

HIGHER RANK NUMERICAL HULLS OF MATRICES

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Abstract. For any $n \times n$ matrix A , we use the joint higher rank numerical range, $\Lambda_k(A, \dots, A^m)$, to define the *higher rank numerical hull* of A . We characterize the higher rank numerical hulls of Hermitian matrices. Also, the higher rank numerical hulls of unitary matrices are studied.

1. Introduction and preliminaries

The higher rank numerical range was introduced by Choi, Kribs and Zyczkowski, in connection to the construction of quantum error correction code in the study of quantum information theory [1]. In quantum computing, information is stored in qubits (quantum bits). Mathematically, the state of a qubit is represented by a 2×2 rank one Hermitian matrix Q satisfying $Q^2 = Q$. A state of N -qubits Q_1, \dots, Q_N is represented by their tensor products in M_n with $n = 2^N$.

Let $M_{n,k}(\mathbb{C})$ be the set of $n \times k$ complex matrices ($M_n(\mathbb{C}) := M_{n,n}(\mathbb{C})$) and let $\mathcal{U}_n(\mathbb{C})$ be the set of $n \times n$ unitary matrices. Motivated by the study of convergence of iterative methods in solving linear systems (e.g., see [8]), researchers studied the *polynomial numerical hull of order m* of a matrix $A \in M_n(\mathbb{C})$, which is defined and denoted by

$$V^m(A) = \{ \xi \in \mathbb{C} : |p(\xi)| \leq \|p(A)\| \text{ for all } p(z) \in \mathcal{P}_m[\mathbb{C}] \},$$

where $\mathcal{P}_m[\mathbb{C}]$ is the set of complex polynomials with degree at most m . The *joint numerical range* of $(A_1, A_2, \dots, A_m) \in M_n(\mathbb{C}) \times \dots \times M_n(\mathbb{C})$ is denoted by

$$W(A_1, A_2, \dots, A_m) = \{ (x^* A_1 x, x^* A_2 x, \dots, x^* A_m x) : x \in \mathbb{C}^n, x^* x = 1 \}.$$

By the result in [5]

$$V^m(A) = \{ \zeta \in \mathbb{C} : (\zeta, \zeta^2, \dots, \zeta^m) \in \text{conv}(W(A, A^2, \dots, A^m)) \},$$

where $\text{conv}(X)$ denotes the convex hull of $X \subseteq \mathbb{C}^m$. Throughout the paper k, m and n are considered as natural numbers and I_k is the $k \times k$ identity matrix.

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Let $k \geq 1$. The *rank- k numerical range* (see [1]) and the *rank- k spectrum* of a matrix $A \in M_n(\mathbb{C})$ are denoted by $\Lambda_k(A)$, and $\sigma_k(A)$ respectively, as follows:

$$\Lambda_k(A) = \{\lambda \in \mathbb{C} : \exists X \in M_{n,k}, X^*AX = \lambda I_k, X^*X = I_k\}, \quad (1)$$

$$\sigma_k(A) = \{\lambda \in \mathbb{C} : \dim(\ker(\lambda I_n - A)) \geq k\}. \quad (2)$$

In the following we state some properties:

- (i) $\sigma_k(A) \subseteq \Lambda_k(A) \subseteq \Lambda_{k-1}(A) \subseteq \cdots \subseteq \Lambda_1(A) = W(A)$, $k \geq 2$.
- (ii) $\Lambda_k(\alpha A + \beta I) = \alpha \Lambda_k(A) + \beta$ for all $\alpha, \beta \in \mathbb{C}$.
- (iii) The higher rank numerical range is convex [9].
- (iv) Rank- k numerical range of every $n \times n$ complex matrix is non-empty if $k < n/3 + 1$. Also, if $k \geq n/3 + 1$, an $n \times n$ complex matrix is given for which the rank- k numerical range is empty [6, Theorems 1, 2].
- (v) Rank- k numerical range of every $n \times n$ normal matrix is a convex polygon determined by the eigenvalues [7, Corollary 2.4].

