Extremal digraphs whose walks with the same initial and terminal vertices have distinct lengths

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Abstract Let D be a digraph of order n in which any two walks with the same initial vertex and the same terminal vertex have distinct lengths. We prove that D has at most $(n+1)^2/4$ arcs if n is odd and $n(n+2)/4$ arcs if n is even. The digraphs attaining this maximum size are determined.

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1 Introduction and Main Results

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

For a given positive integer n, let $\Theta(n)$ denote the set of digraphs of order n in which any two walks with the same initial vertex and the same terminal vertex have distinct lengths. Thus, for a digraph D on the vertices $1, 2, \ldots, n$, $D \in \Theta(n)$ if and only if for

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every pair of vertices i, j and for every positive integer k there is at most one walk of length k from i to j. Let $\theta(n)$ denote the maximum size of a digraph in $\Theta(n)$.

We consider the following problem.

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

The motivation for studying Problem 1 is to explore the relation between the size and the walks of a digraph. Intuitively $\theta(n)$ cannot be very large compared with n^2, while the structure of the extremal digraphs attaining $\theta(n)$ seems unclear. Recall that a square upper triangular matrix is called *strict* if its diagonal entries are zero. Throughout we denote by $J_{r,t}$ the $r \times t$ matrix with each entry equal to 1 and abbreviate $J_{t,t}$ as J_t. Our solution to Problem 1 is contained in the following main result.

Theorem 1 *Let n be a positive integer. Then*

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

A digraph $D \in \Theta(n)$ has size $\theta(n)$ if and only if the adjacency matrix of D is permutation similar to

$$\begin{pmatrix} U & E & J_{r,t} \\ 0 & P & J_{s,t} \\ 0 & 0 & 0 \end{pmatrix} \tag{1}$$

or its transpose, where P is a permutation matrix and it does appear, U is a strictly upper triangular matrix, there is exactly one entry 1 in each row of $(U\ E)$, $t = (n-1)/2$ if n is odd and $t = n/2 - 1$ or $n/2$ if n is even.

The corresponding theorem on loopless digraphs follows from Theorem 1 immediately: For $n \geq 2$ the maximum size remains $\theta(n)$ and the extremal digraphs attaining $\theta(n)$ are those whose adjacency matrices are permutation similar to the matrix in (1) or its transpose with the additional condition that P has zero diagonal entries. The four extremal loopless digraphs of order 5 are shown in Figure 1.

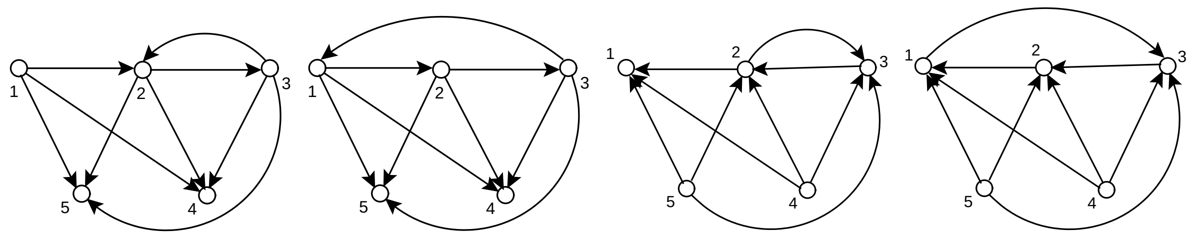

Figure 1: The extremal loopless digraphs of order 5

Denote by $M_{m,n}\{0,1\}$ the set of $m \times n$ 0-1 matrices, and abbreviate $M_{n,n}\{0,1\}$ as $M_n\{0,1\}$. For a given positive integer n, denote

$$\Gamma(n) = \{A \in M_n\{0,1\} | A^k \in M_n\{0,1\} \text{ for every positive integer } k\}$$

and denote by $f(A)$ the number of 1's in a matrix A. Define $\gamma(n) = \max\{f(A)|A \in \Gamma(n)\}$.

It is well known [2, p.72] that for $A \in M_n\{0,1\}$ and a given positive integer k, $A^k \in M_n\{0,1\}$ if and only if for every pair of vertices i, j (not necessarily distinct) there is at most one walk of length k from i to j in the digraph of A. Thus, considering the adjacency matrix of a digraph we see that Problem 1 is equivalent to the following

Problem 2. For a given positive integer n, determine $\gamma(n)$ and determine the matrices in $\Gamma(n)$ that attain $\gamma(n)$.

The solution to Problem 2 is the following equivalent matrix version of Theorem 1:

Theorem 2 *Let n be a positive integer. Then*

$$\gamma(n) = \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases}$$

For a matrix $A \in \Gamma(n)$, $f(A) = \gamma(n)$ if and only if A is permutation similar to

$$\begin{pmatrix} U & E & J_{r,t} \\ 0 & P & J_{s,t} \\ 0 & 0 & 0 \end{pmatrix} \tag{2}$$

or its transpose, where P is a permutation matrix and it does appear, U is a strictly upper triangular matrix, there is exactly one entry 1 in each row of $(U\ E)$, $t = (n-1)/2$ if n is odd and $t = n/2 - 1$ or $n/2$ if n is even.

