SOME CONVEXITY THEOREMS FOR MATRICES

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Introduction. The *numerical range* of a bounded linear operator A on a complex Hilbert space H is the set $W(A) = \{(Af, f) : \|f\| = 1\}$. Because it is convex and its closure contains the spectrum of A, the numerical range is often a useful tool in operator theory. However, even when H is two-dimensional, the numerical range of an operator can be large relative to its spectrum, so that knowledge of $W(A)$ generally permits only crude information about A. P. R. Halmos **[2]** has suggested a refinement of the notion of numerical range by introducing the k-numerical ranges

$$W_k(A) = \left\{\frac{1}{k}\operatorname{tr}(PA) : P = \text{projection of rank } k\right\}$$

for $k = 1, 2, 3, \ldots$. It is clear that $W_1(A) = W(A)$. C. A. Berger **[2]** has shown that $W_k(A)$ is convex.

In Section 1 of this paper we obtain a few additional results about k-numerical ranges, including a description of $W_k(A)$ for normal matrices A. In Section 2 we introduce another generalized numerical range $\mathscr{W}(A)$, which by definition consists of the diagonals of all matrices that are unitarily equivalent to A. A theorem of Horn [3] shows that $\mathscr{W}(A)$ is convex if A is a Hermitian matrix; this can fail for normal matrices of order $\geqq 3$ **[5, 7]**. By computing the convex hull of $\mathscr{W}(A)$ for normal matrices A, we obtain a generalization of a result of F. John **[4]**. Finally, in Section 3 we exploit the connection between $\mathscr{W}(A)$ and k-numerical ranges to obtain a simple proof of Horn's result.

1. k-numerical ranges. Throughout the paper H is a complex Hilbert space of dimension $n < \infty$, and A is a linear operator on H. We begin by listing some elementary properties of $W_k(A)$.

THEOREM 1.1. *For any operator A on H,*

(i) *$W_k(A)$ is convex and compact.*
(ii) $(n-k)W_{n-k}(A) = \operatorname{tr}(A) - kW_k(A) \qquad (k = 1, 2, \ldots, n-1).$
(iii) *$W_k(U^{-1}AU) = W_k(A)$ if U is unitary.*
(iv) $W_n(A) = (1/n)\operatorname{tr}(A)$, $W_1(A) = W(A)$.
(v) *$W_k(A)$ contains each normalized sum*

$$\frac{1}{k}(\lambda_{i_1} + \lambda_{i_2} + \ldots + \lambda_{i_k})$$

of eigenvalues of A.
(vi) $W_{k+1}(A) \subset W_k(A) \qquad (k = 1, 2, \ldots, n-1).$

Proof. As mentioned in the Introduction, the convexity of $W_k(A)$ was proved by Berger. The rest of (i) follows from the continuity of the trace and the compactness of the set of rank

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k projections. Statements (ii), (iii), and (iv) are clear from the definition. Assertion (v) is an immediate consequence of (iii) and the fact that A is unitarily equivalent to a matrix in triangular form. The inclusion in (vi) will follow from Theorem (1.2) and the fact that if $O \leqq X \leqq I$ and $\operatorname{tr}(X) = k+1$, then

$$\frac{1}{k+1}\operatorname{tr}(XA) = \frac{1}{k}\operatorname{tr}(YA),$$

where

$$Y = \frac{k}{k+1}X.$$

Note that if $k = 1$, then (v) reduces to the familiar fact that the numerical range contains the spectrum.

THEOREM 1.2.

$$W_k(A) = \left\{\frac{1}{k}\operatorname{tr}(XA) : 0 \leqq X \leqq I, \operatorname{tr}(X) = k\right\}.$$

In order to prove Theorem 1.2 we need two lemmas.

LEMMA 1.3. *Let P_k be the set of n-tuples $\langle p_1, p_2, \dots, p_n\rangle$ satisfying $0 \leqq p_i \leqq 1$, $\sum_i p_i = k$. Then P_k is compact and convex, and the set* Ext(P_k) *of extreme points of P_k consists of all vectors with k coordinates equal to* 1 *and the rest equal to* 0.

