Nilpotent $0 - 1$ Matrices

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1 Introduction

In this note, we prove the following result:

Theorem A. *Let $\mathbf{A}_k$ be an $n \times n$ matrix obtained by switching k random entries of $\mathbf{0}$ from 0 to 1. Then*

$$\mathbb{P}\left[\mathbf{A}_k^2 = \mathbf{0}\right] = \frac{1}{\binom{n^2}{k}} \sum_{s=1}^{k} \sum_{t=1}^{k} \binom{n}{s} \binom{n-s}{t} \sum_{i=0}^{s} \sum_{j=0}^{t} (-1)^{i+j} \binom{s}{i} \binom{t}{j} \binom{(s-i)(t-j)}{k}.$$

This result generalizes the $k = 2$ case as discussed at [1].

2 Proof of Theorem A

We begin with some several elementary definitions in graph theory.

Definition 1. The *adjacency matrix* of a *directed graph* with vertices $\{v_1, \ldots, v_n\}$ is an $n \times n$ matrix $\mathbf{M}$ with entries given by

$$m_{ij} = \begin{cases} 1, & \text{if there is a directed edge } v_i \to v_j, \\ 0, & \text{otherwise,} \end{cases}$$

where $1 \le i, j \le n$. Note that $\mathbf{A}_{ii} = 1$ indicates there is a loop at v_i.

Definition 2. The *adjacency matrix* of a *directed bipartite graph* with bipartition (U, W), where $U = \{u_1, \ldots, u_m\}$ and $W = \{w_1, \ldots, w_n\}$, is the $m \times n$ matrix $\mathbf{M}$ with entries given by

$$m_{ij} = \begin{cases} 1, & \text{if there is a directed edge } u_i \to w_j, \\ 0, & \text{otherwise,} \end{cases}$$

where $1 \le i \le m$ and $1 \le j \le n$.

Definition 3. A *walk of length k* is a sequence of vertices $v_1, \ldots, v_k$ (possibly with repetition) such that there exists an edge $v_i \to v_{i+1}$ for all $1 \le i \le k-1$.

We now prove some helpful results.

Proposition 4. *Let $\mathbf{A}$ be the adjacency matrix of a directed graph with vertices $V = \{1, \ldots, n\}$. Then a_{ij}^m counts the number of walks of length m from i to j.*

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Proof. For $1 \le i, j \le n$, let $\mathbf{1}_{ij}$ be the $n \times n$ matrix whose (i, j)-entry is 1, and all other entries are 0. Suppose there are k edges, and label them as

$$E = \left\{(i_1, j_1), \ldots, (i_k, j_k)\right\}.$$

Then we may decompose $\mathbf{A}$ as

$$\mathbf{A} = \sum_{(i,j)\in E} \mathbf{1}_{ij} = \sum_{t=1}^{k} \mathbf{1}_{i_t j_t}.$$

Now consider higher powers of $\mathbf{A}$. Since

$$\mathbf{1}_{ab}\mathbf{1}_{cd} = \begin{cases} \mathbf{1}_{ad}, & \text{if } b = c, \\ \mathbf{0}, & \text{otherwise,} \end{cases}$$

one can inductively show that

$$\mathbf{1}_{i_{t_1} j_{t_1}} \ldots \mathbf{1}_{i_{t_m} j_{t_m}} = \begin{cases} \mathbf{1}_{i_{t_1} j_{t_m}}, & \text{if } j_{t_r} = i_{t_{r+1}} \text{ for all } 1 \le r \le m-1,] \\ \mathbf{0}, & \text{otherwise.} \end{cases}$$

Thus,

$$\mathbf{A}^m = \sum_{(t_1,\ldots,t_m)\in \mathcal{P}_m} \mathbf{1}_{i_{t_1} j_{t_m}},$$

where $\mathcal{P}_m$ is the set of all length m sequences of edges (i_{t_r}, j_{t_r}) such that $j_{t_r} = i_{t_{r+1}}$ for all $1 \le r \le m-1$. But each sequence in $\mathcal{P}_m$ describes a walk of length m from (i_{t_1}, j_{t_1}) to (i_{t_m}, j_{t_m}):

$$i_{t_1} \longrightarrow j_{t_1} = i_{t_2} \longrightarrow j_{t_2} = \cdots = i_{t_m} \longrightarrow j_{t_m},$$

and adds 1 to the (i_{t_1}, j_{t_m}) entry in $\mathbf{A}^m$. Thus, a_{ij}^m counts the number of walks of length m from i to j. □

Proposition 5. *Let S and T be disjoint sets of size s and t respectively. The number of ways to draw k arrows from S to T such that*

- *every element of S is the tail of at least one arrow, and*
- *every element of T is the head of at least one arrow,*

is given by

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

Proof. We may view the given set-up as a directed bipartite graph (S, T, E) with $|E| = k$. Let $\mathbf{M}$ be the adjacency matrix of this graph. By construction, every row and every column of $\mathbf{M}$ must have at least one non-zero entry. It thus suffices to count the number of $s \times t$ matrices with entries in $\{0, 1\}$ with no all-zero rows or columns, and exactly k 1's.

