

# Nilpotent Matrices

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## 1 Introduction

Let  $n$  and  $k$  be non-negative integers, and define  $\mathcal{A}(n, k)$  to be the set of all  $n \times n$   $(0, 1)$ -matrices containing exactly  $k$  ones that square to  $0$ . In this note, we investigate the function  $f(n, k) = k! |\mathcal{A}(n, k)|$ .

		$k$									
		0	1	2	3	4	5	6	7	8	9
$n$	0	1									
	1	1									
	2	1	2								
	3	1	6	6							
	4	1	12	36	32	6					
	5	1	20	120	280	280	120	20			
	6	1	30	300	1320	2910	3492	2400	960	210	20

Table 1:  $|\mathcal{A}(n, k)|$  for small values of  $n$  and  $k$ . ([A052296](#))

## 2 Preliminaries

### 2.1 Graph Theory

We begin with some several elementary definitions in graph theory.

**Definition 1** (Adjacency Matrices).

- Let  $(V, E)$  be a *directed graph* whose vertices are indexed as  $V = \{v_1, \dots, v_n\}$ . Its adjacency matrix is the  $n \times n$  matrix  $\mathbf{M}$  with entries given by

$$\mathbf{M}_{ij} = \begin{cases} 1, & \text{if } (v_i, v_j) \in E, \\ 0, & \text{otherwise,} \end{cases}$$

where  $i, j \in [n]$ .

- Let  $(U, W, E)$  be a *directed bipartite graph* whose partite sets are indexed as  $U = \{u_1, \dots, u_m\}$  and  $W = \{w_1, \dots, w_n\}$ . Its adjacency matrix is the  $m \times n$  matrix  $\mathbf{M}$  with entries given by

$$\mathbf{M}_{ij} = \begin{cases} 1, & \text{if } (u_i, w_j) \in E, \\ 0, & \text{otherwise,} \end{cases}$$

where  $i \in [m]$  and  $j \in [n]$ .

**Definition 2.** A *directed walk of length  $n$*  is a sequence of vertices  $v_1, \dots, v_{n+1}$  (possibly with repetition) such that there exists a directed edge  $(v_i, v_{i+1})$  for all  $1 \leq i \leq n$ .

It is well-known that powers of an adjacency matrix are closely related to directed walks.

**Proposition 3.** Let  $\mathbf{M}$  be the adjacency matrix of a directed graph whose vertices are indexed as  $V = \{v_1, \dots, v_n\}$ . Then  $(\mathbf{M}^k)_{ij}$  counts the number of directed walks of length  $k$  from  $v_i$  to  $v_j$ .

## 2.2 Combinatorics

The *Stirling numbers of the first and second kind* are written as  ${}[n]_k$  and  $\{n\}_k$ , respectively. The *falling factorial* is written as  $(x)_n = x(x-1)\dots(x-n+1)$ . We write  $[n]$  to mean the set  $\{1, \dots, n\}$ .

Throughout this paper, we make use of the following well-known combinatorial identities.

**Proposition 4** ([2, 5]). Let  $n$  and  $k$  be non-negative integers with  $n \geq k$ , and  $x$  a non-negative real number.

$$(4.1) \quad \binom{n}{k} = \frac{(n)_k}{k!},$$

$$(4.2) \quad \{n\}_k = \frac{1}{k!} \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} i^n,$$

$$(4.3) \quad (x)_n = \sum_{k=0}^n (-1)^{n-k} [n]_k x^n,$$

$$(4.4) \quad \sum_{k=0}^n \{n\}_k (x)_k = x^n.$$

**Definition 5.** The *Stirling transform* of a sequence  $\{a_n\}_{n \geq 0}$ , denoted  $\mathcal{S}[\{a_n\}_{n \geq 0}]$ , is defined to be the sequence  $\{b_n\}_{n \geq 0}$  given by

$$b_n = \sum_{k=0}^{\infty} \{n\}_k a_k.$$

The inverse transform, denoted  $\mathcal{S}^{-1}[\{b_n\}_{n \geq 0}]$ , is

$$a_n = \sum_{k=0}^{\infty} (-1)^{n-k} [n]_k b_k.$$

**Example 6.** From [Identity \(4.4\)](#), we see that  $\mathcal{S}[\{(x)_n\}_{n \geq 0}] = \{x^n\}_{n \geq 0}$ . Conversely, [Identity \(4.3\)](#) tells us that  $\mathcal{S}^{-1}[\{x^n\}_{n \geq 0}] = \{(x)_n\}_{n \geq 0}$ .