We will prove Theorem 2 in Section 2. A related problem with a fixed length of walks is studied in [3, 5].

2 Proof of Theorem 2

To prove Theorem 2 we need several lemmas. Denote the digraph of $A \in M_n\{0,1\}$ by $D(A)$. Use the notation $i \xrightarrow[d_{ij}]{W_{ij}} j$ to indicate that the walk W_{ij} from i to j is of length d_{ij}. If there is a walk W_{ij} from i to j of length d_{ij} and a walk W_{jk} from j to k of length d_{jk}, we write $i \xrightarrow[d_{ij}]{W_{ij}} j \xrightarrow[d_{jk}]{W_{jk}} k$, and so on.

Lemma 3 *Let $D \in \Theta(n)$ with $n \geq 2$. Then D is strongly connected if and only if D is a cycle.*

Proof. If D is a cycle, then it is clearly strongly connected. Conversely suppose $D \in \Theta(n)$ is strongly connected. To prove that D is a cycle it suffices to show that the outdegree of each vertex of D is 1. Since D is strongly connected, the outdegree of each vertex is at least 1. To the contrary suppose that the outdegree of some vertex i is at least 2 and $i \to j$, $i \to k$ are two arcs in D.

Case 1. $j = i$ or $k = i$. Without loss of generality we assume $j = i$. Since D is strongly connected, there is a walk W_{ki} of length d_{ki} from k to i. Then there are at least two walks of length $d_{ki} + 1$ from i to i:

$$i \to k \xrightarrow[d_{ki}]{W_{ki}} i \quad \text{and} \quad i \to i \to \cdots \to i,$$

which contradicts the condition $D \in \Theta(n)$.

Case 2. $j \neq i$ and $k \neq i$. There is a path W_{ji} of length d_{ji} from j to i and a path W_{ki} of length d_{ki} from k to i. Let $d = \text{lcm}(d_{ji} + 1, d_{ki} + 1)$, the least common multiple. Then there are at least two walks of length d from i to i :

$$W_1: \quad i \to j \xrightarrow[d_{ji}]{W_{ji}} i \to j \xrightarrow[d_{ji}]{W_{ji}} i \to \cdots \to i \to j \xrightarrow[d_{ji}]{W_{ji}} i$$

$$W_2: \quad i \to k \xrightarrow[d_{ki}]{W_{ki}} i \to k \xrightarrow[d_{ki}]{W_{ki}} i \to \cdots \to i \to k \xrightarrow[d_{ki}]{W_{ki}} i$$

where there are $\frac{d}{d_{ji}+1}$ cycles $i \to j \xrightarrow[d_{ji}]{W_{ji}} i$ in W_1 and $\frac{d}{d_{ki}+1}$ cycles $i \to k \xrightarrow[d_{ki}]{W_{ki}} i$ in W_2, which contradicts the condition $D \in \Theta(n)$. Thus we have proved that the outdegree of each vertex is 1. □

We denote by C_n the basic circulant matrix of order n, i.e., $C_1 = 1$ and for $n \geq 2$

$$C_n = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ 1 & & & 0 \end{pmatrix}.$$

Note that the basic circulant matrices are permutation matrices. Since a matrix $A \in M_n\{0,1\}$ is irreducible if and only if $D(A)$ is strongly connected, we have the following corollary. For brevity we will write PS to mean "permutation similar".

Corollary 4 *Let $A \in \Gamma(n)$ with $n \geq 2$. Then A is irreducible if and only if A is PS to C_n.*

When we say that a matrix is of a certain block form, some blocks may be void, i.e., do not appear unless we emphasize that they appear. For example, the following block form with U, P, V square

$$\begin{pmatrix} U & B & H \\ 0 & P & K \\ 0 & 0 & V \end{pmatrix}$$

includes the two forms

$$\begin{pmatrix} P & K \\ 0 & V \end{pmatrix}, \quad P$$

which correspond respectively to the case when U does not appear and the case when both U and V do not appear. Thus, the precise form in this example depends on whether the diagonal blocks appear (of course, at least one of them does appear).

Lemma 5 *Let $A \in \Gamma(n)$. Then A is PS to a matrix of the form*

$$\begin{pmatrix} U & B & H \\ 0 & P & K \\ 0 & 0 & V \end{pmatrix} \tag{3}$$

where U, V are square strictly upper triangular matrices and P is a permutation matrix if they appear.

Proof. We use induction on the order n. The lemma holds trivially for the case $n = 1$. Now let $n \geq 2$ and assume that the lemma holds for matrices in $\Gamma(n-1)$.

