Digraphs that have at most one walk of a given length with the same endpoints[1]

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Abstract. Let $\Theta(n,k)$ be the set of digraphs of order n that have at most one walk of length k with the same endpoints. Let $\theta(n,k)$ be the maximum number of arcs of a digraph in $\Theta(n,k)$. We prove that if $n \geq 5$ and $k \geq n-1$ then $\theta(n,k) = n(n-1)/2$ and this maximum number is attained at D if and only if D is a transitive tournament. $\theta(n,n-2)$ and $\theta(n,n-3)$ are also determined.

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1. Introduction

Digraphs in this paper allow loops but do not allow multiple arcs. We follow the terminology in [1] and [2]. The number of the vertices of a digraph is called its *order* and the number of the arcs its *size*. For digraphs, cycles and walks will mean directed cycles and directed walks respectively.

For given positive integers n, k, let $\Theta(n,k)$ denote the set of the digraphs D on vertices $1, 2, \ldots, n$ such that for any i, j with $1 \leq i, j \leq n$, D has at most one walk of length k from i to j. Let $\theta(n,k)$ denote the maximum size of a digraph in $\Theta(n,k)$. In 2007 the second-named author posed the following problem at a seminar:

Problem 1. *For given positive integers n, k, determine $\theta(n,k)$ and determine the digraphs in $\Theta(n,k)$ that attain the size $\theta(n,k)$.*

Note that the possible sizes of the digraphs in $\Theta(n,k)$ are the integers in the interval $[0,\ \theta(n,k)]$. In fact, if $D \in \Theta(n,k)$ has size $\theta(n,k)$ and m is an integer in $[0,\ \theta(n,k)]$, then deleting any $\theta(n,k)-m$ arcs in D we obtain a digraph $D_1 \in \Theta(n,k)$

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with size m. The motivation for studying Problem 1 is to explore the relation between the size and the walks of a digraph. Intuitively digraphs in $\Theta(n,k)$ cannot have very large sizes.

The case $k = 2$ of Problem 1 has been solved by Wu [5] whose result is

$$\theta(n,2) = \begin{cases} \frac{n^2+4n-1}{4}, & \text{if } n \text{ is odd,} \\ \frac{n^2+4n-4}{4}, & \text{if } n \text{ is even and } n \neq 4, \\ 8, & \text{if } n = 4 \end{cases}$$

and the digraphs attaining this largest size are also determined in [5].

A digraph is said to be *transitive* if for every three distinct vertices v_i, v_j, v_k the condition that (v_i, v_j) and (v_j, v_k) are arcs implies that (v_i, v_k) is an arc. It is clear that a tournament of order n is transitive if and only if its vertices can be labeled as $1, 2 \ldots, n$ such that (i, j) is an arc if and only if $i < j$. Two useful references on tournaments are [3, 4]. Our main result is the following

Theorem 1. *Let n, k be given integers with $n \geq 5$ and $k \geq n-1$. Then $\theta(n,k) = n(n-1)/2$ and a digraph $D \in \Theta(n,k)$ has size $n(n-1)/2$ if and only if D is a transitive tournament.*

Throughout we denote by $M_n\{0,1\}$ the set of 0-1 matrices of order n. For given positive integers n, k denote $\Gamma(n,k) = \{A \in M_n\{0,1\} | A^k \in M_n\{0,1\}\}$. Denote by $f(A)$ the number of $1'$s in a matrix A. Define

$$\gamma(n,k) = \max\{f(A) | A \in \Gamma(n,k)\}.$$

Considering the adjacency matrix of a digraph we see that Problem 1 is equivalent to the following

Problem 1'. *For given positive integers n, k, determine $\gamma(n,k)$ and determine the matrices in $\Gamma(n,k)$ that attain $\gamma(n,k)$.*

Of course, $\theta(n,k) = \gamma(n,k)$.

We denote by

$$T_n = \begin{pmatrix} 0 & 1 & \cdots & 1 \\ & \ddots & \ddots & \vdots \\ & & 0 & 1 \\ & & & 0 \end{pmatrix},$$

the upper triangular tournament matrix of order n. A digraph of order n is a transitive tournament if and only if its adjacency matrix is permutation similar to T_n. Thus, Theorem 1 is equivalent to the following

Theorem 1'. *Let n, k be given integers with $n \geq 5$ and $k \geq n-1$. Then $\gamma(n,k) = n(n-1)/2$ and a matrix $A \in \Gamma(n,k)$ satisfies $f(A) = n(n-1)/2$ if and only if A is permutation similar to T_n.*

In Section 2 we prove Theorem 1'. In Section 3 we determine $\gamma(n, n-2)$ and $\gamma(n, n-3)$.

