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ENUMERATION OF SYMMETRIC MATRICES

BY HANSRAJ GUPTA

1. Introduction. Let $H(n, r)$ denote the number of $n \times n$ matrices $[a_{ij}]$ where the a_{ij} are non-negative integers that satisfy

$$\sum_{i=1}^{n} a_{ij} = r = \sum_{j=1}^{n} a_{ij}, \qquad 1 \le i, \quad j \le n. \tag{1.1}$$

Anand, Dumir and Gupta [1] conjectured that for a given n and any r,

$$H(n, r) = \sum_{t=0}^{\binom{n-1}{2}} c_t \binom{r+n+t-1}{n+2t-1}, \tag{1.2}$$

where the c_t depend on n alone. This would imply that

$$\sum_{r=0}^{\infty} H(n, r)x^r = (1-x)^{-(n-1)^2-1}\psi(x), \tag{1.3}$$

where $\psi(x)$ is a symmetric polynomial in x of degree $(n-1)(n-2)$. It appears that the coefficients in $\psi(x)$ are positive integers. In particular, we have

$$\sum_{r=0}^{\infty} H(1, r)x^r = (1-x)^{-1},$$

$$\sum_{r=0}^{\infty} H(2, r)x^r = (1-x)^{-2},$$

$$\sum_{r=0}^{\infty} H(3, r)x^r = (1-x)^{-5}(1 + x + x^2)$$

and probably

$$\sum_{r=0}^{\infty} H(4, r)x^r = (1-x)^{-10}(1 + 14x + 87x^2 + 148x^3 + 87x^4 + 14x^5 + x^6).$$

Carlitz [2] has considered the analogous problem for symmetric matrices. Here, we shall be concerned with the case $r = 2$, not considered by Carlitz.

2. Let $S(n)$ denote the number of $n \times n$ symmetric matrices $[a_{ij}]$, where the a_{ij} satisfy

$$a_{ij} = a_{ji} = 0, 1 \text{ or } 2; \qquad 1 \le i, j \le n;$$

and

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$$\sum_{i=1}^{n} a_{ij} = 2.$$

With regard to the elements in the first row, we need consider matrices of the following four forms only:

(i) $a_{11} = 2;\ a_{1j} = 0,\ j \neq 1;$
(ii) $a_{12} = 2;\ a_{1j} = 0,\ j \neq 2;$
(iii) $a_{11} = a_{12} = 1;\quad a_{1j} = 0,\ j \neq 1, 2;$
(iv) $a_{12} = a_{13} = 1;\quad a_{1j} = 0,\ j \neq 2, 3.$

In what follows, to illustrate our points, we shall give only the relevant portions of the matrices under consideration. If we denote the number of matrices of types (i) – (iv), in our set, by $\alpha(n)$, $\beta(n)$, $\gamma(n)$ and $\delta(n)$ respectively; then it is easy to see that

$$\boxed{S(n) = \alpha(n) + (n-1)\{\beta(n) + \gamma(n)\} + \binom{n-1}{2}\delta(n).} \tag{2.1}$$

3. Relations between $\alpha(n), \beta(n), \gamma(n), \delta(n)$ **and** $S(n)$.

3.1. We readily see that

$$\boxed{\alpha(n) = S(n-1).} \tag{3.1}$$

For removing the first row and the first column from any matrix of type (i), we are left with a desirable matrix with $(n-1)$ rows and as many columns.

3.2. Again, we have

$$\boxed{\beta(n) = S(n-2).} \tag{3.2}$$

For removing the first two rows and the first two columns from any matrix of type (ii), we are left with a desirable matrix with $(n-2)$ rows and an equal number of columns.

3.3. In the case of matrices of the type (iii), we have to consider two subcases:

(a) When $a_{22} = 1$. The contribution to $\gamma(n)$ in this case is $S(n-2)$.