If A is irreducible, then A is a permutation matrix by Corollary 4 and the lemma holds. Next suppose that A is reducible. Then A is PS to

$$G = \begin{pmatrix} A_1 & A_{12} & \cdots & A_{1s} \\ 0 & A_2 & \cdots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_s \end{pmatrix}, \quad (4)$$

where $s \geq 2$ and $A_i \in M_{n_i}\{0,1\}$ is irreducible [2, p.57]. $A \in \Gamma(n)$ implies $G \in \Gamma(n)$. From

$$G^k = \begin{pmatrix} A_1^k & & * \\ & \ddots & \\ 0 & & A_s^k \end{pmatrix}, \quad k = 1, 2, \ldots$$

we deduce $A_i \in \Gamma(n_i)$ for each $1 \leq i \leq s$. We first show that the block matrix G in (4) has the following three properties:

i) For $1 \leq i \leq s$, if A_i's order $n_i \geq 2$, then A_i is PS to C_{n_i}. This follows from Corollary 4.

Denote

$$\begin{aligned} \Omega &= \{t | A_t \neq 0,\ 1 \leq t \leq s\} \\ &= \{t | n_t \geq 2,\ 1 \leq t \leq s\} \cup \{t | n_t = 1,\ A_t = 1,\ 1 \leq t \leq s\}. \end{aligned}$$

ii) For $i \in \Omega$, denote the cycle or loop in $D(G)$ corresponding to $D(A_i)$ by W_i. Then for $i, j \in \Omega$, $i \neq j$, there is no walk connecting W_i and W_j in $D(G)$. In particular, $A_{ij} = 0$ for such pairs i, j.

To the contrary, assume that there is a walk W_{pq} of length k from p to q , where p and q are vertices in W_i and W_j respectively. Note that the lengths of W_i and W_j are n_i and n_j respectively. Let $d = \text{lcm}(n_i, n_j)$. Then we have the following two walks from vertex p to vertex q of the same length $d + k$ in $D(G)$

$$\begin{aligned} W: &\quad p \xrightarrow[n_i]{W_i} p \xrightarrow[n_i]{W_i} p \rightarrow \cdots \rightarrow p \xrightarrow[n_i]{W_i} p \xrightarrow[k]{W_{pq}} q, \\ W': &\quad p \xrightarrow[k]{W_{pq}} q \xrightarrow[n_j]{W_j} q \xrightarrow[n_j]{W_j} q \rightarrow \cdots \rightarrow q \xrightarrow[n_j]{W_j} q, \end{aligned}$$

where there are d/n_i cycles or loops $p \xrightarrow[n_i]{W_i} p$ in W and d/n_j cycles or loops $q \xrightarrow[n_j]{W_j} q$ in W'. This is a contradiction.

iii) If $A_i = 0$, then either $A_{ij} = 0$ for all $j \in \Omega$ or $A_{ji} = 0$ for all $j \in \Omega$.

To the contrary, assume that $A_i = 0$ with $n_i = 1$, $A_{ij} \neq 0$ and $A_{ki} \neq 0$ with $j, k \in \Omega$. Let $G = (g_{uv})$ and suppose that A_i lies in the m-th row of G (and hence in the m-th column). Then A_{ij} has an entry $g_{mp} = 1$ and A_{ki} has an entry $g_{qm} = 1$. Define W_j and W_k as in ii) above. Then W_k and W_j are connected by the walk $q \to m \to p$, which contradicts ii).

If G is nonsingular, then every A_i is nonsingular. From i) and ii) we deduce that G is a permutation matrix and hence it has the form (3) with U, V void.

Next we consider the case that G is singular. We will show that G has either a zero row or a zero column. Suppose G has no zero column. Since G is singular, at least one block matrix A_i on the diagonal of G is a zero matrix (of order 1 by i)). Let A_{i_1} be the first zero matrix among $A_1, A_2, \ldots, A_s$. Then $i_1 \geq 2$ and $1, \ldots, i_1 - 1 \in \Omega$, since $A_1 = 0$ contradicts the assumption that G has no zero column. Since G is block upper triangular and the i_1-th block column is not a zero column, there exists some $1 \leq t_0 \leq i_1 - 1$ such that $A_{t_0, i_1} \neq 0$. By iii) we get $A_{i_1, j} = 0$ for all $j \in \Omega$. If the i_1-th block row of G is not a zero row, there exists some $i_2 > i_1$ such that $A_{i_1, i_2} \neq 0$. Hence $i_2 \notin \Omega$, i.e., $A_{i_2} = 0$. We deduce that $A_{i_2, j} = 0$ for all $j \in \Omega$, since otherwise for some $t \in \Omega$ with $t > i_2$, there would be a walk connecting W_{t_0} and W_t in $D(G)$, which contradicts ii). Now if the i_2-th block row of G is not a zero row, then there exists some $i_3 > i_2$ such that $A_{i_2, i_3} = 1$ and $A_{i_3} = 0$. Continuing in this way we will finally find a zero row, since the order n is finite.