**Proposition 7** ([1]). Suppose  $\mathcal{S}[\{a_n\}_{n \geq 0}] = \{b_n\}_{n \geq 0}$  and define the exponential generating functions

$$A(x) = \sum_{n=0}^{\infty} \frac{a_n}{n!} x^n \quad \text{and} \quad B(x) = \sum_{n=0}^{\infty} \frac{b_n}{n!} x^n.$$

Then  $B(x) = A(e^x - 1)$ .

## 3 Properties of $f(n, k)$

### 3.1 Generating Function

**Theorem A.** Let  $F(x; n) = \sum_{k=0}^{\infty} f(n, k) x^k / k!$  be the exponential generating function of the sequence  $\{f(n, k)\}_{k \geq 0}$ . Then

$$F(x; n) = \sum_{i=0}^n \binom{n}{i} ((1+x)^{n-i} - 1)^i.$$

This result appears in [3], but a proof was omitted. We provide a proof here for completeness.

*Proof.* Note that

$$F(x; n) = \sum_{k=0}^{\infty} \frac{f(n, k)}{k!} x^k = \sum_{k=0}^{\infty} |\mathcal{A}(n, k)| x^k.$$

We thus find the ordinary generating function for  $|\mathcal{A}(n, k)|$ .

Let  $\mathbf{A} \in \bigcup_{k \geq 0} \mathcal{A}(n, k)$ . If  $\mathbf{A}_{ij} = 1$ , then  $\mathbf{A}_{jm} = 0$  for all  $m \in [n]$ ; if  $\mathbf{A}_{jm} = 1$  for some  $m \in [n]$ , we obtain the contradiction

$$(\mathbf{A}^2)_{im} = \sum_{t=1}^n \mathbf{A}_{it} \mathbf{A}_{tm} \geq \mathbf{A}_{ij} \mathbf{A}_{jm} = 1 \neq 0.$$

That is to say, if column  $j$  has a 1, then row  $j$  must be all zeroes.

Given two complementary sets  $A$  and  $B = [n] \setminus A$ , we let  $A$  be the indices of columns that *must* have a 1, and  $B$  the indices of rows that *could* have a 1. We now count the number of ways to construct  $\mathbf{A}$  given some choice of  $A$ . Within each column  $j \in A$ , we can only place 1's in the rows indexed by  $B$ . Since the column cannot be all zeroes, this amounts to choosing a non-empty subset of  $B$ . Hence, the generating function recording all possibilities for that particular column  $j$  is

$$\sum_{i=1}^{|B|} \binom{|B|}{i} x^i = (1+x)^{|B|} - 1.$$

As the choices for different columns in  $A$  are independent, the ordinary generating function over all columns is

$$\left( (1+x)^{|B|} - 1 \right)^{|A|}.$$

Fix  $|A| = i$ , so  $|B| = n - i$ . There are  $\binom{n}{i}$  choices for  $A$ . Summing over all possible sizes  $i$ , we finally obtain the generating function

$$F(x; n) = \sum_{i=0}^n \binom{n}{i} \left( (1+x)^{n-i} - 1 \right)^i.$$

□

**Corollary 8.** Let  $S(n) = \sum_{k=0}^n |\mathcal{A}(n, k)|$  be the total number of  $n \times n$  matrices that square to  $\mathbf{0}$ . Then

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

$n$	0	1	2	3	4	5	6
$S(n)$	1	1	3	13	87	841	11643

Table 2:  $S(n)$  for small values of  $n$ . (A001831)

### 3.2 Formulas

In this subsection, we give several formulas for  $f(n, k)$ . We begin with the following combinatorial lemma.