(b) When $a_{22} = 0$. Removing the first row and the first column, we are left with a matrix reducible to the form

$$\begin{matrix} 0 & 1 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & 0 & 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & & & & & \\ 0 & 0 & & & & & \\ 0 & 0 & & & & & \\ \cdot & \cdot & & & & & \end{matrix}$$

If we replace the zero at the top left corner by 1, this becomes an $(n-1) \times (n-1)$ matrix of type (iii). The contribution to $\gamma(n)$ in this case, therefore, is

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$(n-2)\,\gamma(n-1)$. We, thus, have

(3.3) $$\boxed{\gamma(n) = S(n-2) + (n-2)\,\gamma(n-1).}$$ *

3.4. In the case of matrices of type (iv), a number of subcases arise. We consider these and note the contribution to $\delta(n)$ in each case.

(a) When $a_{22} = 1 = a_{33}$. In this case, the matrix is of the form:

$$\begin{array}{l} 0\ 1\ 1\ 0\ 0\ \cdot\ \cdot \\ 1\ 1\ 0\ 0\ 0\ \cdot\ \cdot \\ 1\ 0\ 1\ 0\ 0\ \cdot\ \cdot \\ 0\ 0\ 0 \\ 0\ 0\ 0 \\ \cdot\ \cdot\ \cdot \end{array}$$

The contribution to $\delta(n)$ is $S(n-3)$.

(b) When $a_{23} = 1 = a_{32}$. The contribution to $\delta(n)$ is again $S(n-3)$.

(c) When the matrix is reducible to the form:

$$\begin{array}{l} 0\ 1\ 1\ 0\ 0\ \cdot\ \cdot \\ 1\ 0\ 0\ 1\ 0\ \cdot\ \cdot \\ 1\ 0\ 0\ 1\ 0\ \cdot\ \cdot \\ 0\ 1\ 1\ 0\ 0\ \cdot\ \cdot \\ 0\ 0\ 0\ 0 \\ \cdot\ \cdot\ \cdot\ \cdot \end{array}$$

The contribution to $\delta(n)$ is $(n-3)\,S(n-4)$.

(d) When the matrix is reducible to one of the two forms:

$$\begin{array}{l} 0\ 1\ 1\ 0\ 0\ \cdot\ \cdot \\ 1\ 1\ 0\ 0\ 0\ \cdot\ \cdot \\ 1\ 0\ 0\ 1\ 0\ \cdot\ \cdot \\ 0\ 0\ 1 \\ 0\ 0\ 0 \\ \cdot\ \cdot\ \cdot \end{array} \qquad \begin{array}{l} 0\ 1\ 1\ 0\ 0\ \cdot\ \cdot \\ 1\ 0\ 0\ 1\ 0\ \cdot\ \cdot \\ 1\ 0\ 1\ 0\ 0\ \cdot\ \cdot \\ 0\ 1\ 0 \\ 0\ 0\ 0 \\ \cdot\ \cdot\ \cdot\ \cdot \end{array}$$

Removing the first two or the first and third rows and the same columns, we are left with an $(n-2) \times (n-2)$ matrix of the type:

$$\begin{array}{l} 0\ 1\ 0\ \cdot\ \cdot \\ 1\ 0\ 0\ \cdot\ \cdot \\ 0\ 0 \\ \cdot\ \cdot \end{array}$$

The contribution to $\delta(n)$ in either case, is $(n-3)\,\gamma(n-2)$.

(e) Finally, when the matrix is reducible to one of the two forms:

$$\begin{array}{llllllll} 0&1&1&0&0&0&\cdot&\cdot\\ 1&0&0&1&0&0&\cdot&\cdot\\ 1&0&0&0&1&0&\cdot&\cdot\\ 0&1&0\\ 0&0&1\\ 0&0&0\\ \cdot&\cdot&\cdot \end{array} \qquad \begin{array}{llllllll} 0&1&1&0&0&0&\cdot&\cdot\\ 1&0&0&0&1&0&\cdot&\cdot\\ 1&0&0&1&0&0&\cdot&\cdot\\ 0&0&1\\ 0&1&0\\ 0&0&0\\ \cdot&\cdot&\cdot \end{array}$$