If G has a zero row, then G and hence A is PS to a matrix of the form

$$\begin{pmatrix} Y & * \\ 0 & 0 \end{pmatrix}$$

where Y is of order $n - 1$. $A \in \Gamma(n)$ implies $Y \in \Gamma(n - 1)$. Applying the induction hypothesis to Y shows that A is PS to a matrix of the form (3). If G has a zero column, then G and hence A is PS to a matrix of the form

$$\begin{pmatrix} 0 & * \\ 0 & Z \end{pmatrix}$$

where Z is of order $n - 1$. $A \in \Gamma(n)$ implies $Z \in \Gamma(n - 1)$. Applying the induction hypothesis to Z shows that A is PS to a matrix of the form (3). This completes the proof.

□

We remark that the properties i) and ii) in the above proof have already been observed in [4, Theorem 4.7].

Since every permutation matrix is PS to a direct sum of basic circulant matrices, the next corollary follows from Lemma 5 immediately.

Corollary 6 *Let $A \in \Gamma(n)$. Then A is symmetric if and only if A is PS to* $\mathrm{diag}(A_1, A_2, \ldots, A_k)$, *where each A_i is* 0, *or* 1, *or* C_2.

Corollary 6 shows that the graph version of Problem 1 is trivial.

Let $T_n\{0,1\}$ be the set of all the $n \times n$ strictly upper triangular 0-1 matrices whose squares are also 0-1 matrices. For a matrix A, denote by $A^k(i,j)$ the (i,j) entry of A^k. Recall that $f(A)$ denotes the number of 1's in a matrix A.

Lemma 7 *Let n be a positive integer. Then*

$$\max\{f(A) | A \in T_n\{0,1\}\} = \begin{cases} \frac{(n-1)(n+3)}{4} & \textit{if } n \textit{ is odd,} \\ \frac{n(n+2)}{4} - 1 & \textit{if } n \textit{ is even.} \end{cases}$$

Proof. i) If n is even, let $n = 2m$. We first prove

$$f(A) \le m^2 + m - 1 \text{ for all } A \in T_{2m}\{0,1\}. \tag{5}$$

Use induction on m. When $m = 1$,

$$A_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

is the only nonzero matrix in $T_2\{0,1\}$ and $f(A_0) = 1 = m^2 + m - 1$. Now let $m \ge 2$ and assume that (5) is true for all positive integers less than m.

Partition $A \in T_{2m}\{0,1\}$ as

$$A = \begin{pmatrix} 0 & a^T & \alpha \\ 0 & B & b \\ 0 & 0 & 0 \end{pmatrix},$$

where $a, b \in M_{2(m-1),1}\{0,1\}$, $\alpha = 0$ or 1. $A \in T_{2m}\{0,1\}$ implies $B \in T_{2(m-1)}\{0,1\}$. Then by the induction hypothesis,

$$f(B) \le (m-1)^2 + (m-1) - 1.$$

In the sequel we will repeatedly use the fact that if x, y are vectors in $\{0,1\}^d$ and their inner product $\langle x, y\rangle \le 1$, then x and y altogether have at most $d+1$ components equal to 1.

Note that $A^2(1, 2m) = a^T b \le 1$, which implies that there are at most $2m-1$ ones in a and b. We have

$$f(a) + f(b) + f(\alpha) \le 2m.$$

Thus

$$f(A) = f(B) + f(a) + f(b) + f(\alpha) \le (m-1)^2 + (m-1) - 1 + 2m = m^2 + m - 1,$$

proving (5).

On the other hand, take

$$A_1 = \begin{pmatrix} U_1 & J_m \\ 0 & 0 \end{pmatrix} \in M_{2m}\{0,1\},$$

where

$$U_1 = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix} \in M_m\{0,1\}.$$

A direct computation shows that $A_1 \in T_{2m}\{0,1\}$ and $f(A_1) = m^2 + m - 1$. Thus we have proved

$$\max\{f(A) | A \in T_n\{0,1\}\} = m^2 + m - 1 = \frac{n(n+2)}{4} - 1$$

when n is even.

ii) If n is odd, let $n = 2m+1$ for some nonnegative integer m. Noting that $T_1\{0,1\} = \{0\}$, a similar induction on m shows that

$$f(A) \le m^2 + 2m, \text{ for all } A \in T_{2m+1}\{0,1\}.$$

On the other hand, take

$$A_2 = \begin{pmatrix} U_2 & J_{m+1,m} \\ 0 & 0 \end{pmatrix} \in M_{2m+1}\{0,1\},$$

where

$$U_2 = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix} \in M_{m+1}\{0,1\}.$$

Then $A_2 \in T_{2m+1}\{0,1\}$ and $f(A_2) = m^2 + 2m$. Thus we have proved

$$\max\{f(A)|A \in T_n\{0,1\}\} = m^2 + 2m = \frac{(n-1)(n+3)}{4}$$

when n is odd. □

Lemma 8 *Let*

$$A = \begin{pmatrix} U & B \\ 0 & P \end{pmatrix} \in M_n\{0,1\} \tag{6}$$

where U is a strictly upper triangular matrix and P is a permutation matrix such that $A^2 \in M_n\{0,1\}$. Then

$$f(A) \leq \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases}$$

If n is odd, equality holds if and only if $U = 0$ and $B = J_{(n-1)/2,(n+1)/2}$. If n is even, equality holds if and only if $U = 0$ and $B = J_{n/2}$ or $B = J_{n/2-1,n/2+1}$.