2. Proof of Theorem 1'

The digraph of a matrix $A = (a_{ij})$ of order n, denoted $D(A)$, is the digraph on vertices $1, 2, \ldots, n$ in which (i,j) is an arc with tail i and head j if and only if $a_{ij} \neq 0$. It is clear that for $A \in M_n\{0,1\}$, $A \in \Gamma(n,k)$ if and only if $D(A) \in \Theta(n,k)$. A p-cycle is a cycle of length p.

For a matrix $A = (a_{ij})$ of order n and integers $1 \leq i_1 < i_2 < \cdots < i_t \leq n$, we denote by $A[i_1, \ldots, i_t]$ the principal submatrix of A indexed by $i_1, \ldots, i_t$ and we denote by $A(i)$ the principal submatrix of A of order $n-1$ obtained by deleting the i-th row and i-th column.

Let A^T denote the transpose of a matrix A. We will use the following fact repeatedly: $A \in \Gamma(n,k)$ if and only if $PAP^T \in \Gamma(n,k)$ for any permutation matrix P if and only if $A^T \in \Gamma(n,k)$.

Lemma 1. *Let $A \in \Gamma(n,k)$. Then the following statements on $D(A)$ hold.*

(i) If $k \geq 2$, two loops cannot be connected by an arc. If $k \geq 3$, two loops cannot be connected by a walk of length 2.

(ii) If $k \geq 2$, a loop and a 2-cycle are disjoint. If $k \geq 3$, a loop and a 2-cycle cannot be connected by an arc.

(iii) If $k \geq 3$, a loop and a 3-cycle are disjoint.

(iv) If $k \geq 2$, two 2-cycles are disjoint. If $k \geq 3$, two 2-cycles cannot be connected by an arc.

(v) If $k \geq 2$, there do not exist i, j, t with $i \neq j$ such that $i \to i$ and $i \to t$ are arcs, and $i \to j \to t$ is a walk.

Proof. We just prove (v) and omit the similar and easy verifications of the remaining items. If $t = j$, (v) is one case in (i); if $t = i$, (v) is one case in (ii). Now we suppose that i, j, t are distinct such that $i \to i$ and $i \to t$ are arcs, and $i \to j \to t$ is a walk. Then we will have the following two distinct walks of length k from i to t :

$$\begin{cases} i \to \cdots \to i \to j \to t \\ i \to \cdots \to i \to i \to t, \end{cases}$$

which contradicts the assumption that $A^k \in M_n\{0, 1\}$. □

Lemma 2. *If $A \in \Gamma(n, k)$ and B is a principal submatrix of A of order m, then $B \in \Gamma(m, k)$.*

Proof. Deleting any $n - m$ vertices of $D(A)$ together with the arcs incident with them we obtain a digraph in $\Theta(m, k)$. The result is also clear from the matrix viewpoint. □

Lemma 3. *If $k \geq 2$, then $\gamma(2, k) = 2$.*

Proof. By Lemma 1 (i) and (ii) we have $\gamma(2, k) \leq 2$. Considering any permutation matrix of order 2 we conclude that $\gamma(2, k) = 2$. □

Lemma 4. *If $k \geq 3$, then $\gamma(3, k) = 4$.*

Proof. Let $A = (a_{ij}) \in \Gamma(3, k)$. Suppose $f(A) \geq 5$. Considering the distribution of the ones in the four disjoint sets of A's entries $\{a_{11}, a_{22}, a_{33}\}$, $\{a_{12}, a_{21}\}$, $\{a_{13}, a_{31}\}$, $\{a_{23}, a_{32}\}$, we deduce that there exist i_1, j_1, i_2, j_2 with $\{i_1, j_1\} \neq \{i_2, j_2\}$ and

$$a_{i_1 j_1} = a_{j_1 i_1} = 1 = a_{i_2 j_2} = a_{j_2 i_2}.$$

We distinguish three cases: $i_1 = j_1, i_2 = j_2$; $i_1 = j_1, i_2 \neq j_2$; $i_1 \neq j_1, i_2 \neq j_2$.

Case 1: $i_1 = j_1, i_2 = j_2$. By permutation similarity transform if necessary, without loss of generality (WLOG) we assume $i_1 = j_1 = 1$ and $i_2 = j_2 = 2$. Considering the principal submatrices of A of order 2, using Lemmas 2 and 3 we have

$$a_{12} = a_{21} = 0,\ a_{13} + a_{31} + a_{33} \leq 1,\ a_{23} + a_{32} \leq 1.$$

Hence

$$f(A) = 2 + (a_{13} + a_{31} + a_{33}) + (a_{23} + a_{32}) \leq 4,$$

a contradiction.

Case 2: $i_1 = j_1, i_2 \neq j_2$. WLOG suppose $i_1 = j_1 = 1$. By Lemma 1(ii), $i_2 \neq 1, j_2 \neq 1$. Thus $a_{23} = a_{32} = 1$. Considering $A[2,3]$ and using Lemmas 2 and 3 we have $a_{22} = a_{33} = 0$. Now

$$A = \begin{pmatrix} 1 & a_{12} & a_{13} \\ a_{21} & 0 & 1 \\ a_{31} & 1 & 0 \end{pmatrix}.$$

By Lemma 1(ii), $a_{12} = a_{13} = a_{21} = a_{31} = 0$. Hence $f(A) = 3$, a contradiction.