**Lemma 9.** *The number of directed bipartite graphs  $(S, T, E)$  with exactly  $k$  edges and no isolated vertices is given by*

$$\frac{s! t!}{k!} \sum_{i=0}^k (-1)^{k-i} \begin{bmatrix} k \\ i \end{bmatrix} \begin{Bmatrix} i \\ s \end{Bmatrix} \begin{Bmatrix} i \\ t \end{Bmatrix},$$

where  $s = |S|$  and  $t = |T|$ .

*Proof.* By considering the adjacency matrix, there is a one-to-one correspondence between directed bipartite graphs with exactly  $k$  edges and no isolated vertices, and  $s \times t$   $(0, 1)$ -matrices with exactly  $k$  1's and no all-zero rows or columns.

Let  $\#$  denote the number of such matrices (equivalently, the number of graphs). We count  $\#$  using inclusion-exclusion. Let  $R_i$  and  $C_j$  denote the events that the  $i$ th row and  $j$ th column, respectively, are all zero. Then the number of matrices with no all-zero rows or columns is

$$\# = \sum_{A \subseteq S} \sum_{B \subseteq T} (-1)^{|A|+|B|} \left| \bigcap_{a \in A} R_a \cap \bigcap_{b \in B} C_b \right|.$$

Grouping the terms by the sizes of  $A$  and  $B$  gives

$$\# = \sum_{i=0}^s \sum_{j=0}^t \sum_{\substack{A \subseteq S \\ |A|=i}} \sum_{\substack{B \subseteq T \\ |B|=j}} (-1)^{i+j} \left| \bigcap_{a \in A} R_a \cap \bigcap_{b \in B} C_b \right|.$$

Fix  $|A| = i$  and  $|B| = j$ . There are  $\binom{s}{i}$  choices for  $A$  and  $\binom{t}{j}$  choices for  $B$ . Consider the event  $\bigcap_{a \in A} R_a \cap \bigcap_{b \in B} C_b$ , in which the rows indexed by  $A$  and columns indexed by  $B$  are all zero. There are  $(s-i)(t-j)$  remaining positions to place the  $k$  1's in, so

$$\left| \bigcap_{a \in A} R_a \cap \bigcap_{b \in B} C_b \right| = \binom{(s-i)(t-j)}{k}.$$

Substituting these values into our expression for  $\#$  yields

$$\# = \sum_{i=0}^s \sum_{j=0}^t (-1)^{i+j} \binom{s}{i} \binom{t}{j} \binom{(s-i)(t-j)}{k}.$$

Applying the combinatorial identities listed in [Proposition 4](#) finishes the proof.

$$\begin{aligned}
\# &= \sum_{i=0}^s \sum_{j=0}^t (-1)^{i+j} \binom{s}{i} \binom{t}{j} \binom{(s-i)(t-j)}{k} \\
&\stackrel{(4.1)}{=} \sum_{i=0}^s \sum_{j=0}^t (-1)^{i+j} \binom{s}{i} \binom{t}{j} \frac{((s-i)(t-j))_k}{k!} \\
&\stackrel{(4.3)}{=} \frac{1}{k!} \sum_{i=0}^s \sum_{j=0}^t (-1)^{i+j} \binom{s}{i} \binom{t}{j} \sum_{m=0}^k (-1)^{k-m} \binom{k}{m} (s-i)^m (t-j)^m \\
&= \frac{s! t!}{k!} \sum_{m=0}^k (-1)^{k-m} \binom{k}{m} \left[ \frac{1}{s!} \sum_{i=0}^s (-1)^i \binom{s}{i} (s-i)^m \right] \left[ \frac{1}{t!} \sum_{j=0}^t (-1)^j \binom{t}{j} (t-j)^m \right] \\
&\stackrel{(4.4)}{=} \frac{s! t!}{k!} \sum_{m=0}^k (-1)^{k-m} \binom{k}{m} \left\{ \begin{matrix} m \\ s \end{matrix} \right\} \left\{ \begin{matrix} m \\ t \end{matrix} \right\}.
\end{aligned}$$

□

With this result, we are ready to find a formula for  $f(n, k)$ .