Proof. Let U be of order r and P be of order s with $r + s = n$.

We first consider the case $r \leq s$. We assert that $f(A) \leq (r+1)s$ and equality holds if and only if $U = 0$ and $B = J_{r,s}$.

Let $A = (a_{ij})$. If $U = 0$, obviously $f(A) \leq (r+1)s$. Suppose $U \neq 0$ and that among the rows of U, the i_0-th row has the largest number t of nonzero entries which are $a_{i_0,j_1} = a_{i_0,j_2} = \cdots = a_{i_0,j_t} = 1$ with $1 \leq j_1 < j_2 < \cdots < j_t \leq r$. i_0 is less than each of $j_1, j_2, \ldots, j_t$, since U is strictly upper triangular. Suppose in P, $a_{i_{r+1},r+1} = \cdots = a_{i_n,n} = 1$ where $i_{r+1}, i_{r+2}, \ldots, i_n$ are a permutation of $r+1, r+2, \ldots, n$.

Since $A^2 \in M_n\{0,1\}$, for $r+1 \leq v \leq n$ we have

$$\begin{aligned} A^2(i_0, v) &= a_{i_0,j_1}a_{j_1,v} + a_{i_0,j_2}a_{j_2,v} + \cdots + a_{i_0,j_t}a_{j_t,v} + a_{i_0,i_v}a_{i_v,v} \\ &= a_{j_1,v} + a_{j_2,v} + \cdots + a_{j_t,v} + a_{i_0,i_v} \leq 1. \end{aligned}$$

Thus, for each v with $r+1 \leq v \leq n$, there are at least t zeros among $a_{j_1,v}, \ldots, a_{j_t,v}, a_{i_0,i_v}$. Note that $i_0, j_1, j_2, \ldots, j_t$ are distinct and $i_{r+1}, \ldots, i_n$ are a permutation of $r+1, \ldots, n$. It follows that B has at least $(n-r)t = st$ zero entries and $f(B) \leq rs - st$. On the other hand, since the last row of U is a zero row, $f(U) \le (r-1)t < st$. Therefore

$$\begin{aligned} f(A) &= f(U) + f(B) + f(P) \\ &< st + (rs - st) + s \\ &= (r+1)s. \end{aligned}$$

The equality case part of the assertion is obvious. Hence

$$\begin{aligned} f(A) &\le (r+1)s \\ &= \frac{(n+1)^2}{4} - \left(s - \frac{n+1}{2}\right)^2 \\ &\le \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

If n is odd, equality holds if and only if $U = 0$ and $B = J_{r,s}$ with $s = (n+1)/2$, i.e., $B = J_{(n-1)/2,(n+1)/2}$. If n is even, equality holds if and only if $U = 0$ and $B = J_{r,s}$ with $s = n/2$ or $s = n/2 + 1$, i.e., $B = J_{n/2}$ or $B = J_{n/2-1,n/2+1}$.

Next we complete the proof by showing that if $r > s$, then

$$f(A) < \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases} \tag{7}$$

First note that if P is PS to a matrix Q, then A is PS to a matrix of the form (6) with U unchanged and P replaced by Q. Since every permutation matrix is PS to a direct sum of basic circulant matrices, without loss of generality we assume that P is a direct sum of m basic circulant matrices. We use induction on the number m to prove (7). If $m = 0$, i.e., P is void, then $A = U \in T_n\{0,1\}$ and by Lemma 7,

$$f(A) \le \begin{cases} \frac{(n-1)(n+3)}{4} < \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} - 1 < \frac{n(n+2)}{4} & \text{if } n \text{ is even,} \end{cases}$$

proving (7). Now suppose $m \ge 1$ and assume that (7) holds for $m-1$. Let the m-th (the last) basic circulant matrix in the direct sum of P be C_k which is of order k. Re-partition A as

$$A = \begin{pmatrix} U_1 & E & H \\ 0 & A_1 & W \\ 0 & 0 & C_k \end{pmatrix},$$

where U_1 is of order k and A_1 is of form (6). Since $r > s$, A_1 is not void, i.e., it does appear. $A^2 \in M_n\{0,1\}$ implies $A_1^2 \in M_{n-2k}\{0,1\}$. Applying the induction hypothesis to A_1 we have

$$f(A_1) < \begin{cases} \frac{(n-2k+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{(n-2k)(n-2k+2)}{4} & \text{if } n \text{ is even.} \end{cases}$$

In order to prove (7), it suffices to show that

$$f(U_1) + f(E) + f(H) + f(W) + f(C_k) \leq k(n-k+1), \tag{8}$$

since then

$$\begin{aligned} f(A) &= f(A_1) + f(U_1) + f(E) + f(H) + f(W) + f(C_k) \\ &< \begin{cases} \frac{(n-2k+1)^2}{4} + k(n-k+1) & \text{if } n \text{ is odd} \\ \frac{(n-2k)(n-2k+2)}{4} + k(n-k+1) & \text{if } n \text{ is even} \end{cases} \\ &= \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

If the order $k = 1$, then $U_1 = 0$. From $A^2(1,n) = EW + HC_1 \leq 1$ we deduce that

$$\begin{aligned} f(U_1) + f(E) + f(H) + f(W) + f(C_1) &= f(E) + f(H) + f(W) + f(C_1) \\ &\leq (n-1) + 1 = n. \end{aligned}$$

Hence (8) holds. Next we suppose $k \geq 2$. Now the diagonal entries of C_k are zero.