Case 3: $i_1 \neq j_1, i_2 \neq j_2$. Since $1 \leq i_1, j_1, i_2, j_2 \leq 3$, two of these four indices are equal. This contradicts Lemma 1(iv).

Therefore $f(A) \leq 4$. On the other hand,

$$B = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \in \Gamma(3,k)$$

with $f(B) = 4$. Note that B is idempotent. This proves $\gamma(3,k) = 4$. □

Lemma 5. *If $k \geq 3$, then $\gamma(4,k) = 6$.*

Proof. Suppose that there exists an $A = (a_{ij}) \in \Gamma(4,k)$ with $f(A) \geq 7$. Denote $w(i) = \sum_{j=1}^{4}(a_{ij} + a_{ji}) - a_{ii}$. Recall that $A(i)$ denotes the principal submatrix obtained by deleting the i-th row and i-th column of A. If there is some t with $w(t) \leq 2$, then by Lemma 4,

$$f(A) = w(t) + f(A(t)) \leq 2 + 4 = 6,$$

contradiction. So $w(i) \geq 3$ for each $i = 1,2,3,4$.

We distinguish two cases according to whether $D(A)$ has loops.

Case 1: Each diagonal entry of A is 0. Since the union of the 6 sets

$$\{a_{12}, a_{21}\}, \{a_{13}, a_{31}\}, \{a_{14}, a_{41}\}, \{a_{23}, a_{32}\}, \{a_{24}, a_{42}\}, \{a_{34}, a_{43}\}$$

contains at least 7 entries equal to 1, at least one set contains two $1'$s. WLOG, suppose $a_{12} = a_{21} = 1$. Note that $w(1) \geq 3$. Using permutation similarity transforms and taking transpose if necessary, there are essentially the following two different cases according to the entries in the first row and first column of A :

$$\text{Subcase 1:} \quad A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & a_{23} & a_{24} \\ a_{31} & a_{32} & 0 & a_{34} \\ a_{41} & a_{42} & a_{43} & 0 \end{pmatrix}$$

and

$$\text{Subcase 2:} \quad A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & a_{23} & a_{24} \\ a_{31} & a_{32} & 0 & a_{34} \\ a_{41} & a_{42} & a_{43} & 0 \end{pmatrix}.$$

Subcase 1. By Lemma 1(iv), $a_{31} = a_{41} = 0$, $a_{23} + a_{32} \leq 1$, $a_{24} + a_{42} \leq 1$, $a_{34} + a_{43} \leq 1$.

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & a_{23} & a_{24} \\ 0 & a_{32} & 0 & a_{34} \\ 0 & a_{42} & a_{43} & 0 \end{pmatrix}$$

Then from

$$4 + (a_{23} + a_{32}) + (a_{24} + a_{42}) + (a_{34} + a_{43}) = f(A) \geq 7$$

we get

$$a_{23} + a_{32} = 1,\ a_{24} + a_{42} = 1,\ a_{34} + a_{43} = 1.$$

If $a_{34} = 1$, since one of a_{24} and a_{42} is equal to 1, we will have two distinct walks of length k with the same endpoints in $D(A)$ as shown below:

$$a_{24} = 1 \Rightarrow \begin{cases} \cdots \to 2 \to 1 \to 3 \to 4 \\ \cdots \to 2 \to 1 \to 2 \to 4 \end{cases}$$

$$a_{42} = 1 \Rightarrow \begin{cases} \cdots \to 1 \to 2 \to 1 \to 2 \\ \cdots \to 1 \to 3 \to 4 \to 2 \end{cases}$$

Here $\cdots \to$ means a walk of length $k-3$ constructed by using the cycle $1 \to 2 \to 1$. In the sequel we omit similar explanations. So $a_{34} = 0$ and hence $a_{43} = 1$.

Since

$$a_{23} = 1 \Rightarrow \begin{cases} \cdots \to 2 \to 1 \to 2 \to 3 \\ \cdots \to 2 \to 1 \to 4 \to 3 \end{cases}$$

we must have $a_{23} = 0$. Consequently $a_{32} = 1$. But

$$a_{32} = 1 \Rightarrow \begin{cases} \cdots \to 1 \to 2 \to 1 \to 2 \\ \cdots \to 1 \to 4 \to 3 \to 2 \end{cases}$$

Contradiction.