**Theorem B.**

$$f(n, k) = \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} \sum_{0 \leq s, t \leq i} \left\{ \begin{matrix} i \\ s \end{matrix} \right\} \left\{ \begin{matrix} i \\ t \end{matrix} \right\} (n)_{s+t}.$$

*Proof.* By [Proposition 3](#), there is a one-to-one correspondence between  $\mathcal{A}(n, k)$  and the set of all directed graphs  $(V, E)$  with  $|V| = n$  and  $|E| = k$  that do not contain any directed walks of length 2. We count the number of such graphs.

Let  $S$  and  $T$  be the sets of vertices with non-zero outdegree and indegree respectively. Since all walks are of length one, the sets  $S$  and  $T$  are disjoint. Thus, for fixed sizes  $s = |S|$  and  $t = |T|$ , there are  $\binom{n}{s} \binom{n-s}{t}$  ways to choose  $S$  and  $T$  from  $V$ . Next, [Lemma 9](#) tells us that for any choice of  $S$  and  $T$ , there are

$$\frac{s! t!}{k!} \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} \left\{ \begin{matrix} i \\ s \end{matrix} \right\} \left\{ \begin{matrix} i \\ t \end{matrix} \right\}$$

ways to draw  $k$  edges from vertices in  $S$  to vertices in  $T$ . Enumerating over all possible sizes  $s$  and  $t$ , the number of directed graphs (and thus matrices) is

$$|\mathcal{A}(n, k)| = \sum_{s=0}^k \sum_{t=0}^k \binom{n}{s} \binom{n-s}{t} \frac{s! t!}{k!} \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} \left\{ \begin{matrix} i \\ s \end{matrix} \right\} \left\{ \begin{matrix} i \\ t \end{matrix} \right\}.$$

Writing  $\binom{n}{s} \binom{n-s}{t}$  as  $(n)_{s+t} / s! t!$  and noting that the summand vanishes when  $s, t > i$ , we obtain

$$f(n, k) = k! |\mathcal{A}(n, k)| = \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} \sum_{0 \leq s, t \leq i} \left\{ \begin{matrix} i \\ s \end{matrix} \right\} \left\{ \begin{matrix} i \\ t \end{matrix} \right\} (n)_{s+t}.$$

□

*Remark.* [Theorem B](#) generalizes the  $k = 2$  case as discussed by the author in [\[7\]](#).

Applying [Identity \(4.4\)](#) to the formula given by [Theorem B](#), the triple sum collapses to the following double sum expression for  $f(n, k)$ .

**Proposition 10.**

$$f(n, k) = \sum_{i=0}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{s=0}^i \begin{Bmatrix} i \\ s \end{Bmatrix} (n)_s (n-s)_i^i.$$

*Proof.* Write  $(n)_{s+t} = (n)_s (n-s)_t$ . By [Theorem B](#), this gives

$$\begin{aligned} f(n, k) &= \sum_{i=0}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{s=0}^i \begin{Bmatrix} i \\ s \end{Bmatrix} (n)_s \sum_{t=0}^i \begin{Bmatrix} i \\ t \end{Bmatrix} (n-s)_t \\ &\stackrel{(4.4)}{=} \sum_{i=0}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{s=0}^i \begin{Bmatrix} i \\ s \end{Bmatrix} (n)_s (n-s)_i^i. \end{aligned}$$

□

Next, we use [Theorem B](#) to write  $f(n, k)$  as a polynomial in  $n$ , with coefficients depending on  $k$ .