For $\alpha, \beta \subseteq \{1, 2, \ldots, n\}$, denote by $A[\alpha|\beta]$ the submatrix of A whose rows are indexed by α and whose columns are indexed by β. For integers $p \leq q$, the notation $p : q$ or $\{p : q\}$ will mean the set of integers in the interval $[p, q]$. Let $A = (a_{ij})$. We distinguish two cases.

Case 1. $a_{k,n-k+1} = 0$. Note that U_1 is strictly upper triangular. Since $A^2 \in M_n\{0,1\}$, for $1 \leq i \leq k$,

$$A^2(i, n-i+1) = a_{i,i+1}a_{i+1,n-i+1} + \cdots + a_{i,n-i+1}a_{n-i+1,n-i+1} + \cdots \leq 1$$

which implies

$$f(A[i|i+1 : n-i+1]) + f(A[i+1 : n-i+1|n-i+1]) \leq n - 2i + 2. \tag{9}$$

On the other hand, since $a_{k,n-k+1} = a_{n-k+1,n-k+1} = 0$ and

$$A^2(k, n-k+1) = a_{k,k+1}a_{k+1,n-k+1} + \cdots + a_{k,n-k+1}a_{n-k+1,n-k+1} + \cdots \leq 1$$

we deduce

$$f(A[k|k+1:n-k+1])+f(A[k+1:n-k+1|n-k+1])\leq n-2k+1. \tag{10}$$

Using the special structure of C_k, (9) and (10) we have

$$\begin{aligned}
&f(U_1)+f(E)+f(H)+f(W)+f(C_k)\\
&=\sum_{i=1}^{k}\{f(A[i|i+1:n-i+1])+f(A[i+1:n-i+1|n-i+1])\}+a_{n,n-k+1}\\
&\leq\sum_{i=1}^{k}(n-2i+2)-1+a_{n,n-k+1}\\
&=\sum_{i=1}^{k}(n-2i+2)=k(n-k+1).
\end{aligned}$$

Case 2. $a_{k,n-k+1}=1$.

$$A^2(1,n-k+1)=a_{1,2}a_{2,n-k+1}+\cdots+a_{1,n}a_{n,n-k+1}\leq 1$$

implies

$$f(A[1|2:n])+f(A[2:n|n-k+1])\leq n. \tag{11}$$

For $2\leq i\leq k-1$, since $a_{n-k+1,n-i+2}=0$,

$$\begin{aligned}
A^2(i,n-i+2) &= a_{i,i+1}a_{i+1,n-i+2}+\cdots+a_{i,n-k}a_{n-k,n-i+2}\\
&\quad +a_{i,n-k+2}a_{n-k+2,n-i+2}+\cdots+a_{i,n-i+2}a_{n-i+2,n-i+2}\leq 1
\end{aligned}$$

implies

$$\begin{aligned}
&f(A[i|\{i+1:n-i+2\}\setminus\{n-k+1\}])+f(A[i+1:n-i+2|n-i+2])\\
&\leq n-2i+2.
\end{aligned} \tag{12}$$

Since $a_{k,n-k+1}=a_{n-k+1,n-k+2}=1$ and

$$\begin{aligned}
A^2(k,n-k+2) &= a_{k,k+1}a_{k+1,n-k+2}+\cdots+a_{k,n-k+1}a_{n-k+1,n-k+2}+a_{k,n-k+2}a_{n-k+2,n-k+2}\\
&\leq 1
\end{aligned}$$

we deduce

$$\begin{aligned}
&f(A[k|\{k+1:n-k+2\}\setminus\{n-k+1\}])+f(A[k+1:n-k+2|n-k+2])\\
&\leq n-2k+2.
\end{aligned} \tag{13}$$

By (11), (12) and (13) we have

$$\begin{aligned}
&f(U_1) + f(E) + f(H) + f(W) + f(C_k) \\
&= f(A[1|2:n]) + f(A[2:n|n-k+1]) \\
&\quad + \sum_{i=2}^{k} \{ f(A[i|\{i+1:n-i+2\} \setminus \{n-k+1\}]) + f(A[i+1:n-i+2|n-i+2]) \} \\
&\le n + \sum_{i=2}^{k} (n-2i+2) \\
&= \sum_{i=1}^{k} (n-2i+2) = k(n-k+1).
\end{aligned}$$

□

Proof of Theorem 2. Let $A \in \Gamma(n)$. By Lemma 5, A is PS to a matrix of the form (3). It suffices to consider the case that A has form (3).

