Matrices with all diagonal entries lying on the boundary of the numerical range

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Abstract

For an $n \times n$ complex matrix A, we study the value $k(A)$, which is the maximum size of an orthonormal set $\{x_1, \dots, x_k\}$ such that $x_j^* A x_j$ lie on the boundary of $W(A)$ for $j = 1, \dots, k$. We give a complete characterization of matrices A with $k(A) = n$, and determine when such a matrix has reducing subspaces. Furthermore, we characterize companion matrices and nonnegative upper triangular the Toeplitz matrices A with $k(A) = n$.

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1 Introduction

Let M_n be the set of $n \times n$ complex matrices. For $A \in M_n$, the numerical range of A is defined by

$$W(A) = \{x^* A x : x \in \mathbb{C}^n,\ x^* x = 1\}.$$

The numerical range is a useful tool for studying matrices and operators; see [11] and its references. It is known that the $W(A)$ is a compact convex subset of $\mathbb{C}$. There are interesting interplay between the analytic and algebraic properties of a matrix $A \in M_n$ and the geometric properties of its numerical range. In particular, one may deduce useful information the matrix A if the numerical range of a matrix has some special boundary points. For instance, if μ is an eigenvalue of A lying on the boundary, then A is unitarily similar to $[\mu] \oplus A_1$ with $A_1 \in M_{n-1}$. The same conclusion holds if μ is a boundary point of $W(A)$ attaining the operator norm of A or if μ is a sharp point of the numerical range, i.e., there are two different support lines passing through μ . As a result, a matrix $A \in M_n$ is unitary if and only if all the eigenvalues of A have modluls one and lie on the boundary of $W(A)$, equivalently, $W(A)$ lies inside the unit disk and there is a unitary $U \in M_n$ such that $U^* A U$ is a diagonal matrix with all diagonal entries lying on the unit circle. More generally, if $A \in M_n$ has $n-1$ eigenvalues lying on the boundary of $W(A)$ or if the boundary of $W(A)$ is a polygon with at least $n-1$ vertices, then A is normal.

The results mentioned in the last paragraph concern boundary points of $W(A)$ with some special spectral or geometrical properties. Recently, researchers considered the maximum size of an orthonormal set $\{x_1, \dots, x_k\} \subseteq \mathbb{C}^n$ such that $x_j^* A x_j \in \partial W(A)$, the boundary of $W(A)$. Denote this number by $k(A)$, which is referred to as the GW-number of A. Clearly, $k(A)$ is the maximum number of diagonal entries of a matrix of the form U^*AU for a unitary matrix $U \in M_n$ lying in $\partial W(A)$.

The GW-number was first introduced by Gau and Wu [7], who proved that (i) $2 \le k(A) \le n$ for all $A \in M_n$, (ii) $k(B) = 2$ for any 2×2 matrix B, and (iii) $k(C) = \lceil n/2 \rceil$ for all $C \in S_n$, where S_n denotes the set of matrices $X \in M_n$ whose eigenvalues all lie in the open unit disk and for which $\mathrm{rank}(I_n - X^*X) = 1$. Researchers have obtained interesting results on the GW-number for various classes of matrices, including weighted shift matrices, nonnegative matrices, almost normal matrices, tridiagonal Toeplitz matrices, and arrowhead matrices; see [1, 2, 3, 8, 9, 10].

We are interested in the case when $k(A) = n$. For a normal matrix A, if all eigenvalues of A lie on $\partial W(A)$, then $k(A) = n$. On the other extreme, consider the matrix

$$B = \begin{pmatrix} 0 & 1 & \cdots & 1 \\ & 0 & \ddots & \vdots \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in M_n.$$

It is easy to verify that B is unitarily irreducible and that $(B + B^*)/2$ is unitarily similar to $(-\frac{1}{2})I_{n-1} \oplus [(n-1)/2]$, and hence $k(B) = n$.

In this paper, we give a complete characterization of matrices $A \in M_n$ with $k(A) = n$. Moreover, we show that this condition leads to further structural results for special classes of matrices. In Section 2, we present the full characterization of all A with $k(A) = n$. In Section 3, we study when such matrices admit nontrivial reducing subspaces. In Section 4, we characterize companion matrices and nonnegative upper triangular Toeplitz matrices A satisfying $k(A) = n$. These results refine and extend earlier work on matrices with diagonal entries lying on the boundary of the numerical range and provide additional insight into the interaction between numerical range geometry and matrix structure.

2 Characterization of matrices with GW-number equal to n

Suppose $A = (a_{rs})$ with $k = k(A)$ diagonal entries lying on the boundary of $W(A)$. We may apply a permutation similarity, and assume that the first n_1 diagonal entries lie on a support line L_1, the next n_2 diagonal entries lie on the support line L_2, and so on. Then we may assume that $A = (A_{rs})_{1 \le r,s \le \ell+1}$ such that the diagonal entries of A_{jj} lie on a support line L_j for $j = 1, \dots, \ell$. We have the following.

Lemma 2.1. *Suppose $A = (A_{rs})_{1 \le r,s \le \ell+1} \in M_n$ such that $A_{jj} \in M_{n_j}$ for $j = 1, \dots, \ell$ such that the diagonal entries of A_{jj} lie on a support line L_j of $W(A)$ for ℓ distinct support lines of $W(A)$. Then there are ℓ distinct $t_1, \dots, t_\ell \in [0, 2\pi)$ such that $e^{it_j}W(A)$ lies on the left side of $e^{it_j}L_j$, which is parallel to $i\mathbb{R}$, for $j = 1, \dots, \ell$. Moreover, $e^{it_j}A_{jj} = d_jI_{n_j} + iG_{jj}$ for some $d_j \in \mathbb{R}$, $G_{jj} = G_{jj}^*$, and $-e^{it_j}A_{js} = e^{-it_j}A_{sj}^*$ for $1 \le j \le \ell$ and $j \ne s$. Consequently, $A_{js} = 0$ if L_j and L_s are not parallel.*

Proof. Since the diagonal entries of A_{11} lie on a support line L_1, there exists $t_1 \in [0, 2\pi)$ such that $e^{it_1}W(A)$ lies on the left side of $e^{it_1}L_1$. So, $\mathrm{Re}(e^{it_1}A)$ has largest eigenvalue equal d_1. Consequently, $\mathrm{Re}(e^{it_1}A) = d_1 I_{n_1} \oplus D$ for some $D = D^*$ with eigenvalues strictly smaller than d_1. So, $e^{it_1}A_{11} = d_1 I_{n_1} + iG_{11}$ with $G_{11} = G_{11}^*$. Moreover, $-e^{it_1}A_{1s} = e^{-it_1}A_{s1}^*$ for $1 < s \le \ell + 1$. We can apply the same argument to the diagonal blocks $A_{22}, \ldots, A_{\ell\ell}$. Thus, for each $j = 1, \ldots, \ell$, we obtain

$$-e^{it_j}A_{js} = e^{-it_j}A_{sj}^* \quad \text{for } 1 \le j \le \ell \text{ and } j \ne s.$$

Now, suppose L_j and L_s are not parallel. Then, from the equation $-e^{it_j}A_{js} = e^{-it_j}A_{sj}^*$ and $-e^{it_s}A_{sj} = e^{-it_s}A_{js}^*$, we have $-e^{2it_s}A_{js} = A_{sj}^* = -e^{2it_j}A_{js}$. Thus, $A_{js}(e^{2it_s} - e^{2it_j}) = 0$. This implies that either $A_{js} = 0$, or $e^{2it_s} = e^{2it_j}$. If $e^{2it_s} = e^{2it_j}$, then $e^{2i(t_s - t_j)} = 1$, which implies that $t_s - t_j = 0$ or $t_s - t_j = \pi$. This is a contradiction because L_j and L_s are not parallel. Therefore, we have $A_{js} = 0$. □

Corollary 2.2. *Let $A = (a_{rs}) \in M_n$ with a_{11}, a_{22} lying on two non-parallel support lines of $W(A)$. Then the leading 2×2 principal submatrix B of A is a diagonal matrix so that $W(B)$ is a line segment.*

Theorem 2.3. *Let $A \in M_n$. Then $k(A) = n$ if and only if A is unitarily similar to $e^{i\theta_1}A_1 \oplus \cdots \oplus e^{i\theta_k}A_k$ with $A_j \in M_{n_j}$ for $j = 1, \ldots, k$ for distinct $\theta_1, \ldots, \theta_k \in [0, 2\pi)$ such that:*

(a) *$A_j - a_j I_{n_j}$ is skew-Hermitian for some $a_j \in \mathbb{R}$ so that $e^{i\theta_j}W(A_j)$ is a line segment lying on a support line of $W(A)$ parallel to $e^{i\theta_j}(i\mathbb{R})$.*

(b) *$A_j - (a_j I_{r_j} \oplus b_j I_{n_j - r_j})$ is skew-Hermitian with $a_j > b_j$ such that the diagonal entries of $e^{i\theta_j}A_j$ lie on two support lines of $W(A)$ that are parallel to $e^{i\theta_j}(i\mathbb{R})$.*

Proof. Suppose $U^*AU = (a_{ij})$ such that $a_{11}, \ldots, a_{nn} \in \partial W(A)$. We may apply a permutation similarity and assume that $(e^{i\theta_1}I_{n_1} \oplus \cdots \oplus e^{i\theta_k}I_{n_k})U^*AU$ has real diagonal entries. By Lemma 2.1, we see that A has the asserted form.

Conversely, if A is unitarily similar $e^{i\theta_1}A_1 \oplus \cdots \oplus e^{i\theta_k}A_k$ satisfying (a) and (b), then all the diagonal entries of $e^{i\theta_j}A_j$ lie on the boundary of $W(A)$. Thus, $k(A) = n$. □

A matrix $A \in M_n$ has a non-trivial reducing subspace $V \subseteq \mathbb{C}^n$ if $A(V) \subseteq V$ and $A^*(V) \subseteq V$. Evidently, A has a nontrivial reducing subspace if and only if A is unitarily similar to $B \oplus C$, where $B \in M_r, C \in M_{n-r}$ with $1 \le r \le n/2$. We also say that $A \in M_n$ is unitarily reducible. By Theorem 2.3, we have the following.

Corollary 2.4. *Let $A \in M_n$ be unitarily irreducible. Then $k(A) = n$ if and only if there is $t \in [0, 2\pi)$ such that $e^{it}A$ is unitarily similar to $H + iG$ with $H = (aI_k \oplus bI_{n-k})$, $G^* = G$ for some $1 \le k < n$ and two distinct real numbers a and b.*

By Theorem 2.3, we also have the following.