The contribution to $\delta(n)$ in either case, is $(n-3)(n-4)/2$ times what it would be from the $(n-2) \times (n-2)$ matrix

$$\begin{array}{lllll} 0&1&1&0&\cdot\ \cdot\\ 1\\ 1\\ 0\\ \cdot \end{array}$$

It is, therefore, $(n-3)(n-4)\,\delta(n)/2$ in each case. We, thus, have (3.4) $\delta(n) = 2\,S(n-3) + (n-3)\,S(n-4) + 2\,(n-3)\,\gamma(n-2) + (n-3)(n-4)\,\delta(n-2)$, which in view of (3.3),

$$\delta(n) = (n-3)\,S(n-4) + 2\,\gamma(n-1) + (n-3)(n-4)\,\delta(n-2).$$

4. Recursion formulae for $S(n)$ and $\gamma(n)$. The results obtained in §3, can be written:

(4.1) $$S(n) = \gamma(n+2) - n\,\gamma(n+1),$$

(4.2) $$\delta(n) - (n-3)(n-4)\,\delta(n-2) = (n-3)\,S(n-4) + 2\,\gamma(n-1).$$

Also, from (2.1) and (3.3), we have

(4.3) $$\binom{n-1}{2}\delta(n) = S(n) - (n-1)S(n-2) - \gamma(n+1).$$

Multiplying the two sides of (4.2) by $(n-1)(n-2)/2$, and making use of (4.3), we get

$$\begin{aligned} S(n) - (n-1)S(n-2) - \gamma(n+1) - (n-1)(n-2)\\ \cdot\{S(n-2) - (n-3)S(n-4) - \gamma(n-1)\}\\ = (1/2)(n-1)(n-2)(n-3)S(n-4) + (n-1)(n-2)\gamma(n-1). \end{aligned}$$

Hence

(4.4) $$\gamma(n+1) = S(n) - (n-1)^2\,S(n-2) + (1/2)\,(n-1)\,(n-2)\,(n-3)\,S(n-4).$$

From (4.1) and (4.4), we now have

$$S(n+1) = (n+1)S(n) + n^2S(n-1) - n(n-1)^2S(n-2) - 3\binom{n}{3}S(n-3) + 12\binom{n}{4}S(n-4); \tag{4.5}$$

and

$$\gamma(n+2) = (n+1)\gamma(n+1) + (n-1)^2\gamma(n) - (n-1)^2(n-2)\gamma(n-1) - 3\binom{n-1}{3}\gamma(n-2) + 12\binom{n-1}{4}\gamma(n-3). \tag{4.6}$$

Since $S(1) = 1 = \gamma(2)$, we take

$$S(0) = 1 = \gamma(1);$$

and

$$S(-m) = 0 \text{ for } m > 0, \gamma(-m) = 0 \text{ for } m \geq 0.$$

5. As an analogous problem, we find $S^*(n)$, the number of matrices $[a_{ij}]$, $1 \leq i, j \leq n$, such that

$$a_{ij} = a_{ji} = 0 \text{ or } 1,$$

$$\sum_{i=1}^{n} a_{ij} = 2.$$

Defining $\gamma^*(n)$ and $\delta^*(n)$ in the obvious way, and proceeding as in the preceding sections, we get

$$S^*(n) = (n-1)\gamma^*(n) + (1/2)(n-1)(n-2)\,\delta^*(n); \tag{5.1}$$

$$\gamma^*(n) = S^*(n-2) + (n-2)\gamma^*(n-1); \tag{5.2}$$

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and

$$\delta^*(n) = 2\gamma^*(n-1) + (n-3)S^*(n-4) + (n-3)(n-4)\,\delta^*(n-2). \tag{5.3}$$

Eliminating $\gamma^*(n)$ and $\delta^*(n)$ from these relations, we obtain without any particular difficulty

$$S^*(n+1) = n\left\{S^*(n) + nS^*(n-1) - (n-1)(n-3)S^*(n-2) - \binom{n-1}{2}S^*(n-3) - 3\binom{n-1}{3}S^*(n-4)\right\}. \tag{5.4}$$

We take $S^*(0) = 1$ and $S^*(-m) = 0$ for $m > 0$.