Proof. If $p = \langle p_1, p_2, \dots, p_n\rangle$ belongs to P_k and if $0 < p_1 < 1$, $0 < p_i < 1$ for some $i \neq 1$, because k is an integer. If $\varepsilon = \min\{p_1, p_i, 1-p_1, 1-p_i\}$, then $p = \frac{1}{2}(p' + p'')$, where

$$p' = \langle p_1 - \varepsilon, p_2, \dots, p_i + \varepsilon, \dots, p_n\rangle,$$

$$p'' = \langle p_1 + \varepsilon, p_2, \dots, p_i - \varepsilon, \dots, p_n\rangle.$$

Since p', p'' belong to P_k, it follows that p is not an extreme point of P_k. The same argument clearly works for the other coordinates of p. Hence if p is an extreme point, then each p_i is either 0 or 1. Thus exactly k coordinates of p equal 1 and the others are 0. Conversely, it is clear that each such vector is an extreme point of P_k.

LEMMA 1.4. *The convex hull of the set of Hermitian projections of rank k consists of those operators X satisfying $O \leqq X \leqq I$,* $\operatorname{tr}(X) = k$.

Proof. Suppose $O \leqq X \leqq I$ and $\operatorname{tr}(X) = k$. By the spectral theorem we can write $X = \sum_{i=1}^{n} \lambda_i E_i$, where the E_i are mutually orthogonal projections of rank 1, and the λ_i are the eigenvalues of X. Then $0 \leqq \lambda_i \leqq 1$ and $\sum_{i=1}^{n} \lambda_i = k$, and Lemma 1.3 implies that X is a convex combination of projections of rank k.

The converse follows from the obvious fact that the set of operators X satisfying $O \leqq X \leqq I$ and $\operatorname{tr}(X) = k$ is convex and contains the projections of rank k.

There is another way of expressing Lemma 1.4 which seems of independent interest. Let $\mathscr{C}_k$ be the positive cone generated by the projections of rank k, i.e., $\mathscr{C}_k$ is the smallest set that contains all such projections and is closed with respect to addition and multiplication by non-negative scalars.

COROLLARY. $\mathscr{C}_k = \{X \geqq 0 : \operatorname{tr}(X) \geqq k \| X \|\}$.

Proof of Theorem 1.2. If $O \leqq X \leqq I$ and $\operatorname{tr}(X) = k$, then by Lemma 1.4 $X = \sum_i a_i F_i$ is a convex combination of projections of rank k. Hence

$$\frac{1}{k}\operatorname{tr}(XA) = \frac{1}{k}\sum_i a_i \operatorname{tr}(F_i A)$$

is a convex combination of the points $(1/k)\operatorname{tr}(F_i A) \in W_k(A)$. Using Berger's result that $W_k(A)$ is convex, we find that $(1/k)\operatorname{tr}(XA) \in W_k(A)$. This proves one of the inclusions asserted in Theorem 1.2. The other is trivial.

THEOREM 1.5. *If A is a normal operator on H, then*

$$\operatorname{Ext} W_k(A) \subset \left\{\frac{1}{k}(\lambda_{i_1} + \lambda_{i_2} + \ldots + \lambda_{i_k})\right\},$$

the set of normalized k-fold sums of eigenvalues of A.

Proof. By the spectral theorem, we can suppose that $A = \sum_{i=1}^{n} \lambda_i E_i$, where the E_i are mutually orthogonal projections of rank 1.

Suppose that $\lambda = (1/k)\operatorname{tr}(PA)$ belongs to $W_k(A)$.
Then

$$\lambda = \frac{1}{k}\operatorname{tr}(P(\sum_i \lambda_i E_i)) = \frac{1}{k}\sum_i \lambda_i \operatorname{tr}(PE_i).$$

Since $\operatorname{tr}(PE_i) = \operatorname{tr}(P^2 E_i) = \operatorname{tr}(PE_i P) \geqq 0$, the n-tuple with coordinates $\operatorname{tr}(PE_i)$ belongs to P_k. By Lemma 1.3 there are numbers a_i, x_{ij} such that

$$0 \leqq a_i \leqq 1, \qquad \sum a_i = 1, \qquad \operatorname{tr}(PE_j) = \sum_i a_i x_{ij},$$

where, for each i, exactly k of the x_{ij} are 1 and the others are 0.