Corollary 2.5. *Let $A \in M_n$ be such that $e^{it}A = (aI_k \oplus bI_{n-k}) + iG$, where $a, b, t \in \mathbb{R}$ with $a \geq b$. and $G^* = G = \begin{pmatrix} G_{11} & G_{12} \\ G_{12}^* & G_{22} \end{pmatrix}$. Then $k(A) = n$. In particular, the diagonal entries of $aI_k + iG_{11}$ lie on the right support line of $e^{it}W(A)$ parallel to $i\mathbb{R}$, and the diagonal entries of $bI_{n-k} + iG_{22}$ lie on the left support line of $e^{it}W(A)$ parallel to $i\mathbb{R}$.*

Note that a matrix in the form of Corollary 2.5 may or may not be unitarily irreducible.

The following result [2, Theorem 6] is also a consequence of Theorem 2.3.

Corollary 2.6. *Let $A \in M_n$ be such that $k(A) = n$. If, in addition, A is unitarily similar to the direct sum $A_1 \oplus \cdots \oplus A_m$, where $A_j \in M_{n_j}$ for $j = 1, \ldots m$, and $n = n_1 + \cdots + n_m$, then $k(A_j) = n_j$ for all $1 \leq j \leq m$.*

3 Reducibility of matrices with GW-number equal to n

In this section, we study the reducibility of matrices $A \in M_n$ with $k(A) = n$ under unitary similarity. By Theorem 2.3, we may assume that A only has one irreducible component of type (b) because a matrix of type (a) is normal and unitarily diagonalizable. So, we focus on matrices A in the form

$$\begin{pmatrix} aI_k & \\ & bI_{n-k} \end{pmatrix} + iG \qquad \text{with} \quad a \neq b, \quad G^* = G = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}, \ G_{11} \in M_k. \tag{3.1}$$

Now, suppose A is in the form (3.1). There are unitary matrices $U \in M_k$ and $V \in M_{n-k}$ such that $U^*G_{11}U = \operatorname{diag}(a_1, \ldots, a_k)$ with $a_1 \geq \cdots \geq a_k$ and $V^*G_{22}V = \operatorname{diag}(b_1, \ldots, b_{n-k})$ with $b_1 \geq \cdots \geq b_{n-k}$. We may replace A by $(U \oplus V)^*A(U \oplus V)$ and assume that

$$G_{11} = \operatorname{diag}(a_1, \ldots, a_k) \ \text{ with } a_1 \geq \cdots \geq a_k, \ G_{22} = \operatorname{diag}(b_1, \ldots, b_{n-k}) \ \text{ with } b_1 \geq \cdots \geq b_{n-k}. \tag{3.2}$$

Of course, by Corollary 2.5, we have $a + ia_1, \ldots, a + ia_k$ lie on a support line of $W(A)$ parallel to $i\mathbb{R}$, and $b + ib_1, \ldots, b + ib_{n-k}$ lie on the other support line of $W(A)$ parallel to $i\mathbb{R}$.

Denote by $\{e_1, \ldots, e_n\}$ the standard basis for $\mathbb{R}^n$. We have the following.

Theorem 3.1. *Suppose $A \in M_n$ has the form (3.1) with G_{11}, G_{22} satisfying (3.2). Let $V_1 = \operatorname{span}\{e_1, \ldots, e_k\}$, $V_2 = \operatorname{span}\{e_{k+1}, \ldots, e_n\}$. Then A is unitarily reducible if and only if any one of the following conditions holds.*

(a) *G has a proper invariant (reducing) subspace spanned by vectors in $V_1 \cup V_2$.*

(b) *There is a unitary matrix $U = U_1 \oplus U_2$ with $U_1 \in M_k$ such that $U_i^*G_{ii}U_i$ is permutationally similar to G_{ii} for $i = 1, 2$ and $U_1^*G_{12}U_2$ has one of the following form:*

$$\text{(b.1)} \ \begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix} \textit{ for some nonzero } R_1, R_2, \qquad \text{(b.2)} \ [R_1 \ 0] \ , \qquad \text{(b.3)} \ \begin{bmatrix} 0 \\ R_2 \end{bmatrix}.$$

In the latter two cases, A has reducing eigenvalues.

(c) *There is a unitary matrix* $U = U_1 \oplus U_2$ *with* $U_1 \in M_k$ *such that* U^*AU *is permutationally similar to a direct summand and* $U_i^* G_{ii} U_i = G_{ii}$ *for* $i = 1, 2$.

Proof. Let $G_{11} = D_1, G_{22} = D_2, G_{12} = R$. Without loss of generality, we may assume that $(a, b) = (1, -1)$.

The equivalence (b) $\Leftrightarrow$ (c) is clear. Suppose $U^*AU = B \oplus C$ with $B \in M_r$. Then we may assume $(B + B^*)/2 = I_p \oplus -I_q$ with $p + q = r$ so that the first p columns of U is in V_1 and the next q columns of U is in V_2. Thus, these columns will be an invariant (reducing) subspace of G. Thus condition (a) holds.

Suppose (a) holds. Let $\tilde{V}_1 \subseteq V_1$ and $\tilde{V}_2 \subseteq V_2$ be such that $\tilde{V}_1 \cup \tilde{V}_2$ be a reducing subspace of A. Suppose U is unitary with the first k_1 columns spanning $\tilde{V}_1$, which together with the next $k - k_1$ columns forming a basis for V_1. Then the next k_2 columns forming a basis for $\tilde{V}_2$. Then U has the form $U_1 \oplus U_2$ such that $U_1^* D_1 U_1 = B_1 \oplus C_1$, $U_2^* D_2 U_2 = B_2 \oplus C_2$, and $U_1^* R U_2$ has one of the three forms according to the 3 cases:

$$(1)\ 1 \le k_1 < k \text{ and } 1 \le k_2 < n - k, \quad (2)\ k_1 = 0, \quad (3)\ k_2 = 0.$$

If $k_1 < k$, we can further replace U_1 by a unitary matrix of the form $U_1(X_1 \oplus X_2) \in M_k$ with $X_1 \in M_{k_1}$ such that $U_1^* D_1 U_1$ is in diagonal form. Similarly, if $k_2 < n - k$, we can further replace U_2 by a unitary matrix of the form $U_2(Y_1 \oplus Y_2) \in M_k$ with $Y_1 \in M_{k_2}$ such that $U_2^* D_2 U_2$ is in diagonal form. With the modified U_1 and U_2, we get condition (b).

If (b) holds, then clearly A is unitarily reducible. □

Corollary 3.2. *Suppose* $A \in M_n$ *has the form* (3.1) *satisfying any of the following conditions.*

(a) *Suppose* G_{11}, G_{22} *satisfy* (3.2) *such that* $a_1, \ldots, a_k$ *and* $b_1, \ldots, b_{n-k}$ *are distinct.*

(b) *Suppose* $n = 2k$ *and* $G_{12} = s_1 E_{11} + \cdots + s_k E_{kk} \in M_k$ *such that* $s_1 > \cdots > s_k \ge 0$.

(c) *Suppose* $n = 2k + 1$ *and* $G_{12} = s_1 E_{11} + \cdots + s_k E_{kk} \in M_k$ *such that* $s_1 > \cdots > s_k > 0$.

Then A *is unitarily reducible if and only if* A *is permutationally similar to a direct sum.*

Proof. (a) We only need to prove the necessary condition. Assume that A is unitarily reducible. By Theorem 3.1, there is a unitary matrix $U = U_1 \oplus U_2 \in M_k \oplus M_{n-k}$ such that U^*AU is permutationally similar to a direct sum, and $U_i^* G_{ii} U_i$ is permutationally similar to G_{ii} for $i = 1, 2$. Since G_{ii} is a diagonal matrix with distinct diagonal elements, so U_i is a permutation matrix for $i = 1, 2$. This proves the desired result.

The proof of (b) and (c) are similar. □

By Theorem 3.1, we see that A will have reducing eigenvalues if (b.2) or (b.3) holds. We have a more explicit description of this situation as shown in the following.

Theorem 3.3. *Suppose $A \in M_n$ has the form* (3.1) *with G_{11}, G_{22} satisfying* (3.2)*, and $G_{12} = R$ has columns $r_1, \ldots, r_{n-k} \in \mathbb{C}^k$ and R^t has columns $s_1, \ldots, s_k \in \mathbb{C}^{n-k}$. Then the following conditions are equivalent.*

(a) *A has a reducing eigenvalue.*

(b) *A has a reducing eigenvalue $a + ia_j$ or $b + ib_j$ for some j.*

(c) *One of the following holds.*

(c.1) *$s_j = 0$ or $r_j = 0$,*

(c.2) *There is $p \geq 1$ such that $a_j = a_{j+p}$ and $\operatorname{rank}[s_j \ldots s_{j+p}] \leq p$,*

(c.3) *There is $p \geq 1$ such that $b_j = b_{j+p}$ and $\operatorname{rank}[r_j \ldots r_{j+p}] \leq p$ for some j.*

In particular, when $p \geq \min\{k, n-k\}$, if $a_j = a_{j+p}$ or $b_j = b_{j+p}$ for some j, then condition (c) *is satisfied, and so are* (a) *and* (b).

Proof. Let $G_{11} = D_1, G_{22} = D_2, G_{12} = R$.

(a) $\Rightarrow$ (b). Assume that A is unitarily similar to $B \oplus [\alpha]$. By Theorem 3.1, there is a unitary matrix $U = U_1 \oplus U_2$ such that U^*AU is permutationally similar to $B \oplus [\alpha]$ and $U_i^* D_i U_i = D_i$ for $i = 1, 2$. Hence, we have that α is a diagonal element of U^*AU and the diagonal elements are either $a + ia_j$ or $b + ib_j$, which leads to the conclusion.