Subcase 2. If $a_{23} = a_{24} = 1$, then interchanging rows 1 and 2 and columns 1 and 2 we transform A to subcase 1. So we need consider only the case when $a_{23}+a_{24} \leq 1$. By Lemma 1(iv), $a_{31} = 0$.

a) Suppose $a_{24} = 1$. Then $a_{23} = 0$. By Lemma 1(iv), $a_{42} = 0$.

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & a_{32} & 0 & a_{34} \\ a_{41} & 0 & a_{43} & 0 \end{pmatrix}$$

Since $w(3) \geq 3$, at least two of a_{32}, a_{34}, a_{43} are equal to 1. But $a_{34} = a_{43} = 1$ is impossible by Lemma 1(iv). So $a_{32} = 1$ and exactly one of a_{34} and a_{43} is equal to 1 and the other is equal to 0. From $f(A) \geq 7$ we get $a_{41} = 1$. But then

$$\begin{cases} \cdots \to 2 \to 1 \to 3 \to 2 \\ \cdots \to 2 \to 4 \to 1 \to 2, \end{cases}$$

contradiction.

b) Suppose $a_{24} = 0$.

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & a_{23} & 0 \\ 0 & a_{32} & 0 & a_{34} \\ a_{41} & a_{42} & a_{43} & 0 \end{pmatrix}$$

By Lemma 1(iv), $a_{23} + a_{32} \leq 1$, $a_{34} + a_{43} \leq 1$. From

$$3 + (a_{23} + a_{32}) + (a_{34} + a_{43}) + a_{41} + a_{42} = f(A) \geq 7$$

we deduce $a_{41} = a_{42} = 1$, $a_{23} + a_{32} = 1$, $a_{34} + a_{43} = 1$. But

$$a_{23} = 1 \Rightarrow \begin{cases} 4 \to 2 \to 1 (\to \cdots) \to 3 \\ 4 \to 1 \to 2 (\to \cdots) \to 3 \end{cases}$$

So $a_{23} = 0$ and $a_{32} = 1$. Again

$$a_{32} = 1 \Rightarrow \begin{cases} 4 \to 2 \to 1 \to 2 \to \cdots \\ 4 \to 1 \to 3 \to 2 \to \cdots \end{cases}$$

Contradiction.

Case 2: There is a diagonal entry equal to 1. WLOG suppose $a_{11} = 1$. Using permutation similarity transform, taking transpose if necessary and noting that $w(1) \geq 3$, there are essentially the following three different cases.

Subcase 1. The first row of A has four $1'$s. By Lemma 1(v), $a_{ij} = 0$, $2 \leq i \leq 4$, $1 \leq j \leq 4$. Hence $f(A) = 4$, contradiction.

Subcase 2. The first row of A has three $1'$s. WLOG suppose $a_{12} = a_{13} = 1$. By Lemma 1(v), $a_{ij} = 0$, $2 \leq i \leq 3$, $1 \leq j \leq 3$.

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & a_{24} \\ 0 & 0 & 0 & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}$$

By Lemma 1(ii), $a_{24} + a_{42} \leq 1$, $a_{34} + a_{43} \leq 1$. Using Lemmas 2 and 3, and considering $A[1,4]$ we have $a_{41} + a_{44} \leq 1$. Hence

$$f(A) = 3 + (a_{24} + a_{42}) + (a_{34} + a_{43}) + (a_{41} + a_{44}) \leq 6,$$

contradiction.

Subcase 3. The first row of A has two $1'$s. WLOG suppose $a_{12} = 1$. Using

Lemmas 2 and 3, and considering $A[1,2]$ we have $a_{21} = a_{22} = 0$.

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}$$

The case $a_{31} = a_{41} = 1$ can be converted to subcase 2 by taking transpose and using permutation similarity transform. Note that $w(1) \geq 3$. We need consider only the case when exactly one of them is equal to 1. WLOG suppose $a_{31} = 1$, $a_{41} = 0$. By Lemma 1 (iii) and (i), $a_{23} = a_{33} = 0$.

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & a_{24} \\ 1 & a_{32} & 0 & a_{34} \\ 0 & a_{42} & a_{43} & a_{44} \end{pmatrix}$$

By Lemma 1(ii), $a_{24} + a_{42} \leq 1$, $a_{34} + a_{43} \leq 1$. Then from

$$3 + a_{32} + a_{44} + (a_{24} + a_{42}) + (a_{34} + a_{43}) = f(A) \geq 7$$

we obtain

$$a_{32} = a_{44} = 1,\ a_{24} + a_{42} = 1,\ a_{34} + a_{43} = 1.$$

By Lemma 1(i) we have $a_{24} = a_{43} = 0$. Now

$$a_{44} = a_{34} = a_{42} = 1 \Rightarrow \begin{cases} 3 \to 1 \to \cdots \to 1 \to 2 \\ 3 \to 4 \to \cdots \to 4 \to 2, \end{cases}$$

contradiction.