We use induction on the order n. For $n = 1$ and $n = 2$, the theorem is easy to verify. Now let $n \ge 3$ and assume that the theorem holds for matrices of order less than n. Suppose $A \in \Gamma(n)$ is of form (3):

$$A = \begin{pmatrix} U & B & H \\ 0 & P & K \\ 0 & 0 & V \end{pmatrix}$$

where $U \in M_r\{0,1\}$ and $V \in M_t\{0,1\}$ are strictly upper triangular matrices, and $P \in M_s\{0,1\}$ is a permutation matrix.

If $s = 0$, by Lemma 7 we have

$$f(A) < \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases}$$

If $s \ge 1$ and $r = 0$ or $t = 0$, the theorem holds by Lemma 8, where for the case $r = 0$ in applying Lemma 8 we have used the fact that the transpose of

$$\begin{pmatrix} P & K \\ 0 & V \end{pmatrix}$$

is PS to a matrix of the form (6).

Now suppose $s, r, t \geq 1$. Further partition A as

$$A = \begin{pmatrix} 0 & a_1^T & a_2^T & a_3^T & \alpha \\ 0 & U_1 & B_1 & H_1 & b_1 \\ 0 & 0 & P & K_1 & b_2 \\ 0 & 0 & 0 & V_1 & b_3 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & a^T & \alpha \\ 0 & A_1 & b \\ 0 & 0 & 0 \end{pmatrix}$$

where $a, b \in \{0,1\}^{n-2}$. $A \in \Gamma(n)$ implies $A_1 \in \Gamma(n-2)$. By the induction hypothesis, we have

$$f(A_1) \leq \begin{cases} \frac{(n-1)^2}{4} & \text{if } n \text{ is odd} \\ \frac{(n-2)n}{4} & \text{if } n \text{ is even} \end{cases}$$

and equality holds if and only if A_1 is PS to a matrix of the form (2) or its transpose with n there replaced by $n-2$. Since $A^2(1,n) = a^T b \leq 1$, we have

$$f(a) + f(b) + f(\alpha) \leq (n-1) + 1 = n.$$

Thus

$$\begin{aligned} f(A) &= f(A_1) + f(a) + f(b) + f(\alpha) \\ &\leq \begin{cases} \frac{(n-1)^2}{4} + n & \text{if } n \text{ is odd} \\ \frac{(n-2)n}{4} + n & \text{if } n \text{ is even} \end{cases} \\ &= \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd,} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even.} \end{cases} \end{aligned} \tag{14}$$

Suppose equality holds in (14). Then A_1 is PS to a matrix of the form (2) or its transpose, $\alpha = 1$ and $f(a) + f(b) = n-1$. Let $A = (a_{ij})$. $f(a) + f(b) = n-1$ and $a^T b \leq 1$ imply that $a_{1i} + a_{in} \geq 1$ for $2 \leq i \leq n-1$ and there is exactly one i such that $a_{1i} + a_{in} = 2$. Next we show that A is PS to a matrix of the form (2) or its transpose. We need only consider the case when A_1 is PS to a matrix of the form (2), since the case when A_1 is PS to a matrix of the transposed form of (2) can be converted to the former case by permutation similarity transform and taking transpose. Note that if $A_2 = QA_1Q^T$ for a permutation matrix Q, then A is PS to

$$\begin{pmatrix} 0 & (Qa)^T & \alpha \\ 0 & A_2 & Qb \\ 0 & 0 & 0 \end{pmatrix}.$$

Thus, without loss of generality we may suppose

$$A_1 = \begin{pmatrix} U_1 & B_1 & J_{p,q} \\ 0 & P & J_{s,q} \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and } A = \begin{pmatrix} 0 & a_1^T & a_2^T & a_3^T & 1 \\ 0 & U_1 & B_1 & J_{p,q} & b_1 \\ 0 & 0 & P & J_{s,q} & b_2 \\ 0 & 0 & 0 & 0 & b_3 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

where $s \geq 1$ and there is exactly one entry 1 in each row of (U_1, B_1), $q = (n-3)/2$ if n is odd and $q = (n-2)/2 - 1$ or $(n-2)/2$ if n is even. Note that P is of order s. We distinguish three cases.

Case 1. $q = 0$. Since $q = (n-3)/2$ if n is odd and $q = (n-2)/2 - 1$ or $(n-2)/2$ if n is even, we get $n = 3$ or $n = 4$.

If $n = 3$ then $s = 1$ and $p = 0$. $f(A) = 4$ implies $a_2 = b_2 = 1$. Hence

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

which has the form (2).

If $n = 4$, then $s = 2$ or $s = 1$. First consider the case $s = 2$. $f(a_2) + f(b_2) = f(A) - 3 = 3$ implies $a_2 = J_{2,1}$, $f(b_2) = 1$ or $b_2 = J_{2,1}$, $f(a_2) = 1$, which ensures that A has the form (2) or is PS to its transpose. Next consider the case $s = 1$. Then $p = 1$ and

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} & 1 \\ 0 & 0 & 1 & a_{24} \\ 0 & 0 & 1 & a_{34} \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Now $A^2(1,3) = a_{12} + a_{13} \leq 1$ and $a_{12} + a_{13} + a_{24} + a_{34} = 3$ imply that $a_{24} = a_{34} = 1$ and exactly one of a_{12} and a_{13} is 1. Thus A has the form (2).