(b) $\Rightarrow$ (c). Let $U_1^* R U_2 = [r_1' \cdots r_{n-k}']$ and $U_2 = [u_{im}] \in M_{n-k}$. We consider two cases: $b_{j-1} > b_j > b_{j+1}$ and there is a $p \geq 1$ such that $b_{j-1} > b_j = b_{j+p} > b_{j+p+1}$. In the first case, we have $r_j' = 0$ and $[u_{1j} \cdots u_{(n-k)j}]^t = e_j$. Then

$$0 = r_j' = U_1^* R U_2 e_j = U_1^* R e_j = U_1^* r_j.$$

Thus, $r_j = 0$ because U_1 is unitary. In the second case, $r_i' = 0$ for some $j \leq i \leq j+p$ and $U_2' \equiv [u_{im}]_{j \leq i, m \leq j+p}$ is unitary. Then

$$[r_j' \cdots r_{j+p}'] = U_1^* R U_2 [e_j \cdots e_{j+p}] = U_1^* [r_j \cdots r_{j+p}] U_2'.$$

We obtain

$$p \geq \operatorname{rank}[r_j' \cdots r_{j+p}'] = \operatorname{rank}[r_j \cdots r_{j+p}].$$

(c) $\Rightarrow$ (a). The cases where $s_j = 0$ or $r_j = 0$ are clear. Assume that $b_j = b_{j+p}$ and $\operatorname{rank}[r_j \cdots r_{j+p}] \leq p$ for some j. Then, there exists a unitary matrix $U_2' \in M_{p+1}$ such that $[r_j \cdots r_{j+p}] U_2' = [0 \; r_{j+1}' \cdots r_{j+p}']$. Let $U = I_k \oplus I_{j-1} \oplus U_2' \oplus I_{n-k-j-p}$. Then

$$U^*AU = \begin{pmatrix} aI_k & 0 \\ 0 & b_{n-k} \end{pmatrix} + i \begin{pmatrix} D_1 & R_1 \\ R_1^* & D_2 \end{pmatrix},$$

where j-th column of R_1 is equal 0. Thus, U^*AU is permutationally similar to $B \oplus [b + ib_j]$. This proves the case, and the other cases are similar.

Finally, assume that $b_j = b_{j+p}$ and $p \geq \min\{k, n-k\}$. In this case, we have $n - k \geq p + 1 > k$, and then

$$\operatorname{rank}[r_j \cdots r_{j+p}] \leq k \leq p.$$

Thus, (c) holds. The case where $a_j = a_{j+p}$ is similar. $\square$

The following was shown in [2, Theorem 8].

Corollary 3.4. *Suppose $A \in M_n$ satisfies the hypothesis of Theorem 3.3 with $k = 1$ and $R = [r_1, \dots, r_{n-1}]$. Then the following conditions are equivalent.*

(a) *A is unitarily reducible.*

(b) *$r_i = 0$ or $b_i = b_{i+1}$ for some i.*

Proof. By Theorem 3.1 (b), A is unitarily reducible if and only if A is unitarily similar to the direct sum of the two matrices.

$$A_1 = \begin{pmatrix} a & 0 \\ 0 & bI_j \end{pmatrix} + i \begin{pmatrix} a_1 & R_1 \\ R_1^* & D_1 \end{pmatrix} \text{ and } A_2 = bI_{n-1-j} + iD_2,$$

where $D_1 \oplus D_2$ is permutationally similar to D. Thus, A_2 is normal. Therefore, condition (a) is equivalent to A having a reducing eigenvalue. On the other hand, (b) is equivalent to Theorem 3.3 (c). This gives us the desired result. $\square$

Next, we give a description for unitarily reducible matrices in M_n with no reducing eigenvalues.

Theorem 3.5. *Suppose A satisfies the hypothesis of Theorem 3.3 with no reducing eigenvalues. The following conditions are equivalent.*

(a) *A has k direct summands.*

(b) *A is unitarily similar to $A_1 \oplus \cdots \oplus A_k$, where A_i is unitarily irreducible in the following form*

$$\begin{pmatrix} a & 0 \\ 0 & bI_{t_i} \end{pmatrix} + i \begin{pmatrix} a_i & R_i \\ R_i^* & D_{2i} \end{pmatrix}$$

for $i = 1, \dots, k$ and $D_{21} \oplus \cdots \oplus D_{2k}$ is permutationally similar to D_2.

(c) *There is a unitary matrix $U_1 \in M_k$ with $U_1^* D_1 U_1 = D_1$ such that if $b_{j+1} < b_j < b_{j-1}$, then*

$$U_1^* r_j = \alpha_j e_i$$

for some $\alpha_j \neq 0$ and $1 \leq i \leq k$; if $b_{j-1} > b_j = b_{j+p} > b_{j+p+1}$, then we have $p < k$ and $U_1^*[r_j \cdots r_{j+p}][r_j \cdots r_{j+p}]^* U_1$ is a diagonal matrix with $p+1$ non-zero elements. In particular, if $\{a_1, \dots, a_k\}$ are distinct, then $U_1 = I_k$.

Proof. We only consider the case $k = 2$. For $k > 2$, the result can be proven by induction.

$(a) \Rightarrow (b)$. By Theorem 3.1 (b).

$(b) \Rightarrow (c)$. By Theorem 3.1 (c), there exists a unitary matrix $U = U_1 \oplus U_2 \in M_n$ such that $U_1^* D_1 U_1$, $U_2^* D_2 U_2$, and

$$U^*AU = \begin{pmatrix} aI_2 & 0 \\ 0 & bI_{n-2} \end{pmatrix} + i \begin{pmatrix} D_1 & U_1^* R U_2 \\ U_2^* R^* U_1 & D_2 \end{pmatrix}$$

is permutationally similar to $A_1 \oplus A_2$ with

$$A_1 = \begin{pmatrix} a & 0 \\ 0 & bI_{t_1} \end{pmatrix} + i \begin{pmatrix} a_1 & R_1 \\ R_1^* & D_{21} \end{pmatrix} \qquad \text{and} \qquad A_2 = \begin{pmatrix} a & 0 \\ 0 & bI_{t_2} \end{pmatrix} + i \begin{pmatrix} a_2 & R_2 \\ R_2^* & D_{22} \end{pmatrix},$$

where D_{21}, D_{22} are diagonal matrices with distinct entries, and R_1, R_2 have all non-zero elements. Otherwise, by Theorem 3.3, A would have a reducing eigenvalue, which leads to a contraction. Hence, $U_1^* R U_2$ is permutationally similar to $\begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}$. Let $U_1^* R U_2 = [r_1' \cdots r_{n-2}']$ and $U_2 = [u_{im}] \in M_{n-2}$. Then for all $1 \leq j \leq n-2$, $r_j' = \alpha_j e_1$ or $\alpha_j e_2$ for some $\alpha_j \neq 0$. Given $1 \leq j \leq n-2$, consider the following two cases. $b_{j+1} < b_j < b_{j-1}$ and $b_{j-1} > b_j = b_{j+p} > b_{j+p+1}$ for some $p \geq 1$. In the first case, by $U_2^* D_2 U_2 = D_2$, we have $[u_{1j} \cdots u_{(n-2)j}]^t = e_j$. Then

$$U_1^* r_j = U_1^* R e_j = r_j' = \alpha_j e_1 \text{ or } \alpha_j e_2.$$

In the second case, by Theorem 3.3, $1 \leq p < \min\{2, n-2\} \leq 2$. Thus, $p = 1$. Next, we claim that $\langle r_j', r_{j+1}' \rangle = 0$. If not, we may assume that $r_j' = \alpha_j e_1$ and $r_{j+1}' = \alpha_{j+1} e_1$. In this case, both b_j and b_{j+1} would appear on the diagonal of D_{21}, but $b_j = b_{j+1}$. By Theorem 3.3, A_1 has a reducing eigenvalue, which leads to a contradiction. Thus, we conclude that $\langle r_j', r_{j+1}' \rangle = 0$. Since $U_2^* D_2 U_2 = D_2$, we have that $U_2' \equiv [u_{im}]_{j \leq i, m \leq j+1}$ is unitary. Hence $[r_j' \; r_{j+1}'] = U_1^* [r_j \; r_{j+1}] U_2'$ and we obtain that

$$U_1^* [r_j \; r_{j+1}][r_j \; r_{j+1}]^* U_1 = [r_j' \; r_{j+1}'][r_j' \; r_{j+1}']^*,$$

which is a diagonal matrix with non-zero diagonal entries. This completes the proof of part (c).

$(c) \Rightarrow (a)$. Assume that $b_j = b_{j+1}$. In this case, $U_1^* [r_j \; r_{j+1}][r_j \; r_{j+1}]^* U_1$ is a diagonal matrix with non-zero diagonal entries. Let $[r_j \; r_{j+1}]^* U_1 = [s_1 \; s_2]$. Then, the matrix $[s_1/\|s_1\| \; s_2/\|s_2\|] \equiv S$ is a 2×2 unitary matrix. Define $F_1 = I_{j-1} \oplus S \oplus I_{n-2-j-1} \in M_{n-2}$. Then we have

$$\begin{pmatrix} U_1^* & 0 \\ 0 & F_1^* \end{pmatrix} A \begin{pmatrix} U_1 & 0 \\ 0 & F_1 \end{pmatrix} = \begin{pmatrix} aI_2 & 0 \\ 0 & bI_{n-2} \end{pmatrix} + i \begin{pmatrix} D_1 & U_1^* R F_1 \\ F_1^* R^* U_1 & D_2 \end{pmatrix},$$

where $U_1^* R F_1 = U_1^* [r_1 \cdots r_{n-2}] F_1$, and the j-th column is $\alpha_j e_1$, while the $j+1$-th column is $\alpha_{j+1} e_2$ for some $\alpha_j, \alpha_{j+1} \neq 0$. Using a similar reasoning, we can find a unitary matrix $F \in M_{n-2}$ such that $F^* D_2 F = D_2$, and $U_1^* R F$ has each column equal to αe_1 or αe_2 for some $\alpha \neq 0$. Let $U = U_1 \oplus F$. Then the matrix U^*AU is permutationally similar to the direct sum of two matrices. $\square$

Corollary 3.6. *Suppose $A \in M_5$ satisfies the hypothesis of Theorem* 3.3 *with* $(k, n-k) = (2, 3)$. *Then A has a reducing eigenvalue if and only if any of the following holds.*

(a) *The matrix R has a row or a column equal to* 0.

(b) $a_1 = a_2$ *and* $\mathrm{rank}(R) = 1$.

(c) $b_i = b_j$ *for some* $i \neq j$ *and* $\mathrm{rank}([r_i\ r_j]) = 1$.

(d) $b_1 = b_2 = b_3$.