We have proved that $\gamma(4,k) \leq 6$. On the other hand,

$$B = \begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \in \Gamma(4,k)$$

with $f(B) = 6$. Note that B is idempotent. This proves $\gamma(4,k) = 6$. □

Lemma 6. *If $k \geq 4$, then $\gamma(5,k) = 10$. If $A = (a_{ij}) \in \Gamma(5,k)$ satisfies $f(A) = 10$, then $a_{ii} = 0$ for $1 \leq i \leq 5$ and $a_{ij} \neq a_{ji}$ for $1 \leq i < j \leq 5$.*

Proof. Let $B \in \Gamma(5,k)$. Consider the number of $1'$s in all the five principal submatrices $B(i)$ of B of order 4, $i = 1, \dots, 5$. Each off-diagonal entry of B appears 3 times and each diagonal entry of B appears 4 times in these principal submatrices. Suppose B has d diagonal entries equal to 1. By Lemma 2, every $B(i) \in \Gamma(4,k)$ and Lemma 5 gives $f(B(i)) \leq 6$, $i = 1, \dots, 5$. Thus we have

$$3[f(B) - d] + 4d = \sum_{i=1}^{5} f(B(i)) \leq 5 \times 6 = 30.$$

It follows that

$$f(B) \leq 10 - \frac{d}{3} \leq 10.$$

On the other hand, $T_5^4 \in M_5\{0,1\}$ with one entry equal to 1, $T_5^k = 0$ for $k \geq 5$ and $f(T_5) = 10$. This shows $\gamma(5,k) = 10$.

From the above proof we see that $f(A) = 10$ implies that $a_{ii} = 0$ for $1 \leq i \leq 5$ and $f(A(i)) = 6$ for $1 \leq i \leq 5$. Next we show $a_{ij} \neq a_{ji}$ for $i \neq j$.

We first show that for $i \neq j$, $a_{ij} + a_{ji} \leq 1$. To the contrary suppose there exist $i \neq j$ such that $a_{ij} = a_{ji} = 1$. WLOG suppose $a_{12} = a_{21} = 1$. Denote $w(i) = \sum_{j=1}^{5}(a_{ij} + a_{ji}) - a_{ii}$. From $10 = f(A) = w(i) + f(A(i))$ and $f(A(i)) = 6$ we have $w(i) = 4$, $i = 1, \dots, 5$. There exists j with $3 \leq j \leq 5$ such that $a_{1j} = a_{j1} = 0$. Otherwise $w(1) \geq 5$. WLOG suppose $a_{15} = a_{51} = 0$. Then

$$A = \begin{pmatrix} 0 & 1 & a_{13} & a_{14} & 0 \\ 1 & 0 & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & 0 & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & 0 & a_{45} \\ 0 & a_{52} & a_{53} & a_{54} & 0 \end{pmatrix}.$$

Since $w(5) = 4$, considering the three sets

$$\{a_{25}, a_{52}\}, \ \{a_{35}, a_{53}\}, \ \{a_{45}, a_{54}\}$$

we conclude that there exists j such that $a_{j5} = a_{5j} = 1$. By Lemma 1(iv), $j \neq 2$. So $3 \leq j \leq 4$.

Suppose $a_{35} = a_{53} = 1$. By Lemma 1(iv),

$$0 = a_{13} = a_{31} = a_{23} = a_{32} = a_{25} = a_{52}.$$

Thus

$$A = \begin{pmatrix} 0 & 1 & 0 & a_{14} & 0 \\ 1 & 0 & 0 & a_{24} & 0 \\ 0 & 0 & 0 & a_{34} & 1 \\ a_{41} & a_{42} & a_{43} & 0 & a_{45} \\ 0 & 0 & 1 & a_{54} & 0 \end{pmatrix}.$$

Then $f(A(4)) = 4$, which contradicts $f(A(i)) = 6$ for $1 \leq i \leq 5$. In the same way, $a_{45} = a_{54} = 1$ yields a contradiction.

We have proved that for $1 \leq i < j \leq 5$, $a_{ij} + a_{ji} \leq 1$. Note that there are exactly 10 pairs a_{ij}, a_{ji} with $1 \leq i < j \leq 5$. From

$$10 = f(A) = \sum_{1 \leq i < j \leq 5} (a_{ij} + a_{ji})$$

we deduce that for every pair a_{ij}, a_{ji} with $1 \leq i < j \leq 5$ exactly one of them is equal to 1 and the other is equal to 0. Hence $a_{ij} \neq a_{ji}$ for $i \neq j$. □

Lemma 7. *Let $k \geq 4$ and $A \in \Gamma(5, k)$. If $f(A) = 10$, then A is permutation similar to T_5.*

Proof. Let $A = (a_{ij})$. By Lemma 6, $a_{ii} = 0$ for $1 \leq i \leq 5$ and $a_{ij} \neq a_{ji}$ for $1 \leq i < j \leq 5$.