Let $\mathbf{A} = (A_1, \dots, A_m)$ be an m -tuple of $n \times n$ complex matrices. For $1 \leq k \leq n$, the joint rank- k numerical range of \mathbf{A} is denoted by:

$$\Lambda_k(\mathbf{A}) = \{(\lambda_1, \dots, \lambda_m) : \exists X \in M_{n,k}, X^*A_iX = \lambda_i I_k, 1 \leq i \leq m \text{ and } X^*X = I_k\}. \quad (3)$$

In the next section, we use the joint higher rank numerical range to define the higher rank numerical hulls of matrices. Also, we characterize the higher rank numerical hulls of Hermitian matrices. The higher rank numerical hulls of unitary matrices are studied.

2. Higher rank numerical hull

In this section we are going to introduce the notion of higher rank numerical hull of order m for a matrix $A \in M_n(\mathbb{C})$.

DEFINITION 1. Let $A \in M_n(\mathbb{C})$. The *rank- k numerical hull of order m* , is defined and denoted by

$$X_k^m(A) = \{\lambda \in \mathbb{C} : (\lambda, \lambda^2, \dots, \lambda^m) \in \text{conv}(\Lambda_k(A, A^2, \dots, A^m))\}, \quad (4)$$

where $\Lambda_k(A, A^2, \dots, A^m)$ is the joint rank- k numerical range of (A, A^2, \dots, A^m) .

By Greenbaum's results (see (1)) and the convexity result duo to Woerdeman, it is clear that rank-1 numerical hull of order m is the polynomial numerical hull of order m and the rank- k numerical hull of order 1 is the rank- k numerical range. Now, we state some observations which will be used frequently:

LEMMA 2.1. *Let $A \in M_n(\mathbb{C})$. Then*

- i) $\sigma_k(A) \subseteq X_k^m(A) \subseteq X_{k-1}^m(A) \subseteq X_1^m(A) = V^m(A)$, $k \geq 2$.
- ii) $\sigma_k(A) \subseteq X_k^m(A) \subseteq X_k^{m-1}(A) \subseteq X_k^1(A) = \Lambda_k(A)$, $m \geq 2$.
- iii) $X_k^m(A - \mu I) = X_k^m(A) - \mu$

Let $A \in M_n(\mathbb{C})$. Since $X_k^1(A) = \Lambda_k(A)$ and $X_1^m(A) = V^m(A)$, it is enough to study $X_m^k(A)$ for $k, m \geq 2$.

REMARK 1. Assume that $A \in M_n(\mathbb{C})$, and $\Lambda_k(A, A^2, \dots, A^m)$ is convex. Then

$$X_k^m(A) = \{\lambda \in \mathbb{C} : \exists X \in M_{n,k}, X^*A^iX = \lambda^i I_k, 1 \leq i \leq m \text{ and } X^*X = I_k\}. \quad (5)$$

Let $A \in M_n(\mathbb{C})$ be idempotent and let $m \geq 2$. It is clear that $\Lambda_k(A, A^2, \dots, A^m)$ is convex and hence by (5), $X_k^m(A) \subseteq \{\lambda \in \mathbb{C} : \lambda = \lambda^i, 1 \leq i \leq m\} = \{0, 1\}$.

The following Theorem characterizes the rank- k numerical hull of order m for Hermitian matrices.

THEOREM 2.2. *Let $H \in M_n(\mathbb{C})$ be a Hermitian matrix and let $m \geq 2$. Then $X_k^m(H) = \sigma_k(H)$.*

Proof. Let $\lambda \in X_k^m(H)$. By applying [9] to $A = H + iH^2$, it is clear that $\Lambda_k(H, H^2)$ is convex. Hence $(\lambda, \lambda^2) \in \Lambda_k(H, H^2)$. Then, there exists a unitary matrix U such that $U^*HU = \begin{pmatrix} \lambda I_k & B \\ B^* & D \end{pmatrix}$ and $U^*H^2U = \begin{pmatrix} \lambda^2 I_k & E \\ E^* & F \end{pmatrix}$. Thus, $BB^* = 0$ and hence $B = 0$. Therefore, $\lambda \in \sigma_k(H)$. The converse is trivial. \square

By replacing $k = 1$ in Theorem 2.2, we obtain the following Corollary, (see [5]).

