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Can. J. Math., Vol. XXXI, No. 1, 1979, pp. 60–68

LABELED BIPARTITE BLOCKS

F. HARARY AND R. W. ROBINSON

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

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

Received August 5, 1977 and in revised form, February 22, 1978. This research was facilitated by a grant from the Australian Department of Science under the U.S./Australia Cooperative Science Agreement.

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

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

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

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

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

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

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:

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

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

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

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

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

$$(7) \qquad D_p = \frac{M_p}{2} - \sum_{0<i<p} D_i M_{p-i} \binom{p-1}{i-1}.$$

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

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

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

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

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

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

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

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

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

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

where the asterisk on the summation indicates the rather unconventional set of conditions $1 \leqq a \leqq n$, $0 \leqq b \leqq m$, 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

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

where this time the asterisk indicates the following summation conditions: $0 \leqq a \leqq n$, $1 \leqq b \leqq m$, 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 $m \geqq 1$.

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 $\{xC_x(x, y)\}^i \{yC_y(x, y)\}^j$. These numbers are given by the recurrences

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

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

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

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

$$(14) \quad N_{n+1,m} = H_{n,m} - \sum{}^{*} \binom{n}{i}\binom{m}{j} N_{i+1,j} G_{n-i,m-j}^{(i,j)},$$

where the asterisk means that $3 \leqq i \leqq n$, $0 \leqq j \leqq m$, and either $i < n$ or $j < m$. This serves to determine $N_{n+1,m}$ recursively for $n \geqq 0$. 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

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

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	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
165 313	67 263	6 986	7
4 244 481	2 086 099	297 619	8
154 732 801	89 224 635	15 077 658	9
8 005 686 273	5 254 054 111	1 120 452 771	10
587 435 092 993	426 609 529 863	111 765 799 882	11
61 116 916 981 761	47 982 981 969 979	15 350 524 923 547	12
9 011 561 121 239 041	7 507 894 696 005 795	2 875 055 248 515 242	13
1 882 834 327 457 349 633	1 641 072 554 263 066 471	738 416 821 509 929 731	14
557 257 804 202 631 217 153	502 596 525 992 239 961 103	260 316 039 943 139 322 858	15
233 610 656 002 563 147 038 721	216 218 525 837 808 950 623 459	126 430 202 628 042 630 866 787	16
138 681 207 656 726 645 785 559 041	130 887 167 385 831 881 114 006 475	84 814 075 550 928 212 558 332 858	17
116 575 238 610 106 596 799 428 165 633	111 653 218 763 166 828 863 141 636 911	78 847 417 416 749 666 369 637 926 851	18
138 732 780 504 824 441 212 466 218 401 793	134 349 872 458 038 183 085 622 069 028 183	101 857 581 313 647 871 987 176 647 293 514	19
233 733 376 723 912 993 607 453 463 554 293 761	228 228 035 274 548 646 520 045 389 483 662 539	183 373 380 693 566 591 129 149 674 727 445 419	20

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

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

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
562 949 953 421 312	502 757 743 028 605	251 973 418 941 994	7
18 446 744 073 709 551 616	17 309 316 971 673 776 957	10 878 710 974 408 306 717	8
2 417 851 639 229 258 349 412 352	2 333 508 400 614 646 874 734 621	1 727 230 695 707 098 000 548 430	9
1 267 650 600 228 229 401 496 703 205 376	1 243 000 239 291 173 897 659 593 056 765	1 028 983 422 758 641 650 604 161 840 065	10
2 658 455 991 569 831 745 807 614 120 560 689 152	2 629 967 962 392 578 020 413 552 363 565 293 565	2 342 608 062 302 306 704 492 272 616 530 549 874	11
22 300 745 198 530 623 141 535 718 272 648 361 505 980 416	22 170 252 073 745 058 975 210 005 804 934 596 601 690 557	20 683 716 767 972 841 770 515 007 707 311 751 484 424 893	12

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

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

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TABLE 3. Labeled bipartite blocks with and without equal color classes

$B_{m,m}$	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
432 386 386 904 461 704	738 416 821 509 929 731	.5856	7
70 004 505 120 317 453 723 895	126 430 202 628 042 630 866 787	.5537	8
41 988 978 212 639 552 393 332 333 300	78 847 417 416 749 666 369 637 926 851	.5325	9
95 055 430 627 597 798 399 511 262 461 524 570	183 373 380 693 566 591 129 149 674 727 445 419	.5184	10
826 275 345 303 020 411 581 696 428 212 189 429 357 784	1 623 847 327 688 450 079 238 401 833 083 018 045 926 051	.5088	11
27 965 998 400 207 183 955 394 390 590 886 658 323 558 240 477 654	55 669 578 575 421 273 854 874 611 540 671 620 662 810 228 887 603	.5024	12

where i is the residue of p modulo 2 and

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

It is clear that ψ has average value 1 and period 1. It is shown in [8] that $|\psi(x) - 1| \leqq 1.3097 \times 10^{-6}$ 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.

It is straightforward that for $p = 2m$,

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

From this it follows at once that

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

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

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

and

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

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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