Corollary 3.7. *Suppose $A \in M_5$ satisfies the hypothesis of Theorem* 3.3 *with* $(k, n-k) = (2, 3)$ *with no reducing eigenvalues. The following conditions are equivalent.*

(a) *A has* 2 *direct summands.*

(b) *At most two of b_1, b_2, b_3 are equal, and there is a unitary matrix $U_1 \in M_2$ with $U_1^* D_1 U_1 = D_1$ such that if $b_i = b_j$ for some $i \neq j$, then*

$$U_1^*[r_i\ r_j][r_i\ r_j]^* U_1 = \mathrm{diag}(\alpha_i, \alpha_j)$$

for some $\alpha_i, \alpha_{i+1} \neq 0$. Otherwise,

$$U_1^* r_i = \alpha_i e_1 \text{ or } \alpha_i e_2$$

for some $\alpha_i \neq 0$. In particular, if $a_1 \neq a_2$, we have $U = I_2$.

4 Special classes of matrices with GW-number equal to n

We first determine when a companion matrix

$$A = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ a_n & a_{n-1} & \cdots & a_2 & a_1 \end{pmatrix} \in M_n \tag{4.1}$$

will satisfy $k(A) = n$. We always assume that $n \geq 3$ to avoid trivial consideration. We begin with the following.

Theorem 4.1. *Let $n \geq 5$ and $A \in M_n$ be a companion matrix in the form* (4.1). *Then $k(A) = n$ if and only if A is unitary, i.e., $|a_n| = 1$ and $a_1 = \cdots = a_{n-1} = 0$.*

For the proof of Theorem 4.1, we need some basic properties of companion matrices. The first one is a criterion in terms of the eigenvalues for a companion matrix to be unitarily reducible.

Proposition 4.2. [6, Theorem 1.1] *An n-by-n* ($n \geq 2$) *companion matrix A is unitarily reducible if and only if its eigenvalues are of the form:* $a\omega_n^{j_1}, \cdots, a\omega_n^{j_p}, (1/\overline{a})\omega_n^{j_{p+1}}, \cdots, (1/\overline{a})\omega_n^{j_n}$, *where* $a \neq 0$, $\omega_n = e^{2\pi i/n}$, $1 \leq p \leq n-1$, *and* $\{j_1, \cdots, j_p\}$ *and* $\{j_{p+1}, \cdots, j_n\}$ *form a partition of* $\{0, 1, \cdots, n-1\}$. *In this case, A is unitarily similar to a direct sum* $A_1 \oplus A_2$ *with* $\sigma(A_1) = \{a\omega_n^{j_1}, \cdots, a\omega_n^{j_p}\}$ *and* $\sigma(A_2) = \{(1/\overline{a})\omega_n^{j_{p+1}}, \cdots, (1/\overline{a})\omega_n^{j_n}\}$. *In particular, every unitarily reducible companion matrix is invertible.*

The following corollary provides a characterization of companion matrices that are unitary.

Corollary 4.3. [6, Corollary 1.2] *The following conditions are equivalent for an n-by-n companion matrix A of the form* (4.1)*:*

(a) *A is unitary;*

(b) $a_1 = \cdots = a_{n-1} = 0$ *and* $|a_n| = 1$*;*

(c) *the eigenvalues of A are of the form* $a\omega_n^j, j = 0, 1, \cdots, n-1$, *where* $|a| = 1$ *and* $\omega_n = e^{2\pi i/n}$.

For any matrix $B \in M_n$, $\rho(B)$ denotes the spectral radius of B. Let $A \in M_n$ be a unitarily reducible companion matrix, Proposition 4.2 yields that $\rho(A) \geq 1$. Moreover, Corollary 4.3 says that A is unitary if and only if $\rho(A) = 1$. The next result gives a complete characterization of A with $\rho(A) > 1$. Recall that $\mathbb{D}$ denotes the open unit disk,

$$S_n \equiv \{X \in M_n : \sigma(X) \subseteq \mathbb{D} \text{ and } \operatorname{rank}(I_n - X^*X) = 1\},$$

and

$$S_n^{-1} \equiv \{Y \in M_n : \operatorname{rank}(I_n - Y^*Y) = 1 \text{ and } |\lambda| > 1 \text{ for all } \lambda \in \sigma(Y)\}.$$

Note that $Y \in S_n^{-1}$ if and only if Y is invertible and $Y^{-1} \in S_n$.

Proposition 4.4. [4, Corollary 2.3] *Let A be an n-by-n unitarily reducible companion matrix. If A is not unitary, then A is unitarily similar to a direct sum* $B \oplus C$ *with* $B \in S_k$ *and* $C \in S_{n-k}^{-1}$, $1 \leq k \leq n-1$. *In this case, we have* $\sigma(B) = \{a\omega_n^{j_1}, \cdots, a\omega_n^{j_k}\}$ *and* $\sigma(C) = \{(1/\overline{a})\omega_n^{j_{k+1}}, \cdots, (1/\overline{a})\omega_n^{j_n}\}$, *where* $0 < |a| < 1$, $\omega_n = e^{2\pi i/n}$, *and* $\{j_1, \cdots, j_k\}$ *and* $\{j_{k+1}, \cdots, j_n\}$ *form a partition of* $\{0, 1, \cdots, n-1\}$.

The S_n-matrix is completely determined by its eigenvalues.

Proposition 4.5. [5, Corollary 1.3] *An operator is in* S_n *if and only if it has the upper triangular matrix representation* $[t_{ij}]_{i,j=1}^n$, *where* $|t_{ii}| < 1$ *for all i and* $t_{ij} = s_{ij}(1 - |t_{ii}|^2)^{1/2}(1 - |t_{jj}|^2)^{1/2}$ *for* $i < j$ *with*

$$s_{ij} = \begin{cases} \prod_{k=i+1}^{j-1} (-\overline{t}_{kk}) & \text{if } j > i+1, \\ 1 & \text{if } j = i+1. \end{cases}$$

The GW-number of an S_n-matrix can be obtained by the following.

Proposition 4.6. [7, Theorem 4.4] *If A is a matrix of class S_n $(n \geq 3)$, then $k(A) = \lceil n/2 \rceil$, the ceiling of $n/2$.*

The S_n^{-1}-matrix is also completely determined by its eigenvalues.

Proposition 4.7. [4, Theorem 2.4] *An operator is in S_n^{-1} if and only if it has the upper triangular matrix representation $[t_{ij}]_{i,j=1}^n$, where $|t_{ii}| > 1$ for all i and $t_{ij} = s_{ij}(|t_{ii}|^2 - 1)^{1/2}(|t_{jj}|^2 - 1)^{1/2}$ for $i < j$ with*

$$s_{ij} = \begin{cases} \prod_{k=i+1}^{j-1} \bar{t}_{kk} & \text{if } j > i+1, \\ 1 & \text{if } j = i+1. \end{cases}$$

The GW-number of an S_n^{-1}-matrix is unknown, but we can have an upper bound by the following results.

Proposition 4.8. [4, Theorem 2.5] *Let B be an S_n^{-1}-matrix.*

(1) *The maximal eigenvalue of $\mathrm{Re}(e^{i\theta}B)$ is simple for all $\theta \in \mathbb{R}$.*

(2) *$\partial W(B)$ contains no line segment.*

(3) *For any point λ in $\partial W(B)$, the set $\{y \in \mathbb{C}^n : \langle By, y\rangle = \lambda\|y\|^2\}$ is a vector space of dimension one.*

(4) *B is unitarily irreducible.*

(5) *$\partial W(B)$ is a differentiable curve.*

Proposition 4.9. [8, Corollary 3.6] *Let $B \in M_n$ $(n \geq 3)$. If the set $\{y \in \mathbb{C}^n : \langle By, y\rangle = \lambda\|y\|^2\}$ is a vector space of dimension one for all $\lambda \in \partial W(B)$, then $k(B) \leq n - 1$.*

Combine Propositions 4.8 (3) and 4.9, we have the following easy consequence.

Corollary 4.10. *If B is a matrix of class S_n^{-1} $(n \geq 3)$, then $k(B) \leq n-1$.*

Using these, we are able to prove Theorem 4.1.

Proof of Theorem 4.1. If A is unitary, Corollary 4.3 yields $\sigma(A) = \{a, a\omega, \ldots, a\omega^{n-1}\}$, where $|a| = 1$ and $\omega = e^{i2\pi/n}$. In this case, $W(A)$ is a regular n-sided polygon with vertices $\{a, a\omega, \ldots, a\omega^{n-1}\}$. Hence $k(A) = n$.

Conversely, assume that $k(A) = n$. We first show that A is unitarily reducible. Assume the contrary that A is unitarily irreducible. From Corollary 2.4, since $k(A) = n$, after a rotation, we may assume that $\mathrm{Re}\, A$ is unitarily similar to $\alpha I_k \oplus \beta I_{n-k}$, where $\alpha = \max \sigma(\mathrm{Re}\, A)$ and $\beta = \min \sigma(\mathrm{Re}\, A)$. Since $n \geq 5$, it follows that $k \geq 3$ or $n - k \geq 3$. We may assume that $k \geq 3$. Note that the Jordan block

$$J_{n-1} = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in M_{n-1}$$

is the leading principal submatrix of A so that $\operatorname{Re} J_{n-1}$ is the $(n-1)\times(n-1)$ leading principal submatrix of $\operatorname{Re} A$. By interlacing property, $\operatorname{Re} J_{n-1}$ has a multiple eigenvalue α, this contradicts the fact that all eigenvalues of $\operatorname{Re} J_{n-1}$ are simple. Hence A is unitarily reducible.

We next show that A is unitary. On the contrary, suppose that A is not unitary. Then, by Proposition 4.4, A is unitarily similar to $B \oplus C$, where $B \in S_k$ and $C \in S_{n-k}^{-1}$. Since $k(A) = n$, Corollary 2.6 implies that $k(B) = k$ and $k(C) = n-k$. But, if $k \geq 3$, by Proposition 4.6, we have $k(B) = \lceil k/2 \rceil < k = k(B)$, which is a contradiction. Hence we obtain $k \leq 2$. On the other hand, if $n-k \geq 3$, Corollary 4.10 leads to $k(C) \leq n-k-1 < n-k = k(C)$, which is absurd. Therefore, we also have $n-k \leq 2$. These follow that $n = k + (n-k) \leq 2 + 2 = 4$, which contradicts the fact that $n \geq 5$. Hence we conclude that A is unitary. □

The next results concern the cases when $n = 3$ and 4.

Theorem 4.11. *Let $A \in M_3$ be a companion matrix in the form* (4.1). *Then $k(A) = 3$ if and only if there are $\theta, \alpha \in \mathbb{R}$, $d \in \{1, -1\}$ and $z_3 \in \mathbb{C}$ such that*

$$(e^{i3\theta}a_3, e^{i2\theta}a_2, e^{i\theta}a_1) = \left(z_3, -(1+dz_3), \frac{1}{2}(d(1-|z_3|^2) + i\alpha)\right).$$

For the proof of Theorem 4.11, we need a characterization of the GW-numbers of 3-by-3 matrices from [10].