COROLLARY 2.3. *Let H be a Hermitian matrix and let $m \geq 2$. Then $V^m(H) = \sigma(H)$.*

In the following, we study the relationship between $X_k^m(A)$ and two sets $V^m(A)$ and $\Lambda_k(A)$.

PROPOSITION 2.4. *Let $A \in M_n(\mathbb{C})$. Then $X_k^m(A) \subseteq V^m(A) \cap \Lambda_k(A)$. Moreover, $V^m(A) \subseteq X_k^m(I_k \otimes A)$.*

Proof. By Lemma 2.1 (i) and (ii), $X_k^m(A) \subseteq V^m(A) \cap \Lambda_k(A)$. Let $\lambda \in V^m(A)$. Then there exists unit vectors $x_i \in \mathbb{C}^n$, and positive t_i , $i = 1, \dots, l$ such that $\sum_{i=1}^l t_i = 1$ and $\lambda^s = \sum_{i=1}^l t_i x_i^* A^s x_i$, $s = 1, \dots, m$. Define $X_i := I_k \otimes x_i$. Direct computation shows that $\sum_{i=1}^l t_i X_i^* (I_k \otimes A)^s X_i = \lambda^s I_k$, $s = 1, \dots, m$. Hence $(\lambda, \lambda^2, \dots, \lambda^m) \in \text{Conv}(\Lambda_k(I_k \otimes A, I_k \otimes A^2, \dots, I_k \otimes A^m))$. Therefore, $V^m(A) \subseteq X_k^m(I_k \otimes A)$. \square

If A is a scalar matrix, then it is trivial that $X_k^m(A) = V^m(A) \cap \Lambda_k(A)$. But in general $X_k^m(A)$ may or may not be equal to $V^m(A) \cap \Lambda_k(A)$. See the following examples.

EXAMPLE 1. Let $A = \text{diag}(0, 1, -1, i, -i)$. We know that $0 \in V^2(A)$, (see[3]). Also, by [7, Corollary 2.4], $\Lambda_2(A) = \{0\}$. Then $V^2(A) \cap \Lambda_2(A) = \{0\}$. Let $X^* = \begin{pmatrix} 0 & 0.5 & 0.5 & 0.5 & 0.5 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$. Direct computation shows that $0 \in X_2^2(A)$. Thus $X_2^2(A) = V^2(A) \cap \Lambda_2(A)$.

EXAMPLE 2. Let $A = \begin{pmatrix} 2I_2 & J \\ J & 5I_2 \end{pmatrix}$, where $J = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. Since A is Hermitian, by Theorem 2.2, $X_2^2(A) = \sigma_2(A) = \emptyset$. But, it is clear that $2 \in V^2(A) \cap \Lambda_2(A)$. Hence $X_2^2(A) \subsetneq V^2(A) \cap \Lambda_2(A)$.

Now, we characterize $X_k^m(U) \cap \sigma(U)$, for unitary matrices. First, we need the following:

PROPOSITION 2.5. *Let $A \in M_n(\mathbb{C})$ be a normal matrix such that $\sigma(A) = \text{ext}(W(A))$, where $W(A)$ is the numerical range of A and $\text{ext}(S)$ is the set of all extreme points of S . Then $X_k^m(A) \cap \sigma(A) = \sigma_k(A)$.*

Proof. Since $\Lambda_k(A) = X_k^1(A) \supseteq X_k^m(A), m \geq 1$, it is enough to show that $\Lambda_k(A) \cap \sigma(A) = \sigma_k(A)$. Assume $\sigma(A) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$. By [7, Corollary 2.4], we know that

$$\Lambda_k(A) = \bigcap_{1 \leq j_1 < \dots < j_{n-k+1} \leq n} \text{conv}(\{\lambda_{j_1}, \dots, \lambda_{j_{n-k+1}}\}).$$