We proceed by inclusion-exclusion. Consider an arbitrary $s \times t$ matrix with entries in $\{0, 1\}$ and exactly k 1's. Let R_i and C_j be the event that the ith row and jth column is all zero, respectively. By inclusion-exclusion, the number of matrices that avoid all-zero rows and columns is precisely

$$\sum_{A\subseteq[s]} \sum_{B\subseteq[t]} (-1)^{|A|+|B|} \left| \bigcap_{a\in A} R_a \cap \bigcap_{b\in B} C_b \right|.$$

Fix $|A| = i$ and $|B| = j$, and consider the event $\bigcap_{a\in A} R_a \cap \bigcap_{b\in B} C_b$. In this case, all rows with indices in A and all columns with indices in B are forced to be all-zero. This leaves $(s-i)(t-j)$ available positions to place the k 1's in, so

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

Note further that there are $\binom{s}{i}$ possibilities for A and $\binom{t}{j}$ possibilities for B for a total contribution of

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

Enumerating over all possible sizes i and j, we get a final count of

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

as desired. □

We now prove Theorem A.

Proof of Theorem A. We may view $\mathbf{A}_k$ as the adjacency matrix of a directed graph $G = (V, E)$, where $V = \{v_1, \ldots, v_n\}$ and $|E| = k$. By Proposition 4, $\mathbf{A}_k^2 = \mathbf{0}$ if and only if G does not contain any walk of length 2. Equivalently, all walks of G must have length 1.

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 have length one, we have $S \cap T = \varnothing$. 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, Proposition 5 tells us that for any choice of S and T, there are

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

ways to assign k edges from S to T. Enumerating over all possible sizes s and t, the number of valid graphs (and thus matrices) is

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

Since there are $\binom{n^2}{k}$ matrices without restriction, we have the desired result. □

3 Particular Values

For $1 \le k \le 6$, we list the closed-form expressions for $\mathbb{P}\left[\mathbf{A}_k^2 = \mathbf{0}\right]$. We define

$$A_m = \prod_{i=0}^{m-1}(n-i) \quad \text{and} \quad B_m = \prod_{i=0}^{m-1}\left(n^2-i\right).$$

$$\mathbb{P}\left[\mathbf{A}_1^2 = \mathbf{0}\right] = \frac{A_2}{B_1} \tag{$k=1$}$$

$$\mathbb{P}\left[\mathbf{A}_2^2 = \mathbf{0}\right] = \frac{A_3}{B_2}(n-1) \tag{$k=2$}$$

$$\mathbb{P}\left[\mathbf{A}_3^2 = \mathbf{0}\right] = \frac{A_4}{B_3}\left(n^2 - 3n + 4\right) \tag{$k=3$}$$

$$\mathbb{P}\left[\mathbf{A}_4^2 = \mathbf{0}\right] = \frac{A_4}{B_4}\left(n^4 - 10n^3 + 43n^2 - 96n + 86\right) \tag{$k=4$}$$

$$\mathbb{P}\left[\mathbf{A}_5^2 = \mathbf{0}\right] = \frac{A_5}{B_5}\left(n^5 - 15n^4 + 105n^3 - 415n^2 + 886n - 810\right) \tag{$k=5$}$$

$$\mathbb{P}\left[\mathbf{A}_6^2 = \mathbf{0}\right] = \frac{A_5}{B_6}\left(n^7 - 26n^6 + 320n^5 - 2380n^4 + 11341n^3 - 34168n^2 + 59752n - 46440\right) \tag{$k=6$}$$

The following Python snippet yields simplified expressions for fixed k:

```
import sympy as sp

def closed_form(k):
    n = sp.symbols('n', integer=True)

    term = 0

    for S in range(1, k+1):
        for T in range(1, k+1):
            inner = 0
            for I in range(0, S+1):
                for J in range(0, T+1):
                    inner += (-1)**(I+J) * sp.binomial(S, I) * sp.binomial(T, J) * sp.binomial((S-I)*(T-J), k)
            term += sp.binomial(n, S) * sp.binomial(n-S, T) * inner

    expr = term / sp.binomial(n**2, k)
    return sp.simplify(expr)
```

4 Final Remarks

We leave the following questions and extensions for the reader.

- Can the result in Theorem A be further simplified?
- Let

$$\mathbb{P}\left[\mathbf{A}_k^2 = \mathbf{0}\right] = \frac{A_{a_k}}{B_{b_k}}P$$

  for some polynomial P in n.
  - Is $b_k = k$ for all k?
  - What pattern does a_k follow?
  - Are there any patterns to the coefficients of P?
- Determine $\mathbb{P}\left[\mathbf{A}_k^m = \mathbf{0}\right]$ for integers $m > 2$.
- Construct another matrix $\mathbf{B}_k$ independently of $\mathbf{A}_k$. What is $\mathbb{P}[\mathbf{A}_k\mathbf{B}_k = \mathbf{0}]$?

References

[1] Various authors. Determine the probability that $A^2 = O$? Mathematics Stack Exchange. https://math.stackexchange.com/q/4367731. Accessed 2025-09-30.