Proposition 4.12. [10, Proposition 2.11] *Let A be a 3-by-3 matrix. Then $k(A) = 2$ if $W(A)$ is either an elliptic disc, except when A has an eigenvalue on $\partial W(A)$, or an oval region. In all other cases, $k(A) = 3$*

We are now ready to prove Theprem 4.11.

Proof of Theorem 4.11. Suppose that $k(A) = 3$. By Proposition 4.12, either the boundary of the numerical range $\partial W(A)$ contains a line segment, or A has an eigenvalue on $\partial W(A)$. This implies there is a $\theta \in \mathbb{R}$ such that $e^{i\theta}A$ is unitarily similar to $(aI_k \oplus bI_{3-k}) + iG$, where $a, b \in \mathbb{R}$ and $G = G^*$. So, $e^{i\theta}A$ is unitarily similar to $(aI_2 \oplus [b]) + iG$, with $a, b \in \mathbb{R}$ and $G = G^*$. Let $D = \operatorname{diag}(1, e^{i\theta}, e^{i2\theta})$. Then $D(e^{i\theta}A)D^* = \hat{A}$, which can be obtained from A by changing its last row to $(z_3, z_2, z_1) = (e^{i3\theta}a_3, e^{i2\theta}a_2, e^{i\theta}a_1)$. Thus, the eigenvalues of $\operatorname{Re}(\hat{A})$ are $\{a, a, b\}$. Note that the leading 2×2 principal submatrix of $\hat{A}$ is $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, whose real part has spectrum $\{\pm 1/2\}$. Therefore, the interlacing property implies $a \in \{1/2, -1/2\}$. Let $d = 2a \in \{1, -1\}$ and

$$C = 2(\operatorname{Re}(\hat{A}) - aI_3) = \begin{pmatrix} -d & 1 & \bar{z}_3 \\ 1 & -d & 1+\bar{z}_2 \\ z_3 & 1+z_2 & -d+z_1+\bar{z}_1 \end{pmatrix}.$$

Since $\sigma(\operatorname{Re}(\hat{A})) = \{a, a, b\}$, the matrix C must have rank one. This condition implies that

$$z_2 = -1 - dz_3 \quad \text{and} \quad z_1 + \bar{z}_1 = d(1 - |z_3|^2).$$

Conversely, the condition on (a_3, a_2, a_1) ensures that $\mathrm{Re}(e^{i\theta}A)$ is unitarily similar to

$$\mathrm{Re}(\hat{A}) = \frac{1}{2}\begin{pmatrix} 0 & 1 & \bar{z}_3 \\ 1 & 0 & -d\bar{z}_3 \\ z_3 & -dz_3 & d(1-|z_3|^2) \end{pmatrix}.$$

A direct computation shows that $\sigma(\mathrm{Re}(\hat{A})) = \{d/2, d/2, -d(|z_3|^2+1)/2\}$. Therefore, by Corollary 2.5, we have $3 = k(\hat{A}) = k(A)$. This completes the proof. $\square$

Theorem 4.13. *Let $A \in M_4$ be a companion matrix in the form* (4.1). *Then $k(A) = 4$ if and only if there are $\theta, \alpha \in \mathbb{R}$ and $z_4 \in \mathbb{C}$ with $|z_4| = 1$ such that*

$$(e^{i4\theta}a_4, e^{i3\theta}a_3, e^{i2\theta}a_2, e^{i\theta}a_1) = (z_4, 0, -z_4 - 1, i\alpha).$$

For the proof of Theorem 4.13, we need one of Lee's results from [8] on the computation of $k(A)$ for unitarily reducible matrix A, that is, A is unitarily similar to a direct sum $A_1 \oplus A_2$. To formulate this result, we denote by n_j the size of the block A_j and introduce $k_1(A_j)$ as the maximum number k for which there are orthonormal vectors $x_1, \ldots, x_k \in \mathbb{C}^{n_j}$ such that $x_l^* A_j x_l \in \partial W(A) \cap \partial W(A_j)$ for all $1 \le l \le k$; $j = 1, 2$.

Proposition 4.14. [8, Theorem 2.4] *Let $A = B \oplus C$, where $B \in M_k$ and $C \in M_m$. If $\partial W(A)$ consists of at most two line segments, then $k(A) = k_1(B) + k_1(C) \le k(B) + k(C)$. In this case, $k(A) = k(B) + k(C)$ if and only if $k_1(B) = k(B)$ and $k_1(C) = k(C)$. In particular, $k(A) = k + m$ if and only if $k_1(B) = k(B) = k$ and $k_1(C) = k(C) = m$.*

We are now ready to prove Theorem 4.13.

Proof of Theorem 4.13. Assume $k(A) = 4$. First, we want to show that there exists a $\theta \in \mathbb{R}$ such that $e^{i\theta}A$ is unitarily similar to a matrix of the form $(bI_k \oplus cI_{4-k}) + iG$, where $b, c \in \mathbb{R}$ and $G = G^*$. Indeed, if A is unitarily irreducible, since $k(A) = 4$, by Theorem 2.3, we are done. Therefore, it suffices to consider the case that A is unitarily reducible. Then Proposition 4.2 implies that one of the following conditions holds for some $a \neq 0$:

(i) $\sigma(A) = \{a, -1/\overline{a}, i/\overline{a}, -i/\overline{a}\}$, (ii) $\sigma(A) = \{a, ia, -1/\overline{a}, -i/\overline{a}\}$, (iii) $\sigma(A) = \{a, -a, i/\overline{a}, -i/\overline{a}\}$.

Note that if $|a| = 1$, then the three conditions are equivalent to each other, in this case, we have $\sigma(A) = \{a, -a, ia, -ia\}$ and $\det(zI_4 - A) = z - a^4$, thus A is unitary by Corollary 4.3, and $\mathrm{Re}(e^{i\pi/4}\overline{a}A)$ is unitarily similar to $((1/\sqrt{2})I_2 \oplus (-1/\sqrt{2})I_2)$ as required. Therefore, in the following, we always assume that $|a| \neq 1$.

If (i) holds, then A is unitarily similar to a direct sum $A_1 \oplus A_2$ with $\sigma(A_1) = \{a\}$ and $\sigma(A_2) = \{-1/\overline{a}, i/\overline{a}, -i/\overline{a}\}$ by Proposition 4.2. Since $k(A) = 4$, we have $k(A_1) = 1$ and $k(A_2) = 3$ by Corollary 2.6. If $|a| < 1$, we have $A_2 \in S_3^{-1}$ by Proposition 4.4. Moreover, Corollary 4.10 ensure that $k(A_2) \le 3 - 1 = 2 < 3$, which is a contradiction. If $|a| > 1$, we have $A_2 \in S_3$ by Proposition 4.4, and thus $k(A_2) = \lceil 3/2 \rceil = 2 < 3$ by Proposition 4.6, which is absurd. Hence if (i) holds, then $k(A) < 4$, which contradicts our assumption that $k(A) = 4$.

If (ii) holds, then A is unitarily similar to a direct sum $A_1 \oplus A_2$ with $\sigma(A_1) = \{a, ia\}$ and $\sigma(A_2) = \{-1/\overline{a}, -i/\overline{a}\}$ by Proposition 4.2. Without loss of generality, we may assume that $a = re^{i\pi/4}$ where $0 < r = |a| < 1$. Then A_1 is in S_2 and A_2 is in S_2^{-1} by Proposition 4.4. Moreover, from Propositions 4.5 and 4.7, we may assume that

$$A_1 = \begin{pmatrix} re^{i\pi/4} & 1-r^2 \\ 0 & re^{3i\pi/4} \end{pmatrix} \in S_2 \quad \text{and} \quad A_2 = \begin{pmatrix} e^{5i\pi/4}/r & (1/r^2)-1 \\ 0 & e^{7i\pi/4}/r \end{pmatrix} \in S_2^{-1}.$$

Note that both $W(A_1)$ and $W(A_2)$ are elliptical disks, and the major axes of $W(A_1)$ and $W(A_2)$ are parallel and their centers lie on the line $i\mathbb{R}$. Since $r < 1$, the length of the major axis of $W(A_1)$ is less than the length of the major axis of $W(A_2)$, therefore, the arc $\partial W(A) \cap \partial W(A_1)$ is lass than a half of the ellipse $\partial W(A_1)$, if follows that $k_1(A_1) \leq 1 < 2 = k(A_1)$. From Proposition 4.14, we have $k(A) < k(A_1) + k(A_2) = 2 + 2 = 4$. Hence if (ii) holds, then $k(A) < 4$, which contradicts our assumption that $k(A) = 4$.

Finally, if (iii) holds, by Propositions 4.2, 4.4, 4.5, and 4.7, A is unitarily similar to a direct sum $A_1 \oplus A_2$, where

$$A_1 = \begin{pmatrix} a & 1-|a|^2 \\ 0 & -a \end{pmatrix} \quad \text{and} \quad A_2 = \begin{pmatrix} i/\overline{a} & (1/|a|^2)-1 \\ 0 & -i/\overline{a} \end{pmatrix}.$$

Without loss of generality, we may assume that $0 < a < 1$. If $W(A_1)$ is contained in the interior of $W(A_2)$, then $\partial W(A) \cap \partial W(A_1) = \emptyset$ and $\partial W(A) \cap \partial W(A_2) = \partial W(A_2)$, it follows that $k(A) = k(A_2) = 2 < 4$, which contradicts our assumption that $k(A) = 4$. Therefore, $W(A_1)$ is not contained in the interior of $W(A_2)$. Moreover, since the two sets $W(A_1)$ and $W(A_2)$ are elliptical disks centered at the origin, and their major axes of are perpendicular, it follows that $W(A_1)$ and $W(A_2)$ are symmetric with respect to the origin. Moreover, because $W(A_1)$ is not contained in the interior of $W(A_2)$, the two numerical ranges must share two parallel supporting lines. This leads to the conclusion we aim to prove.