Denote the row sum $r(i) = \sum_{j=1}^{5} a_{ij}$, the number of $1'$s in the i-th row. Then $r(i) \leq 4$ and $10 = f(A) = \sum_{i=1}^{5} r(i)$. To prove Lemma 7 it suffices to show

$$\{r(i) | i = 1, 2, 3, 4, 5\} = \{0, 1, 2, 3, 4\}$$

which is equivalent to $r(i) \neq r(t)$ for $i \neq t$. It is easy to see that under the above conditions A is permutation similar to T_5. Here and in the sequel we need the fact that a pair of entries in symmetric positions of a matrix remain in symmetric positions under permutation similarity transforms, that is, if matrices $G = (g_{ij})$ and P are of the same order with P a permutation matrix, $PGP^T = (h_{ij})$ and $h_{st} = g_{ij}$, then $h_{ts} = g_{ji}$, and consequently diagonal entries remain on the diagonal under permutation similarity transforms.

We first note that A cannot have two row sums equal to 4. Otherwise there would exist $i \neq j$ such that $a_{ij} = a_{ji} = 1$. If there are $i \neq t$ such that $r(i) = r(t) = 0$ or $r(i) = r(t) = 1$ then either there exist $1 \leq u \neq v \leq 5$ such that $r(u) = r(v) = 3$ or 2 or A has three row sums equal to 1. Next we show that all these three cases cannot occur.

Case 1: There exist $i \neq t$ such that $r(i) = r(t) = 3$. WLOG suppose $i = 1, t = 2$ and by permutation similarity transform if necessary we may assume

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & a_{34} & a_{35} \\ 0 & 0 & a_{43} & 0 & a_{45} \\ 1 & 0 & a_{53} & a_{54} & 0 \end{pmatrix}.$$

Then

$$a_{34} = 1 \Rightarrow \begin{cases} \cdots \to 2 \to 5 \to 1 \to 2 \to 4 \\ \cdots \to 2 \to 5 \to 1 \to 3 \to 4 \end{cases}$$

$$a_{43} = 1 \Rightarrow \begin{cases} \cdots \to 2 \to 5 \to 1 \to 2 \to 3 \\ \cdots \to 2 \to 5 \to 1 \to 4 \to 3 \end{cases}$$

Hence $a_{34} = a_{43} = 0$ contradicting $a_{34} \neq a_{43}$.

Case 2: There exist $i \neq t$ such that $r(i) = r(t) = 2$. There are essentially the following two cases.

Subcase 1,

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & a_{34} & a_{35} \\ 1 & 0 & a_{43} & 0 & a_{45} \\ 1 & 1 & a_{53} & a_{54} & 0 \end{pmatrix}.$$

Then

$$a_{34} = 1 \Rightarrow \begin{cases} \cdots \to 4 \to 1 \to 2 \to 4 \to 1 \\ \cdots \to 4 \to 1 \to 3 \to 4 \to 1 \end{cases}$$

$$a_{43} = 1 \Rightarrow \begin{cases} 5 \to 2 \to 4 \to 1(\to 2 \to 4 \to 1 \to \cdots) \to 3 \\ 5 \to 1 \to 2 \to 4(\to 1 \to 2 \to 4 \to \cdots) \to 3 \end{cases}$$

Here we may use the 3-cycle $1 \to 2 \to 4 \to 1$ each of whose vertices dominates 3 to obtain the length k of the two different walks. Hence $a_{34} = a_{43} = 0$ contradicting $a_{34} \neq a_{43}$.

Subcase 2,

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & a_{34} & a_{35} \\ 1 & 0 & a_{43} & 0 & a_{45} \\ 1 & 0 & a_{53} & a_{54} & 0 \end{pmatrix}.$$

Then we have

$$\begin{cases} \cdots \to 5 \to 1 \to 2 \to 4 \to 1 \\ \cdots \to 5 \to 1 \to 2 \to 5 \to 1 \end{cases}$$

Contradiction.

Case 3: A has three row sums equal to 1. WLOG suppose $r(1) = r(2) = r(3) = 1$. Since each pair of $\{a_{12}, a_{21}\}, \{a_{13}, a_{31}\}, \{a_{23}, a_{32}\}$ contains exactly one 1, using the condition $r(1) = r(2) = r(3) = 1$ we deduce that $A[1, 2, 3]$ is a permutation matrix and

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} & 0 & 0 \\ a_{21} & 0 & a_{23} & 0 & 0 \\ a_{31} & a_{32} & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & a_{45} \\ 1 & 1 & 1 & a_{54} & 0 \end{pmatrix}.$$

Now the first three column sums are equal to 3. Thus considering the transpose A^T we come to the case 1. This completes the proof. $\square$

Combining Lemmas 6 and 7 we obtain the following

Lemma 8. *Theorem 1' holds for* $n = 5$.

Lemma 8 is the starting point of our proof of Theorem 1'. Another key ingredient is the following lemma.