Let $\lambda \in \sigma(A) \cap \Lambda_k(A)$. Since $\sigma(A) \subseteq \text{ext}(\text{conv}(\{\lambda_1, \dots, \lambda_n\}))$, the algebraic multiplicity of λ is greater than or equal to k . Also, we know that, for normal matrices, the algebraic and geometric multiplicities are the same. Therefore, $\Lambda_k(A) \cap \sigma(A) \subseteq \sigma_k(A)$. The converse is trivial. \square

COROLLARY 2.6. *Let $U \in \mathcal{U}_n(\mathbb{C})$. Then $X_k^m(U) \cap \sigma(U) = \sigma_k(U)$.*

The following example shows that Proposition 2.5 doesn't hold if there exists an eigenvalue which is not an extreme point.

EXAMPLE 3. Let $A = \text{diag}(0, 1, e^{i2\pi/3}, e^{i4\pi/3})$ and let $X^* = \begin{pmatrix} 0 & \sqrt{3}/3 & \sqrt{3}/3 & \sqrt{3}/3 \\ 1 & 0 & 0 & 0 \end{pmatrix}$.

Direct computation shows that $X^*AX = X^*A^2X = 0I_2$, and hence $0 \in \sigma(A) \cap X_2^2(A)$ but $0 \notin \sigma_2(A)$.

Let H be a Hermitian matrix and let $m \geq 2$. By Theorem 2.2, we know that $X_k^m(H) = \sigma_k(H)$. The following Proposition shows that this relation may happen for non Hermitian matrices.

PROPOSITION 2.7. *Suppose $A \in M_n(\mathbb{C})$ is a normal matrix such that $\sigma(A)$ lies in a semi-circle. If $m \geq 2$, then $X_k^m(A) = \sigma_k(A)$.*

Proof. There exists a complex number α such that αA is a unitary matrix. Without loss of generality, we replace αA by A . Let $m \geq 2$. By [4, Theorem 2.8.], $V^m(A) = \sigma(A)$, and by Proposition 2.5, $\Lambda_k(A) \cap \sigma(A) = \sigma_k(A)$. Since $\sigma_k(A) \subseteq X_k^m(A) \subseteq V^m(A) \cap \Lambda_k(A) = \sigma_k(A)$, we obtain that $X_k^m(A) = \sigma_k(A)$. \square

The following definition helps us to study $X_k^m(U)$ for unitary matrices $U \in \mathcal{U}_{2k}(\mathbb{C})$.

DEFINITION 2. Let $A \in M_n(\mathbb{C})$. The rank- (k_1, k_2) numerical range of A , $(k_1 + k_2 = n)$, is defined and denoted by

$$\Lambda_{(k_1, k_2)}(A) = \left\{ (\lambda, \mu) \in \mathbb{C}^2 : \exists U \in \mathcal{U}_n, U^*AU = \begin{pmatrix} \lambda I_{k_1} & * \\ * & \mu I_{k_2} \end{pmatrix} \right\}. \quad (6)$$

Let $U \in \mathcal{U}_n(\mathbb{C})$ be a unitary matrix with distinct eigenvalues. By [2, Theorem 4.7], we know that $\Lambda_{(k_1, k_2)}(U) = \emptyset$, for $k_1 \neq k_2$. Now, we assume $k_1 = k_2$.

THEOREM 2.8. Let $U \in \mathcal{U}_{2k}(\mathbb{C})$ and let $(\lambda, \mu) \in \Lambda_k(U, U^2)$. Thus

- (i) If $\mu = \lambda^2$, then $\lambda \in \sigma_k(U)$.
- (ii) If $\mu \neq \lambda^2$, then $(\lambda, \lambda e^{i\theta}) \in \Lambda_{(k, k)}(U)$, where $0 \leq \theta \leq 2\pi$.