Next, let $D = \operatorname{diag}(1, e^{i\theta}, e^{2i\theta}, e^{3i\theta})$. Then $\hat{A} = D(e^{i\theta}A)D^*$ is just the matrix obtained from A by changing its last row by $(z_4, z_3, z_2, z_1) = (e^{i4\theta}a_4, e^{i3\theta}a_3, e^{i2\theta}a_2, e^{i\theta}a_1)$, i.e.,

$$\hat{A} = \begin{pmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & 0 & 1 \\ z_4 & z_3 & z_2 & z_1 \end{pmatrix}.$$

Then $\operatorname{Re}\hat{A} = (\hat{A} + \hat{A}^*)/2$ is

$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & \overline{z}_4 \\ 1 & 0 & 1 & \overline{z}_3 \\ 0 & 1 & 0 & 1+\overline{z}_2 \\ z_4 & z_3 & 1+z_2 & z_1+\overline{z}_1 \end{pmatrix},$$

and unitarily similar to $bI_k \oplus cI_{4-k}$. The leading 2×2 principal submatrix has eigenvalues $\pm 1/2$. The leading 3×3 principal submatrix has eigenvalues $\{\pm 1/\sqrt{2}, 0\}$. By interlacing property, $\operatorname{Re}\hat{A}$

has no eigenvalue of algebraic multiplicity 3, and its spectrum must be $\{\pm 1/\sqrt{2}, \pm 1/\sqrt{2}\}$, indicating that $\operatorname{tr}(\operatorname{Re}\hat{A}) = 0$. This implies that $\operatorname{Re} z_1 = 0$, so $z_1 = i\alpha$ for some $\alpha \in \mathbb{R}$. Now, consider the eigenvectors associated with $\pm 1/\sqrt{2}$. It can be verified that

$$\begin{pmatrix} \pm\frac{1}{\sqrt{2}} & \frac{1}{2} & 0 \\ \frac{1}{2} & \pm\frac{1}{\sqrt{2}} & \frac{1}{2} \\ 0 & \frac{1}{2} & \pm\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ \mp\sqrt{2} \\ 1 \end{pmatrix} = 0.$$

Therefore,

$$(\operatorname{Re}\hat{A} \pm 1/\sqrt{2} I_4) \begin{pmatrix} 1 \\ \mp\sqrt{2} \\ 1 \\ 0 \end{pmatrix} = 0.$$

This gives

$$\langle \begin{pmatrix} z_4 \\ z_3 \\ 1+z_2 \end{pmatrix}, \begin{pmatrix} 1 \\ \mp\sqrt{2} \\ 1 \end{pmatrix} \rangle = 0,$$

which implies that the vector $(z_4, z_3, 1+z_2)^t$ is orthogonal to both $(1, \sqrt{2}, 1)^t$ and $(1, -\sqrt{2}, 1)^t$. Hence, $(z_4, z_3, 1+z_2)^t = \mu(1, 0, -1)^t$ for some $\mu \in \mathbb{C}$. This gives $z_2 = -z_4 - 1$, and $z_3 = 0$. To determine $|z_4|$, consider the characteristic polynomial of $\operatorname{Re}\hat{A}$. With the above conditions, the matrix becomes

$$\operatorname{Re}\hat{A} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & \bar{z}_4 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -\bar{z}_4 \\ z_4 & 0 & -z_4 & 0 \end{pmatrix}. \tag{4.2}$$

Direct computation of its characteristic polynomial yields

$$(\frac{1}{\sqrt{2}} - \lambda)^2 (\frac{1}{\sqrt{2}} + \lambda)^2 = \det(\operatorname{Re} A - \lambda I_4) = (\frac{1}{\sqrt{2}} - \lambda)(\frac{1}{\sqrt{2}} + \lambda)(\frac{|z_4|^2}{2} - \lambda^2),$$

which implies $|z_4| = 1$.

Conversely, if $(a_4, \ldots, a_1)$ satisfies the condition. Then $e^{i\theta} A$ is unitarily similar to $\hat{A}$ with $\operatorname{Re}\hat{A}$ in the form (4.2) with $|z_4| = 1$. This matrix has eigenvalues $\{\pm 1/\sqrt{2}, \pm 1/\sqrt{2}\}$, and hence $k(A) = 4$ by Corollary 2.5. $\square$

Next, we turns to nonnegative upper triangular Toeplitz matrices.

Theorem 4.15. *Let $a_1 > 0$, $a_j \geq 0$ for $j = 2, \ldots, n-1$, and*

$$A = \begin{pmatrix} 0 & a_1 & a_2 & \cdots & a_{n-1} \\ & 0 & a_1 & \ddots & \vdots \\ & & \ddots & \ddots & a_2 \\ & & & 0 & a_1 \\ & & & & 0 \end{pmatrix} \in M_n.$$

Then $k(A) = n$ if and only if one of the following statements holds:

(a) *$A+A^t$ is unitarily similar to $[(n-1)a_1]\oplus(-a_1)I_{n-1}$. In this case, $a_j = a_1$ for all $2 \le j \le n-1$.*

(b) *n is even and $(A - A^t)/\alpha$ is an orthogonal matrix, where $\alpha = \sqrt{\sum_{j=1}^{n-1} a_j^2}$.*

Proof. Assume that $k(A) = n$. Since $a_1 \neq 0$, then A is unitarily irreducible, thus $k(A) = n$ yields that $\mathrm{Re}(e^{i\theta_0}A)$ is unitarily similar to $aI_k \oplus bI_{n-k}$ for some $\theta_0 \in [0, \pi)$ and $a, b \in \mathbb{R}$. We want to show that either $\theta_0 = 0$ or $\theta_0 = \pi/2$. Indeed, note that since $\{z \in \mathbb{C} : |z| \le a_1/2\} = W\left(\begin{pmatrix} 0 & a_1 \\ 0 & 0 \end{pmatrix}\right) \subseteq W(A)$, it implies that $W(A)$ is not a line segment, thus $|a| \ge a_1/2 > 0$, $|b| \ge a_1/2 > 0$, $ab < 0$, $k \neq 0$ and $k \neq n$. We may assume that $k \ge n-k$, that is, $k \ge n/2$. Let

$$J_n = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in M_n \quad \text{and} \quad V = \begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix} \in M_n,$$

then $A = \sum_{j=1}^{n-1} a_j J_n^j$ and $V^* J_n^j V = J_n^{*j}$ for all j, thus $V^*AV = A^*$. It follows that

$$V^* \mathrm{Re}(e^{i\theta_0}A)V = \frac{1}{2}V^*(e^{i\theta_0}A + e^{-i\theta_0}A^*)V = \frac{1}{2}(e^{i\theta_0}A^* + e^{-i\theta_0}A) = \mathrm{Re}(e^{-i\theta_0}A). \tag{4.3}$$

Since V is unitary, we deduce that $\mathrm{Re}(e^{-i\theta_0}A)$ is also unitarily similar to $aI_k \oplus bI_{n-k}$. Therefore, we have

$$\dim\ker(aI_n - \mathrm{Re}(e^{i\theta_0}A)) = k = \dim\ker(aI_n - \mathrm{Re}(e^{-i\theta_0}A)).$$

We first consider the case that $k > n/2$, then

$$\begin{aligned} & \dim\big(\ker(aI_n - \mathrm{Re}(e^{i\theta_0}A)) \cap \ker(aI_n - \mathrm{Re}(e^{-i\theta_0}A))\big) \\ \ge\ & \dim\ker(aI_n - \mathrm{Re}(e^{i\theta_0}A)) + \dim\ker(aI_n - \mathrm{Re}(e^{-i\theta_0}A)) - n \\ =\ & 2k - n \ge 1. \end{aligned}$$

Let $u \in \ker(aI_n - \mathrm{Re}(e^{i\theta_0}A)) \cap \ker(aI_n - \mathrm{Re}(e^{-i\theta_0}A))$ be a unit vector and L be the line $x = a$. Then $u^*Au \in (e^{i\theta_0}L) \cap (e^{-i\theta_0}L)$ and thus $\theta_0 \neq \pi/2$ because $a \neq 0$ and $(e^{i\pi/2}L) \cap (e^{-i\pi/2}L) = \emptyset$. Note that both the lines $e^{i\theta_0}L$ and $e^{-i\theta_0}L$ are supporting lines of $W(A)$. If $\theta_0 \neq 0$, since $\theta_0 \neq \pi/2$, then these two lines $e^{i\theta_0}L$ and $e^{-i\theta_0}L$ are not parallel, this implies that the point u^*Au is a corner of $W(A)$ and thus u^*Au is a reducing eigenvalue of A, this contradicts the fact that A is unitarily irreducible. Hence we conclude that $\theta_0 = 0$, that is, $\mathrm{Re}\,A$ is unitarily similar to $aI_k \oplus bI_{n-k}$. Note that $\mathrm{Re}\,A$ is a permutationally irreducible nonnegative matrix, its maximal eigenvalue is simple and positive, since $k > n/2$, it forces that $a < 0 < b$ and $n-k = 1$ or $k = n-1$. Moreover, $\mathrm{tr}(\mathrm{Re}\,A) = 0$ yields that $b = -(n-1)a$ and thus $\mathrm{Re}\,A$ is unitarily similar to $aI_{n-1} \oplus [-(n-1)a]$. It following that $\operatorname{Re} A - aI_n$ is a rank one positive semidefinite matrix, in other words, $\operatorname{Re} A - aI_n = yy^*$ for some $y = [y_1\ y_2\ \dots\ y_n]^t \in \mathbb{C}^n$, therefore, we have

$$\begin{pmatrix} -2a & a_1 & a_2 & \cdots & a_{n-1} \\ a_1 & -2a & a_1 & \ddots & \vdots \\ a_2 & a_1 & \ddots & \ddots & a_2 \\ \vdots & \ddots & \ddots & -2a & a_1 \\ a_{n-1} & \cdots & a_2 & a_1 & -2a \end{pmatrix} = 2\operatorname{Re} A - 2aI_n = 2\begin{pmatrix} |y_1|^2 & y_1\overline{y}_2 & \cdots & y_1\overline{y}_n \\ y_2\overline{y}_1 & |y_2|^2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & y_{n-1}\overline{y}_n \\ y_n\overline{y}_1 & \cdots & y_n\overline{y}_{n-1} & |y_n|^2 \end{pmatrix}. \tag{4.4}$$

Compare the entries of the diagonal and the first row, we have $|y_j| = \sqrt{-a}$ for all $1 \le j \le n$, and $a_j = |a_j| = 2|y_1||y_{j+1}| = -2a$ for all $1 \le j \le n-1$. Hence $aI_{n-1} \oplus [-(n-1)a] = (-a_1/2)I_{n-1} \oplus [(n-1)a_1/2]$, that is, $A + A^t = 2\operatorname{Re} A$ is unitarily similar $(-a_1)I_{n-1} \oplus [(n-1)a_1]$ and $a_j = -2a = a_1$ for all $2 \le j \le n-1$, this completes the proof of (a).