**Proposition 11.**

$$f(n, k) = \sum_{p=0}^{2k} \left[ (-1)^p \sum_{i=\lceil p/2 \rceil}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{\substack{0 \leq s, t \leq i \\ s+t \geq p}} (-1)^{s+t} \begin{Bmatrix} i \\ s \end{Bmatrix} \begin{Bmatrix} i \\ t \end{Bmatrix} \begin{Bmatrix} s+t \\ p \end{Bmatrix} \right] n^p.$$

*Proof.* From [Theorem B](#), we have that

$$f(n, k) = \sum_{i=0}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{s=0}^i \begin{Bmatrix} i \\ s \end{Bmatrix} (n)_s (n-s)_i^i.$$

Using [Identity \(4.3\)](#) to expand  $(n)_{s+t}$  as a sum of monomials, we get

$$f(n, k) = \sum_{i=0}^k (-1)^{k-i} \begin{Bmatrix} k \\ i \end{Bmatrix} \sum_{0 \leq s, t \leq i} \begin{Bmatrix} i \\ s \end{Bmatrix} \begin{Bmatrix} i \\ t \end{Bmatrix} \sum_{p=0}^{s+t} (-1)^{s+t-p} \begin{Bmatrix} s+t \\ p \end{Bmatrix} n^p.$$

Interchanging the order of summation so that we sum over  $p$  first yields the desired expression. □

### 3.3 Stirling Transform and Chromatic Polynomials

Let  $P(K_{k,k}, n)$  be the chromatic polynomial of the complete bipartite graph  $K_{k,k}$ . [\[6\]](#) gives the closed-form

$$P(K_{k,k}, n) = \sum_{0 \leq s, t \leq k} \begin{Bmatrix} k \\ s \end{Bmatrix} \begin{Bmatrix} k \\ t \end{Bmatrix} (n)_{s+t}.$$

It follows from [Theorem B](#) that  $\{P(K_{k,k}, n)\}_{k \geq 0}$  is the Stirling transform of  $\{f(n, k)\}_{k \geq 0}$ .

**Proposition 12.**  $P(K_{k,k}, n)$  has exponential generating function

$$\sum_{i=0}^n \begin{Bmatrix} n \\ i \end{Bmatrix} (\mathrm{e}^{xi} - 1)^{n-i}.$$

*Proof.* Let  $G(x; n)$  be the exponential generating function of  $\{P(K_{k,k}, n)\}_{k \geq 0}$ . Since  $\{P(K_{k,k}, n)\}_{k \geq 0}$  is the Stirling transform of  $\{f(n, k)\}_{k \geq 0}$ , we have by [Proposition 7](#) that  $G(x; n) = F(\mathrm{e}^x - 1; n)$ . Using the formula for  $F(x; n)$  given in [Theorem A](#), we see that

$$G(x; n) = \sum_{i=0}^n \begin{Bmatrix} n \\ i \end{Bmatrix} (\mathrm{e}^{xi} - 1)^{n-i}.$$

□

### 3.4 Factorization

**Proposition 13.** For fixed  $n$ , the support of  $f(n, k)$  is  $k = 0, \dots, \lfloor n^2/4 \rfloor$ .

*Proof.* The degree of the  $i$ th term of  $F(x; n)$  is  $i(n - i)$ , which attains a maximum of  $\lfloor n^2/4 \rfloor$  when  $i = \lfloor n/2 \rfloor$ . Thus,  $f(n, k) = 0$  for all  $k > \lfloor n^2/4 \rfloor$ . To show that  $f(n, k)$  is non-zero for  $k = 0, \dots, \lfloor n^2/4 \rfloor$ , it suffices to construct a matrix  $\mathbf{A} \in \mathcal{A}(n, \lfloor n^2/4 \rfloor)$ , since for any  $k < \lfloor n^2/4 \rfloor$  a matrix in  $\mathcal{A}(n, k)$  may be obtained by replacing some of the entries of  $\mathbf{A}$  from 1 to 0.

Let  $\mathbf{0}_{a \times b}$  and  $\mathbf{1}_{a \times b}$  denote the  $a \times b$  blocks whose entries all 0 and 1, respectively. We construct  $\mathbf{A}$  according to the parity of  $n$ .