Proof. Assume that $(\lambda, \mu) \in \Lambda_k(U, U^2)$. Thus, there exists a unitary matrix V such that $V^*UV = \begin{pmatrix} \lambda I_k & B \\ C & D \end{pmatrix}$ and $V^*U^2V = \begin{pmatrix} \mu I_k & B' \\ C' & D' \end{pmatrix}$. Since V^*UV is a unitary matrix, we obtain that

$$C^*C = BB^* = (1 - |\lambda|^2)I_k, \quad \bar{\lambda}B + C^*D = 0, \quad \text{and} \quad BC = (\mu - \lambda^2)I_k. \quad (7)$$

It is readily seen that $BC = CB$ and $|BC| = |B||C|$, where $|B| = (B^*B)^{1/2}$.

- (i) Let $\mu = \lambda^2$. By (7), $BC = 0$, and hence $B = C = 0$. Thus, $|\lambda| = 1$ and $\lambda \in \sigma_k(U)$.
- (ii) Let $\mu \neq \lambda^2$. Then $|\lambda| < 1$. By using (7), we obtain that $\bar{\lambda}BC + C^*CD = \bar{\lambda}(\mu - \lambda^2)I_k + (1 - |\lambda|^2)D = 0$. Thus, $D = \frac{\bar{\lambda}(\lambda^2 - \mu)}{1 - |\lambda|^2}I_k$. If $\lambda = 0$, then B and C are unitary matrices and hence $(0, 0) \in \Lambda_{(k, k)}(U)$. If $\lambda \neq 0$, then by using (7), $B = \frac{\mu - \lambda^2}{1 - |\lambda|^2}C^*$. Also, we know that $|\mu - \lambda^2|I_k = |BC| = |B||C| = (\sqrt{1 - |\lambda|^2}I_k)^2$, so, $\frac{|\mu - \lambda^2|}{1 - |\lambda|^2} = 1$. Thus there exists $0 \leq \theta < 2\pi$ such that $D = \lambda e^{i\theta}I_k$ and hence $(\lambda, \lambda e^{i\theta}) \in \Lambda_{(k, k)}(U)$. \square

THEOREM 2.9. Let $U \in \mathcal{U}_{2k}(\mathbb{C})$ be a unitary matrix with distinct eigenvalues and let $m, k \geq 2$. Then $X_k^m(U) = \emptyset$.

Proof. Let $(\lambda, \mu) \in \Lambda_k(U, U^2)$. Since $\sigma_k(U) = \emptyset$, by Theorem 2.8 (i), $|\lambda| \neq 1$ and $\mu \neq \lambda^2$. Also by [2, Theorem 4.7], and our assumption, $\Lambda_k(U) = \{\lambda\}$ is a singleton. By Theorem 2.8 (ii), $\frac{\bar{\lambda}(\lambda^2 - \mu)}{1 - |\lambda|^2} = \lambda$. Assume that $\lambda \neq 0$. Thus $\mu = \frac{\lambda^2(2|\lambda|^2 - 1)}{|\lambda|^2}$, and hence $\Lambda_k(U, U^2) = \left\{ \left(\lambda, \frac{\lambda^2(2|\lambda|^2 - 1)}{|\lambda|^2} \right) \right\}$. Since $|\lambda| \neq 1$, we obtain that $X_k^m(U) = \emptyset$, $m, k \geq 2$. Now, assume that $\lambda = 0$. By the same manner as in the proof of Theorem 2.8, we

obtain that $BC = \mu I_k$ is unitary matrix. Then $|\mu| = 1$ and $\Lambda_k(U, U^2) = \{(0, \mu)\}$ is a singleton. This means that $X_k^m(U) = \emptyset$, $m, k \geq 2$. \square

COROLLARY 2.10. *Let $D_n = \text{diag}(1, w_n, \dots, w_n^{n-1})$, where $w_n = e^{i2\pi/n}$ and let $m, k \geq 2$. Then $X_k^m(D_{2k}) = \emptyset$.*

REMARK 2. By using [2, Theorem 4.7] and [7, Theorem 2.2], we know that $X_k^1(D_{2k}) = \{0\}$.

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