We next consider the case $k = n/2$. In this case, n is even and $n - k = n/2 = k$. Since A is nilpotent, that is, $\operatorname{tr} \operatorname{Re}(e^{i\theta_0}A) = 0$, we deduce that $b = -a$ and $\operatorname{Re}(e^{i\theta_0}A)$ is unitarily similar to $aI_k \oplus (-a)I_k$. It follows that $(\operatorname{Re}(e^{i\theta_0}A))^2 = a^2 I_n$, or,

$$4a^2 I_n = (e^{i\theta_0}A + e^{-i\theta_0}A^*)^2 = e^{2i\theta_0}A^2 + e^{-2i\theta_0}A^{*2} + AA^* + A^*A. \tag{4.5}$$

We use $(X)_{ij}$ to denote the (i,j)-entry of a matrix $X \in M_n$. Note that $(A^2)_{13} = a_1^2$, $(A^{*2})_{13} = 0 = (A^*A)_{13}$ and $(AA^*)_{13} = \sum_{j=1}^{n-3} a_j a_{j+2}$. Then (4.5) implies that

$$0 = (4a^2 I_n)_{13} = (e^{2i\theta_0}A^2 + e^{-2i\theta_0}A^{*2} + AA^* + A^*A)_{13} = e^{2i\theta_0}a_1^2 + \sum_{j=1}^{n-3} a_j a_{j+2}.$$

Since $a_1 > 0$ and $a_j \ge 0$ for all $2 \le j \le n-1$, it forces that $e^{2i\theta_0} = -1$ or $\theta_0 = \pi/2$. It follows that $\operatorname{Re}(e^{i\theta_0}A) = \operatorname{Re}(iA) = -\operatorname{Im} A$. Hence, $(A - A^t)$ is a multiple of a unitary matrix. Let $\alpha = \sqrt{\sum_{j=1}^{n-1} a_j^2}$ be the norm of the first row of $A - A^t$, we see that $(A - A^t)/\alpha$ is a real unitary matrix, i.e., an real orthogonal matrix. This completes the proof of (b).

Conversely, assume that (a) holds, that is, $a_j = a_1$ for all $2 \le j \le n-1$, then $A + A^t + a_1 I_n = a_1 uu^*$ where $u = [1\ 1\ \dots\ 1]^t \in \mathbb{C}^n$. Since the all one matrix uu^* is unitarily similar to $[n] \oplus 0_{n-1}$, hence $A + A^t$ is unitarily similar to $[(n-1)a_1] \oplus (-a_1)I_{n-1}$ and $k(A) = n$. On the other hand, if (b) holds, then $(A - A^t)/\alpha$ is a skew-Hermitian orthogonal matrix with trace zero, we deduce that $(A - A^t)/\alpha$ is unitarily similar to $iI_{n/2} \oplus (-i)I_{n/2}$, thus $\operatorname{Im} A = (A - A^t)/(2i)$ is unitarily similar to $(\alpha/2)I_{n/2} \oplus (-\alpha/2)I_{n/2}$ and hence $k(A) = n$. This completes the proof. $\square$

One may wonder whether there are matrices satisfying condition (b) in Theorem 4.15. We have the following.

Theorem 4.16. *Let $n = 2k$ $(k \geq 1)$, $a_1 > 0$, $a_j \geq 0$ for $j = 2, \ldots, n-1$, $\alpha = \sqrt{\sum_{j=1}^{n-1} a_j^2}$ and*

$$A = \begin{pmatrix} 0 & a_1 & a_2 & \cdots & a_{n-1} \\ & 0 & a_1 & \ddots & \vdots \\ & & \ddots & \ddots & a_2 \\ & & & 0 & a_1 \\ & & & & 0 \end{pmatrix} \in M_n.$$

Then $(A - A^t)/\alpha$ is an orthogonal matrix if and only if $a_j = a_{n-j}$ and $a_{2j} = 0$ for all $1 \leq j \leq k-1$, and

$$\sum_{i=1}^{n-j} a_i a_{i+j-1} = \sum_{i=1}^{j-2} a_i a_{j-1-i} \quad \text{for all } 3 \leq j \leq k.$$

In particular, if $a_{2j} = 0$ for all $1 \leq j \leq k-1$ and

$$a_{2j-1} = \frac{1}{\sin\left(\frac{(2j-1)\pi}{n}\right)} \quad \text{for } j = 1, \ldots, k,$$

then $(A - A^t)/\alpha$ is an orthogonal matrix.

Proof. Replace A by A/α, we may assume that $\alpha = 1$ and $A - A^t$ is orthogonal. For each $j = 1, \ldots, n$, let $\mathbf{x}_j$ be the jth column of $A - A^t$, then

$$1 = \|\mathbf{x}_j\|^2 = \sum_{i=1}^{j-1} a_i^2 + \sum_{i=1}^{n-j} a_i^2.$$

It follows that $0 = \|\mathbf{x}_{j+1}\|^2 - \|\mathbf{x}_j\|^2 = a_j^2 - a_{n-j}^2$, thus $a_j = a_{n-j}$ for all $1 \leq j \leq n-1$. Moreover, for $2 \leq j \leq k$, we have

$$0 = \mathbf{x}_j^* \mathbf{x}_1 = \sum_{i=1}^{n-j} a_i a_{i+j-1} - \sum_{i=1}^{j-2} a_i a_{j-1-i},$$

or,

$$\sum_{i=1}^{n-j} a_i a_{i+j-1} = \sum_{i=1}^{j-2} a_i a_{j-1-i}.$$

We now show that $a_{2j} = 0$ for all $1 \leq j \leq k-1$. Indeed, for the matrix $A - A^t$, we apply a permutation similarity moving the rows $1, 3, 5, \ldots, n-1$ to the top and row $2, 4, \ldots, n$ to the bottom, and do the same to the columns, we get a matrix $\begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix}$, where

$$A_1 = \begin{pmatrix} 0 & a_2 & a_4 & \cdots & a_{n-2} \\ -a_2 & 0 & a_2 & \ddots & \vdots \\ -a_4 & -a_2 & \ddots & \ddots & a_4 \\ \vdots & \ddots & \ddots & 0 & a_2 \\ -a_{n-2} & \cdots & -a_4 & -a_2 & 0 \end{pmatrix} \quad \text{and} \quad A_2 = \begin{pmatrix} a_1 & a_3 & a_5 & \cdots & a_{n-1} \\ -a_1 & a_1 & a_3 & \ddots & \vdots \\ -a_3 & -a_1 & \ddots & \ddots & a_5 \\ \vdots & \ddots & \ddots & a_1 & a_3 \\ -a_{n-3} & \cdots & -a_3 & -a_1 & a_1 \end{pmatrix}.$$

Let

$$W = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ -1 & & & 0 \end{pmatrix} \in M_k,$$

since $a_j = a_{n-j}$ for all j, it is easily seen that

$$A_1 = \sum_{j=1}^{k-1} a_{2j} W^j \quad \text{and} \quad A_2 = \sum_{j=0}^{k-1} a_{2j+1} W^j.$$

Let $p(z) = \sum_{j=1}^{k-1} a_{2j} z^j$ and $q(z) = \sum_{j=0}^{k-1} a_{2j+1} z^j$, then $A_1 = p(W)$ and $A_2 = q(W)$, thus $A_1 A_2 = A_2 A_1$. Moreover, since $A - A^t$ is orthogonal, we have

$$\begin{aligned} \begin{pmatrix} I_k & 0 \\ 0 & I_k \end{pmatrix} &= \begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix}^t \begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix} \\ &= \begin{pmatrix} -A_1 & -A_2 \\ A_2^t & -A_1 \end{pmatrix} \begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix} = \begin{pmatrix} -A_1^2 + A_2 A_2^t & -2A_1 A_2 \\ A_2^t A_1 + A_1 A_2^t & -A_1^2 + A_2^t A_2 \end{pmatrix}. \end{aligned}$$

This implies that $A_1 A_2 = 0$ and $I_k = A_2 A_2^t - A_1^2$. Therefore, we obtain $A_1 = A_1 A_2 A_2^t - A_1^3 = -A_1^3$, or, $A_1(A_1^2 + I_k) = 0$. We infer that $\sigma(A_1) \subseteq \{0, i, -i\}$. On the other hand, since W is unitary and $W^k = -I_k$, thus $\sigma(W) = \{e^{(2j-1)\pi i/k} : j = 1, \ldots, k\}$ and there is a unitary matrix $U \in M_k$ such that $D \equiv U^* W U = \operatorname{diag}(e^{\pi i/k}, e^{3\pi i/k}, \ldots, e^{(2k-1)i\pi/k})$. It follows that $U^* A_1 U = p(D)$ and $U^* A_2 U = q(D)$, thus we have

$$\begin{pmatrix} U^* & 0 \\ 0 & U^* \end{pmatrix} \begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix} = \begin{pmatrix} p(D) & q(D) \\ -q(D)^* & p(D) \end{pmatrix},$$

that is, the matrix $A - A^t$ is unitarily similar to the direct sum

$$\sum_{j=1}^{k} \oplus \begin{pmatrix} p(e^{(2j-1)\pi i/k}) & q(e^{(2j-1)\pi i/k}) \\ -\overline{q(e^{(2j-1)\pi i/k})} & p(e^{(2j-1)\pi i/k}) \end{pmatrix}.$$

We now check that $q(e^{\pi i/k}) \neq 0$ and $p(e^{\pi i/k}) = 0$. Indeed, since $a_{n-1} = a_1 > 0$, all a_j's are nonnegative and $\sin(j\pi/k) > 0$ for all $1 \leq j \leq k-1$, thus

$$\operatorname{Im}(q(e^{\pi i/k})) = \sum_{j=0}^{k-1} a_{2j+1} \operatorname{Im}(e^{j\pi i/k}) = \sum_{j=0}^{k-1} a_{2j+1} \sin(\frac{j\pi}{k}) \geq a_{n-1} \sin(\frac{(k-1)\pi}{k}) > 0,$$

or, $q(e^{\pi i/k}) \neq 0$. Since the matrix $\begin{pmatrix} A_1 & A_2 \\ -A_2^t & A_1 \end{pmatrix}$ is orthogonal, then the matrix $\begin{pmatrix} p(e^{\pi i/k}) & q(e^{\pi i/k}) \\ -\overline{q(e^{\pi i/k})} & p(e^{\pi i/k}) \end{pmatrix}$ is unitary, we deduce that

$$0 = \begin{pmatrix} p(e^{\pi i/k}) \\ -\overline{q(e^{\pi i/k})} \end{pmatrix}^* \begin{pmatrix} q(e^{\pi i/k}) \\ p(e^{\pi i/k}) \end{pmatrix} = \overline{p(e^{\pi i/k})} \cdot q(e^{\pi i/k}) - q(e^{\pi i/k}) p(e^{\pi i/k}).$$

Since $q(e^{\pi i/k}) \neq 0$, it forces that $p(e^{\pi i/k}) = \overline{p(e^{\pi i/k})}$, or $p(e^{\pi i/k})$ is a real number. But $p(e^{\pi i/k}) \in \sigma(p(D)) = \sigma(A_1) \subseteq \{0, i, -i\}$, hence $p(e^{\pi i/k}) = 0$. It follows that

$$0 = \operatorname{Im}(p(e^{\pi i/k})) = \sum_{j=1}^{k-1} a_{2j} \operatorname{Im}(e^{j\pi i/k}) = \sum_{j=1}^{k-1} a_{2j} \sin(\frac{j\pi}{k}).$$

Note that all a_j's are nonnegative and $\sin(j\pi/k) > 0$ for all $1 \leq j \leq k-1$, hence we conclude that $a_{2j} = 0$ for all $1 \leq j \leq k-1$, this completes the proof of the necessity.