*Case 1:  $n$  is even.* Write  $n = 2m$ , so  $\lfloor n^2/4 \rfloor = m^2$ . Then

$$\mathbf{A} = \begin{pmatrix} \mathbf{0}_{m \times m} & \mathbf{1}_{m \times m} \\ \mathbf{0}_{m \times m} & \mathbf{0}_{m \times m} \end{pmatrix} \in \mathcal{A}(2m, m^2).$$

*Case 2:  $n$  is odd.* Write  $n = 2m + 1$ , so  $\lfloor n^2/4 \rfloor = m^2 + m$ . Then

$$\mathbf{A} = \begin{pmatrix} \mathbf{0}_{m \times m} & \mathbf{1}_{m \times (m+1)} \\ \mathbf{0}_{(m+1) \times m} & \mathbf{0}_{(m+1) \times (m+1)} \end{pmatrix} \in \mathcal{A}(2m + 1, m^2 + m).$$

□

*Remark.* In the case where  $n = 2m$  is even,  $\mathbf{A}$  is the adjacency matrix of the directed complete bipartite graph  $\vec{K}_{m,m}$ . When  $n = 2m + 1$  is odd,  $\mathbf{A}$  is the adjacency matrix of the directed complete bipartite graph  $\vec{K}_{m,m+1}$ .

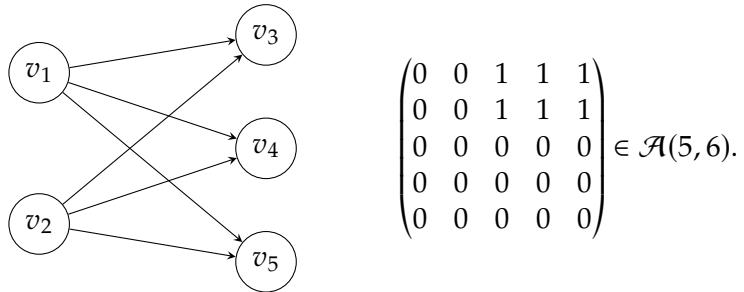


Figure 1: The directed complete bipartite graph  $\vec{K}_{2,3}$  and its adjacency matrix.

**Proposition 14.** Fix  $k$  and let  $\alpha_k = \lceil 2\sqrt{k} \rceil$ . Then  $f(n, k) = (n)_{\alpha_k} P(n, k)$  for some monic polynomial  $P(n, k) \in \mathbb{Z}[n]$  of degree  $2k - \alpha_k$  with no integer roots.

*Proof.* Recall from [Theorem B](#) that

$$f(n, k) = \sum_{i=0}^k (-1)^{k-i} \binom{k}{i} \sum_{0 \leq s, t \leq i} \binom{i}{s} \binom{i}{t} (n)_{s+t}.$$

It is easy to see that  $f(n, k) \in \mathbb{Z}[n]$ . Next, we note that  $\deg((n)_{s+t}) = s + t \leq 2k$ , with equality if and only if  $s = t = i = k$ . The corresponding term is

$$(-1)^{k-k} \binom{k}{k} \binom{k}{k} \binom{k}{k} (n)_{k+k} = (n)_{2k},$$

which is monic. It follows that  $f(n, k)$  is a monic polynomial of degree  $2k$ .

By [Proposition 13](#), we see that  $f(n, k)$  vanishes if and only if  $n \leq \lceil 2\sqrt{k} \rceil = \alpha_k$ . Thus, the only integer roots of  $f(n, k)$  are  $n = 0, 1, \dots, \alpha_k$ , giving the factorization  $f(n, k) = (n)_{\alpha_k} P(n, k)$ , where  $P(n, k) \in \mathbb{Z}[n]$  is a monic polynomial of degree  $2k - \alpha_k$  with no integer roots.  $\square$

$k$	$P(n, k)$
0	1
1	1
2	$-1 + n$
3	$4 - 3n + n^2$
4	$86 - 96n + 43n^2 - 10n^3 + n^4$
5	$-810 + 886n - 415n^2 + 105n^3 - 15n^4 + n^5$
6	$-46440 + 59752n - 34168n^2 + 11341n^3 - 2380n^4 + 320n^5 - 26n^6 + n^7$

Table 3: The polynomials  $P(n, k)$  for  $k = 1, \dots, 6$

## References

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