Lemma 9. *Let $n \geq 4$ and $A \in M_n\{0,1\}$. If all the principal submatrices of A of order $n-1$ are permutation similar to T_{n-1}, then A is permutation similar to T_n.*

Proof. The lemma is equivalent to the following proposition:

Let D be a digraph of order at least 4. If $D - v$ is a transitive tournament for all vertices v, then D is a transitive tournament.

We prove this proposition. Clearly D has no loop, since otherwise one of $D - v$ would have a loop. Furthermore, clearly D is a tournament. It is known [3, Corollary 5a] that a tournament is transitive if and only if it is acyclic. Suppose D is not transitive. Then D contains a cycle of length at least 3, and hence contains a strongly connected subtournament D' of order at least 3. By [3, Theorem 7] which states that a strongly connected tournament of order $m \geq 3$ contains a cycle of each length $k = 3, 4, \ldots, m$, D' contains a triangle (a cycle of length 3). That triangle is in $D - v$ for some vertex v, which contradicts the condition that $D - v$ is transitive. Thus D is a transitive tournament. $\square$

Proof of Theorem 1'. We use induction on the order n. For $n = 5$, the result holds by lemma 8. Suppose the result holds for $n = m - 1$, $m \geq 6$. Now we prove the result for $n = m$ with $k \geq m - 1$.

Let $A \in \Gamma(m, k)$. Denote by $B_1, B_2, \ldots, B_m$ the m principal submatrices of A of order $m - 1$. Then by Lemma 2 $B_i \in \Gamma(m-1, k)$ and by our induction hypothesis

$$f(B_i) \leq \frac{(m-1)(m-2)}{2}, \quad i = 1, \ldots, m \tag{1}$$

where equality holds if and only if B_i is permutation similar to T_{m-1}.

Now we count the number of $1'$s in $B_1, B_2, \ldots, B_m$. Each off-diagonal entry of A appears $m-2$ times and each diagonal entry of A appears $m-1$ times in these principal submatrices. Suppose A has exactly d diagonal entries equal to 1, $d \geq 0$. Using (1) we have

$$(m-2)[f(A) - d] + (m-1)d = \sum_{i=1}^{m} f(B_i) \leq m\frac{(m-1)(m-2)}{2} \tag{2}$$

from which follows

$$f(A) \leq \frac{m(m-1)}{2} - \frac{d}{m-2} \leq \frac{m(m-1)}{2}. \tag{3}$$

Thus, (3) shows that $\gamma(m,k) \le m(m-1)/2$. On the other hand, $T_m^{m-1} \in M_m\{0,1\}$ with the only 1 in the position $(1,m)$ and $T_m^k = 0$ for $k \ge m$. Hence $T_m \in \Gamma(m,k)$. Also, $f(T_m) = m(m-1)/2$. So $\gamma(m,k) = m(m-1)/2$.

Suppose $A \in \Gamma(m,k)$ satisfies $f(A) = m(m-1)/2$ and the m principal submatrices of A of order $m-1$ are $B_1, B_2, \ldots, B_m$. From (3) we deduce $d = 0$, and further from (2) and (1) we deduce $f(B_i) = (m-1)(m-2)/2$ for each $i = 1, 2, \ldots, m$. This implies that each B_i is permutation similar to T_{m-1} by the equality case condition of (1). Applying Lemma 9 we conclude that A is permutation similar to T_m. Conversely, if A is permutation similar to T_m, then $A \in \Gamma(m,k)$ for $k \ge m-1$ and $f(A) = m(m-1)/2$. This completes the proof. □

We remark that Theorem 1' does not hold for $1 \le n \le 4$. The formula $\gamma(n,k) = n(n-1)/2$ is false for $n = 1, 2, 3$ since $\gamma(1,k) = 1$, $\gamma(2,k) = 2$ for $k \ge 2$ and $\gamma(3,k) = 4$ for $k \ge 3$. The formula $\gamma(n,k) = n(n-1)/2$ is true for $n = 4$ and $k \ge 3$, but this largest number of $1'$s can be attained at matrices other than the matrices permutation similar to T_4, say, at

$$B = \begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \in \Gamma(4,k).$$

3. $\gamma(n, n-2)$ and $\gamma(n, n-3)$

In this section we apply Theorem 1' to determine $\gamma(n,n-2)$ and $\gamma(n,n-3)$.

