$ corresponding to just those in which the sizes of the color classes are equal, we present the two sets of numbers in Table 3 up to m=12, along with the ratio $B_{m,m}/B_{2m}$. It is conjectured in the next section that this ratio goes to the limit 0.4697... as $m \to \infty$.

Note. Calculations were carried out on a PDP 11/45, programed by Paul Butler and Albert Nymeyer, with support from the Australian Research Grants Committee.

5. Related problems. The asymptotic evaluation of M_p and C_p has been accomplished in Wright [8] and Read and Wright [6]. For the leading term, the results are

(16)
$$2C_p \sim M_p \sim \sqrt{\frac{2}{p \ln 2}} 2^{p^2/4+p} \psi(i/2),$$

$B_{m,m}$					i		B_{2m}	$B_{m,m}/B_{2m}$	m		
				1					1	1.0000	1
				3					3	1.0000	2
				340					355	.9577	3
			246	295				297	619	.8276	4
		796	058	676		1	120	452	771	.7105	5
9	736	032	295	374	15	350	524	923	547	.6342	6
386	386	904	461	$\frac{432}{704}$	416	821	509	929	738 731	. 5856	7
120	317		$004 \\ 723$		628	042		430 866		.5537	8
			212 333			847 369				. 5325	9
			95 798 524			693 674		591		. 5184	10
	411	581	345 696 357	428	450	623 079 018	238	401	833	.5088	11
			27 183 886			575 611		273		.5024	12

Table 3. Labeled bipartite blocks, with and without equal color classes

where i is the residue of p modulo 2 and

(16')
$$\psi(x) = \sqrt{\frac{\ln 2}{\pi}} \sum_{k=-\infty}^{\infty} 2^{-(x-k)^2}.$$

 $323\ 558\ 240\ 477\ 654$

It is clear that ψ has average value 1 and period 1. It is shown in [8] that $|\psi(x)-1| \leq 1.3097 \times 10^{-6}$ for all x and $\psi(0)-\psi(\frac{1}{2}) > 2.6194 \times 10^{-6}$. Direct computation gives $\psi(0)=1.00000130974\ldots$ and $\psi(\frac{1}{2})=0.99999869026\ldots$ The numerical results of Table 1 lend credence to the obvious conjecture that $B_p \sim C_p$. This can probably be proved in the fashion of [1], since the proof there that most graphs are blocks is based on the rapid growth of the number of labeled graphs.

 $662\ 810\ 228\ 887\ 603$

It is straightforward that for p = 2m,

(17)
$$\binom{2m}{m} 2^{m^2} \sim \frac{\sqrt{(\ln 2)/\pi}}{\psi(0)} M_p$$
.

From this it follows at once that

(18)
$$\frac{1}{2} \binom{2m}{m} C_{m,m} \sim \frac{\sqrt{(\ln 2)/\pi}}{\psi(0)} C_p.$$

If the conjecture $B_p \sim C_p$ is true, then it also follows that

(19)
$$\frac{1}{2} {2m \choose m} 2^{m^2} \sim \frac{1}{2} {2m \choose m} C_{m,m} \sim \frac{1}{2} {2m \choose m} N_{m,m} = B_{m,m}$$

and

(20)
$$B_{m,m} \sim \frac{\sqrt{(\ln 2)/\pi}}{\psi(0)} B_p$$
.

The constant $\sqrt{(\ln 2)/\pi}/\psi(0)$ is just $1/\sum_{k=-\infty}^{\infty} 2^{-k^2}$, which is approximately 0.46971802414.

It is planned to present the counting of unlabeled bipartite blocks in a later communication. Although this is far more difficult than the above labeled enumeration, the cycle index sum methods of [7] can be modified appropriately.

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