Case 2. $q \geq 1$ and $p = 0$, i.e.,

$$A = \begin{pmatrix} 0 & a_2^T & a_3^T & 1 \\ 0 & P & J_{s,q} & b_2 \\ 0 & 0 & 0 & b_3 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Since $A^2(2,n) \le 1$, we get $f(b_3) \le 1$.

If $f(b_3) = 1$, then $A^2(i,n) \le 1$ for $2 \le i \le s+1$ imply $b_2 = 0$. Thus we have $a_2 = J_{s,1}$ and $a_3 = J_{q,1}$. But $A^2(1, n-1) \le 1$ implies $s = f(a_2) \le 1$. We get $s = 1$. Consequently, from

$$f(A_1) = 1 + q = n - 2 = \begin{cases} \frac{(n-1)^2}{4}, & \text{if } n \text{ is odd} \\ \frac{(n-2)n}{4}, & \text{if } n \text{ is even} \end{cases}$$

we deduce $n = 4$ and $q = 1$. Hence

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

which is PS to the transpose of the form (2).

If $f(b_3) = 0$, then $a_3 = J_{q,1}$. $A^2(1, n-1) \le 1$ implies $f(a_2) \le 1$. But $a_2 \ne 0$, since there is exactly one i with $2 \le i \le n-1$ such that $A(1,i) + A(i,n) = 2$. Hence $f(a_2) = 1$ and $b_2 = J_{s,1}$. We have

$$A = \begin{pmatrix} 0 & a_2^T & J_{1,q} & 1 \\ 0 & P & J_{s,q} & J_{s,1} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

which has the form (2).

Case 3. $q \ge 1$ and $p \ge 1$. $A^2(2,n) \le 1$ implies $f(b_3) \le 1$ and $A^2(1, n-1) \le 1$ implies $f(a_1) + f(a_2) \le 1$.

If $f(b_3) = 1$, $A^2(i,n) \le 1$ for $p+2 \le i \le p+1+s$ imply $b_2 = 0$ and hence $a_2 = J_{s,1}$. It follows that $f(a_2) = s$. Since $f(a_1) + f(a_2) \le 1$ and $s \ge 1$, we get $s = 1$ and $a_1 = 0$. Hence $b_1 = J_{p,1}$. From $p + s + q + 2 = n$ we get $p + q = n - 3$. $f(a) + f(b) = n - 1$ implies $f(a_3) = n - p - 3 = q$. Hence $a_3 = J_{q,1}$. $A^2(i,n) \le 1$ for $2 \le i \le p+1$, $f(b_3) = 1$ and $b_1 = J_{p,1}$ imply $U_1 = 0$. Consequently $B_1 = J_{p,1}$. Thus

$$A = \begin{pmatrix} 0 & 0 & 1 & J_{1,q} & 1 \\ 0 & 0 & J_{p,1} & J_{p,q} & J_{p,1} \\ 0 & 0 & 1 & J_{1,q} & 0 \\ 0 & 0 & 0 & 0 & b_3 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

which is PS to the transpose of the form (2).

If $f(b_3) = 0$, we have $a_3 = J_{q,1}$. From $f(a_1) + f(a_2) \leq 1$ and

$$\begin{aligned} n &= f(a_1) + f(a_2) + f(a_3) + f(b_1) + f(b_2) + f(b_3) + 1 \\ &\leq f(a_1) + f(a_2) + q + p + s + 1 \\ &= f(a_1) + f(a_2) + n - 1 \end{aligned}$$

we get $f(a_1) + f(a_2) = 1$ and $f(b_1) + f(b_2) = n - q - 2 = p + s$, which implies $b_1 = J_{p,1}$ and $b_2 = J_{s,1}$, since $b_1 \in \{0,1\}^p$ and $b_2 \in \{0,1\}^s$. Thus

$$A = \begin{pmatrix} 0 & a_1^T & a_2^T & J_{1,q} & 1 \\ 0 & U_1 & B_1 & J_{p,q} & J_{p,1} \\ 0 & 0 & P & J_{s,q} & J_{s,1} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

which has form (2).

On the other hand, if a matrix A is PS to a matrix of the form (2) or its transpose, then

$$f(A) = \begin{cases} \frac{(n+1)^2}{4} & \text{if } n \text{ is odd} \\ \frac{n(n+2)}{4} & \text{if } n \text{ is even} \end{cases}$$

and A is in $\Gamma(n)$. To show $A \in \Gamma(n)$, just observe the interesting property of (U, E) that $UX + EY \in M_{r,m}\{0,1\}$ for any $X \in M_{r,m}\{0,1\}$ and any $Y \in M_{s,m}\{0,1\}$. This completes the proof. □

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