Corollary 10. *Let $n \ge 6$. Then*

$$\gamma(n, n-2) = \frac{n(n-1)}{2} - 1.$$

Proof. Let $A \in \Gamma(n, n-2)$. Suppose $B_1, \ldots, B_n$ are the n principal submatrices of A of order $n-1$. By Lemma 2, each $B_i \in \Gamma(n-1, n-2)$. By assumption, $n-1 \ge 5$. Applying Theorem 1' to B_i we have

$$f(B_i) \le \frac{(n-1)(n-2)}{2}, \quad i = 1, \ldots, n \tag{4}$$

where equality holds if and only if B_i is permutation similar to T_{n-1}. Suppose A has exactly d diagonal entries equal to 1. Counting the number of $1'$s in $B_i, i = 1, \ldots, n$ and using (4) we obtain

$$(n-2)[f(A)-d]+(n-1)d = \sum_{i=1}^{n} f(B_i) \le n\frac{(n-1)(n-2)}{2}. \tag{5}$$

Hence

$$f(A) \le \frac{n(n-1)}{2}.$$

Suppose $f(A) = n(n-1)/2$. Then the inequality in (5) becomes an equality, which implies that (4) becomes an equality for $i = 1, \ldots, n$. Consequently every B_i is permutation similar to T_{n-1}. By Lemma 9, A is permutation similar to T_n. But $T_n^{n-2} \notin M_n\{0,1\}$, so that $A \notin \Gamma(n, n-2)$, contradiction. Thus

$$f(A) \le \frac{n(n-1)}{2} - 1.$$

On the other hand, denote by $J_{s,t}$ the $s \times t$ matrix with all entries equal to 1 and set

$$A_0 = \begin{pmatrix} 0 & J_{2,n-2} \\ 0 & T_{n-2} \end{pmatrix} \in M_n\{0,1\}.$$

Then $f(A_0) = [n(n-1)/2] - 1$ and

$$A_0^{n-2} = \begin{pmatrix} 0 & J_{2,1} \\ 0 & 0 \end{pmatrix} \in M_n\{0,1\}.$$

This proves $\gamma(n, n-2) = [n(n-1)/2] - 1$. □

Corollary 11. *Let $n \ge 7$. Then*

$$\gamma(n, n-3) = \frac{n(n-1)}{2} - 2.$$

Proof. Let $A \in \Gamma(n, n-3)$. Suppose $B_1, \ldots, B_n$ are the n principal submatrices of A of order $n-1$. By Lemma 2, each $B_i \in \Gamma(n-1, n-3)$. By assumption, $n-1 \ge 6$. Applying Corollary 10 to B_i we have

$$f(B_i) \le \frac{(n-1)(n-2)}{2} - 1, \quad i = 1, \ldots, n. \tag{6}$$

Suppose A has exactly d diagonal entries equal to 1. Counting the number of $1'$s in $B_i, i = 1, \dots, n$ and using (6) we obtain

$$(n-2)[f(A)-d] + (n-1)d = \sum_{i=1}^{n} f(B_i) \le n\left[\frac{(n-1)(n-2)}{2} - 1\right].$$

It follows that

$$f(A) \le \frac{n(n-1)}{2} - \frac{n+d}{n-2} < \frac{n(n-1)}{2} - 1.$$

Since $f(A)$ is an integer, we deduce

$$f(A) \le \frac{n(n-1)}{2} - 2.$$

On the other hand, set

$$A_1 = \begin{pmatrix} 0 & J_{2,n-4} & J_{2,2} \\ 0 & T_{n-4} & J_{n-4,2} \\ 0 & 0 & 0 \end{pmatrix} \in M_n\{0,1\}.$$

We have $f(A_1) = [n(n-1)/2] - 2$ and

$$A_1^{n-3} = \begin{pmatrix} 0 & J_{2,2} \\ 0 & 0 \end{pmatrix} \in M_n\{0,1\}.$$

This proves $\gamma(n, n-3) = [n(n-1)/2] - 2$. □

In view of Corollaries 10 and 11, one might conjecture that for $2 \le k \le n-2$,

$$\gamma(n,k) = \frac{n(n-1)}{2} - (n-k-1). \tag{7}$$

This is not the case. As mentioned in the Introduction section, Wu's result [5] on squares already indicates that (7) is false for $k = 2$. In fact, there are other values of $k > 2$ for which (7) is false. Now we show that at least one of $\gamma(10,4)$ and $\gamma(11,4)$ does not satisfy (7). To the contrary, suppose both $\gamma(10,4)$ and $\gamma(11,4)$ satisfy (7), i.e.,

$$\gamma(10,4) = 40, \quad \gamma(11,4) = 49.$$

Let $A \in \Gamma(11,4)$ and suppose $B_1, \dots, B_{11}$ are the principal submatrices of A of order 10. By Lemma 2, each $B_i \in \Gamma(10,4)$. By assumption $f(B_i) \le 40$, $i = 1, \dots, 11$. Suppose A has exactly d diagonal entries equal to 1. As before we have

$$9[f(A)-d] + 10d = \sum_{i=1}^{11} f(B_i) \le 11 \times 40.$$

Hence

$$f(A) \leq \frac{440}{9} - \frac{d}{9} \leq \frac{440}{9} < 49.$$

So $\gamma(11, 4) < 49$, a contradiction.

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