For the proof of the sufficiency, we need to show that $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is an orthonormal set. Indeed, since $a_j = a_{n-j}$ for all $1 \leq j \leq k-1$, we have $\|\mathbf{x}_{j+1}\|^2 - \|\mathbf{x}_j\|^2 = a_j^2 - a_{n-j}^2 = 0$ for all $1 \leq j \leq n-1$. We infer that

$$\|\mathbf{x}_n\|^2 = \|\mathbf{x}_{n-1}\|^2 = \cdots = \|\mathbf{x}_2\|^2 = \|\mathbf{x}_1\|^2 = \sum_{j=1}^{n-1} a_j^2 = \alpha = 1.$$

Next, for $1 \leq i < j \leq n-1$, we have

$$\mathbf{x}_{i+1}^* \mathbf{x}_{j+1} - \mathbf{x}_i^* \mathbf{x}_j = a_i a_j - a_{n-i} a_{n-j} = 0.$$

It follows that

$$\mathbf{x}_i^* \mathbf{x}_j = \mathbf{x}_{i-1}^* \mathbf{x}_{j-1} = \cdots = \mathbf{x}_1^* \mathbf{x}_{j-i+1} \quad \text{for any } 1 \leq i < j \leq n.$$

We now check that $\mathbf{x}_1^* \mathbf{x}_j = 0$ for all $2 \leq j \leq n$. Indeed, for $j = 2$, since $a_{2l} = 0$ for all $1 \leq l \leq k-1$, it implies that $a_l a_{l+1} = 0$ for all $1 \leq l \leq n-2$, thus we obtain

$$\mathbf{x}_1^* \mathbf{x}_2 = \sum_{l=1}^{n-2} a_l a_{l+1} = 0.$$

For $3 \leq j \leq k$, we have

$$\mathbf{x}_1^* \mathbf{x}_j = \sum_{i=1}^{n-j} a_i a_{i+j-1} - \sum_{i=1}^{j-2} a_i a_{j-1-i} = 0,$$

by assumption. For $j = k+1$, note that $n = 2k$ and $a_{k+i} = a_{n-(k+i)} = a_{k-i}$ for all $1 \leq i \leq k-1$, thus

$$\mathbf{x}_1^* \mathbf{x}_{k+1} = \sum_{i=1}^{k-1} a_i a_{k+i} - \sum_{i=1}^{k-1} a_i a_{k-i} = \sum_{i=1}^{k-1} a_i a_{k-i} - \sum_{i=1}^{k-1} a_i a_{k-i} = 0.$$

For $k+2 \leq j \leq n$, let $l = n-j+2$, then $2 \leq l \leq n-k = k$ and

$$\begin{aligned} \mathbf{x}_1^* \mathbf{x}_j &= \sum_{i=1}^{n-j} a_i a_{i+j-1} - \sum_{i=1}^{j-2} a_i a_{j-1-i} = \sum_{i=1}^{l-2} a_i a_{n-l+i+1} - \sum_{i=1}^{n-l} a_i a_{n-l-i+1} \\ &= \sum_{i=1}^{l-2} a_i a_{l-i-1} - \sum_{i=1}^{n-l} a_i a_{l+i-1} = -\mathbf{x}_1^* \mathbf{x}_l = 0. \end{aligned}$$

This completes the proof of the sufficiency.

Finally, assume that $a_{2j} = 0$ for all $1 \le j \le k-1$ and

$$a_{2j-1} = \frac{1}{\sin\left(\frac{(2j-1)\pi}{n}\right)} \quad \text{for } j = 1, \ldots, k.$$

We show that $(A - A^t)/\alpha$ is an orthogonal matrix. Note that $A - A^t$ is permutationally similar to $\begin{pmatrix} 0 & A_2 \\ -A_2^t & 0 \end{pmatrix}$, since $a_{2j} = 0$ for all $1 \le j \le k-1$. Let $\omega_j = e^{(2j-1)\pi i/n}$ for $j = 1, \ldots, k$. Then

$$i \cdot \sum_{l=1}^{k} \overline{\omega}_j^{2l-1} = i \cdot \overline{\omega}_j \sum_{l=1}^{k} (\overline{\omega}_j^2)^{l-1} = i \cdot \overline{\omega}_j \cdot \frac{1 - (\overline{\omega}_j^2)^k}{1 - \overline{\omega}_j^2} = i \cdot \frac{1-(-1)}{\omega_j - \overline{\omega}_j} = \frac{1}{\sin(\frac{(2j-1)\pi}{n})} = a_{2j-1}$$

and $q(e^{(2j-1)\pi i/k}) = \sum_{l=1}^{k} a_{2l-1} \omega_j^{2(l-1)}$ for $1 \le j \le k$. Let

$$F = \begin{pmatrix} 1 & \omega_1^2 & \omega_1^4 \cdots & \omega_1^{2(k-1)} \\ 1 & \omega_2^2 & \omega_2^4 \cdots & \omega_2^{2(k-1)} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \omega_k^2 & \omega_k^4 \cdots & \omega_k^{2(k-1)} \end{pmatrix} \text{ and } Q = \begin{pmatrix} \overline{\omega}_1 & \overline{\omega}_1^3 & \cdots & \overline{\omega}_1^{2k-1} \\ \overline{\omega}_2 & \overline{\omega_2}^3 & \cdots & \overline{\omega}_2^{2k-1} \\ \vdots & \vdots & & \vdots \\ \overline{\omega}_k & \overline{\omega}_k^3 & \cdots & \overline{\omega}_k^{2k-1} \end{pmatrix}.$$

Then $FF^* = kI_k$ and $(\mathrm{diag}(w_1, \ldots, w_k)F)^* = Q$. We deduce that

$$\begin{pmatrix} q(\omega_1^2) \\ q(\omega_2^2) \\ \vdots \\ q(\omega_k^2) \end{pmatrix} = F(\mathrm{diag}(w_1, \ldots, w_k)F)^* \begin{pmatrix} i \\ i \\ \vdots \\ i \end{pmatrix} = k \begin{pmatrix} i\overline{\omega}_1 \\ i\overline{\omega}_2 \\ \vdots \\ i\overline{\omega}_k \end{pmatrix}. \tag{4.6}$$

This implies that the matrix $A_2 = Uq(D)U^*$ has vector of eigenvalues equal to $k(i\overline{\omega}_1, i\overline{\omega}_2, \ldots, i\overline{\omega}_k)^t$, so that $\frac{1}{k}\begin{pmatrix} 0 & A_2 \\ -A_2^t & 0 \end{pmatrix}$ has eigenvalues $\pm i, \ldots, \pm i$ is unitary. It follows that $(A - A^t)/\alpha$, with $\alpha = k$, is a real unitary matrix, and hence is real orthogonal. □

Corollary 4.17. *Let $a \in \mathbb{C} \setminus \{0\}$ and*

$$J_n(a) = \begin{pmatrix} 0 & a & a^2 & \cdots & a^{n-1} \\ & 0 & a & \ddots & \vdots \\ & & \ddots & \ddots & a^2 \\ & & & 0 & a \\ & & & & 0 \end{pmatrix} \in M_n.$$

Then $k(J_n(a)) = n$ if and only if $|a| = 1$.

Proof. Note that $J_n(a)$ is unitarily similar to $J_n(|a|)$. Assume that $k(J_n(|a|)) = n$. Since $|a|^2 \neq 0$, by Theorem 4.15 and Proposition 4.16, we infer that $\mathrm{Re}\, J_n(|a|)$ is unitarily similar to $[(n-1)|a|/2] \oplus (-|a|/2)I_{n-1}$. Moreover, Theorem 4.15 (a) yields that $|a|^2 = |a|$ or $|a| = 1$ as asserted.

Conversely, if $|a| = 1$, then $|a|^j = 1$ for all $1 \le j \le n-1$. Hence $k(J_n(|a|)) = n$ follows from Theorem 4.15 (a), this completes the proof. □

Remark 4.18. We believe that a matrix satisfies Theorem 4.15 (b) must satisfies $a_{2j} = 0$ for all $1 \leq j \leq k-1$ and

$$a_{2j-1} = \frac{c}{\sin\left(\frac{(2j-1)\pi}{n}\right)} \quad \text{for } j = 1, \ldots, k,$$

for some $c > 0$. It would be nice to prove or disprove this statement.

Note that one can use the proof of Theorem 4.15 to show that an irreducible nonnegative strictly upper triangular matrix A satisfies $k(A) = n$ if and only if there is $c > 0$ such that

(a) cA is the upper triangular matrix with all upper triangular entries equal to 1, or

(b) n is even and $c(A - A^t)$ is a skew symmetric orthogonal matrix, so that there is a real orthogonal matrix $P \in M_n$ such that $c(A-A^t) = P^t \begin{pmatrix} 0 & I_k \\ -I_k & 0 \end{pmatrix} P$ has nonnegative upper triangular entries. The matrix cA will be the upper triangular matrix with entries equal to twice of those in $c(A - A^t)$.

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