6. Generating functions.

6.1. Let $T(n)$ denote the number of $n \times n$ symmetric matrices $[a_{ij}]$ which are such that

$$a_{ij} = 0 \text{ or } 1,\ 1 \leq i, j \leq n,$$

and

$$\sum_{i=1}^{n} a_{ij} = 1 = \sum_{j=1}^{n} a_{ij}\,.$$

Then, as Carlitz has shown,

(6.1) $$h(x) = \sum_{n=0}^{\infty} \frac{T(n)}{n!} x^n = \exp\left(x + \frac{x^2}{2}\right).$$

6.2. Let

$$f(x) = \sum_{n=0}^{\infty} \frac{S(n)}{n!} x^n, \quad \text{with} \quad f(0) = 1.$$

Then, in view of (4.5), we have

$$(1 - x - x^2 + x^3)\, f'(x) = (1 + x - x^2 - \tfrac{1}{2} x^3 + \tfrac{1}{2} x^4)\, f(x).$$

This gives

(6.2) $$\frac{f'(x)}{f(x)} = (1 - x^2 + \tfrac{1}{2}x^3)/(1 - x)^2 = \tfrac{1}{2}\{x + (1 - x)^{-1} + (1 - x)^{-2}\}.$$

Hence

(6.3) $$f(x) = (1 - x)^{-\frac{1}{2}} \exp\left(\frac{x^2}{4} + \frac{x}{2(1 - x)}\right).$$

6.3. Let

$$g(x) = \sum_{n=0}^{\infty} \frac{S^*(n)}{n!} x^n, \quad \text{with} \quad g(0) = 1.$$

Then (5.4) gives

(6.4) $$g(x) = (1 - x)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{4} - x + \frac{x}{2(1 - x)}\right).$$

From (6.1), (6.3) and (6.4), we have the interesting relation:

(6.5) $$f(x) = g(x)\, h(x);$$

or what is the same thing

(6.6) $$S(n) = \sum_{k=0}^{n} \binom{n}{k} S^*(n - k) T(k).$$

As a direct consequence of (6.2), we have

(6.7) $$\boxed{S(n + 1) = (2n + 1)S(n) - \binom{n}{2}[2\{S(n - 1) + S(n - 2)\} - (n - 2)S(n - 3)].}$$

Similarly

(6.8) $S^*(n + 1) = n\{$

These formulae are certai

7. For ready reference,
given below.

n	$S(n)$
0	1
1	1
2	3
3	11
4	56
5	348
6	2578

1. H. Anand, V. C. Dumir, H.
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2. L. Carlitz, *Enumeration of*

Allahabad University
Allahabad, India

Similarly

$$\boxed{S^*(n+1) = n\left\{2S^*(n) - (n-2)S^*(n-1) - \binom{n-1}{2}S^*(n-3)\right\}.} \tag{6.8}$$

These formulae are certainly an improvement on those given in §4 and §5.

7. For ready reference, a few values of $S(n)$, $S^*(n)$ and $\gamma(n)$, $\gamma^*(n)$, $T(n)$ are given below.

n	$S(n)$	$S^*(n)$	$T(n)$	$\gamma(n)$	$\gamma^*(n)$
0	1	1	1	0	0
1	1	0	1	1	1
2	3	1	2	1	1
3	11	4	4	2	1
4	56	18	10	7	3
5	348	112	26	32	13
6	2578	820	76	184	70
	985	986	85!	987	1495

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ALLAHABAD UNIVERSITY
ALLAHABAD, INDIA

$S(n)$: no of mxs $n \times n$ symmetric, elements 0, 1 or 2
row sums = 2 Recurrence (6.7)

$S^*(n)$ elements 0 or 1 only, else same Type 2.
— (6.8)

$T(n)$ (0,1)-mxs with row & col sum equal to 1
— type 1
~~recurrence?~~ ~~see Carlitz~~ #85! again

$T_n = T_{n-1} + (n-1)T_{n-2}$

$\gamma(n)$ from (3.3)
$\gamma^*(n)$ from (5.2)