Hence

$$\lambda = \frac{1}{k}\sum_j \lambda_j \operatorname{tr}(PE_j) = \frac{1}{k}\sum_j \lambda_j (\sum_i a_i x_{ij}) = \sum_i a_i \left(\frac{1}{k}\sum_j x_{ij}\lambda_j\right).$$

Now $(1/k)\sum_j x_{ij}\lambda_j$ is, for each i, a normalized k-fold sum of eigenvalues of A. Thus each $\lambda \in W_k(A)$ is a convex combination of normalized k-fold sums of eigenvalues. Since these sums are in $W_k(A)$, the proof is complete.

REMARK. Theorem 1.5 includes the known fact that the extreme points of the numerical range of a normal operator are eigenvalues. This is also true if H is infinite-dimensional [6].

2. Diagonals of matrices. Our interest in k-numerical ranges arose from their connection with an unsolved problem in matrix theory. Given n complex numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, the problem asks for necessary and sufficient conditions on $\mu_1, \mu_2, \ldots, \mu_n$ in order that there exist a normal matrix with eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_n$ and main diagonal $\langle \mu_1, \mu_2, \ldots, \mu_n \rangle$. Equivalently, if A is a given normal matrix, to determine which n-tuples $\langle \mu_1, \mu_2, \ldots \mu_n \rangle$ can serve as the diagonal of some matrix unitarily equivalent to A. Or again, to characterize the *n-dimensional numerical range* $\mathscr{W}(A)$ consisting of n-tuples of the form $\langle (Af_1, f_1), (Af_2, f_2), \ldots, (Af_n, f_n) \rangle$, where the f_i form an orthonormal basis of H. In the case in which A is Hermitian the problem was solved by Horn [3].

THEOREM 2.1. *$\mathscr{W}(A)$ is arcwise connected for any matrix A.*

Proof. If $e_1, e_2, \ldots, e_n$ is a fixed orthonormal basis of H, then any point in $\mathscr{W}(A)$ has the form

$$\langle (U^{-1}AUe_1, e_1), (U^{-1}AUe_2, e_2), \ldots, (U^{-1}AUe_n, e_n) \rangle,$$

where U is a unitary operator on H. The theorem is therefore an immediate consequence of the well known fact that the group of unitary matrices is arcwise connected.

If $\lambda = \langle \lambda_1, \lambda_2, \ldots, \lambda_n \rangle$ is a complex n-tuple and π is a permutation of the numbers $1, 2, \ldots, n$, let λ_π be the n-tuple $\langle \lambda_{\pi(1)}, \lambda_{\pi(2)}, \ldots, \lambda_{\pi(n)} \rangle$, and let $\mathscr{H}(\lambda)$ denote the convex hull of the vectors λ_π.

THEOREM 2.2. *If A is normal with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then $\mathscr{H}(\lambda) = \mathscr{C}\mathscr{W}(A)$ (the convex hull of $\mathscr{W}(A)$).*

Proof. Clearly each λ_π belongs to $\mathscr{W}(A)$ and therefore $\mathscr{H}(\lambda) \subset \mathscr{C}\mathscr{W}(A)$. To complete the proof, it is enough to show that $\mathscr{W}(A) \subset \mathscr{H}(\lambda)$.

If $\mu \in \mathscr{W}(A)$, then there is an orthonormal basis $f_1, f_2, \ldots, f_n$ such that $\mu_i = (Af_i, f_i)$ for $i = 1, 2, \ldots, n$. If $e_1, e_2, \ldots, e_n$ are the eigenvectors of A corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_n$, then a computation shows that $\mu = P\lambda$, where $P_{ij} = |(f_i, e_j)|^2$. Since P is clearly doubly stochastic,† it follows from a theorem of Birkhoff [3] that μ belongs to $\mathscr{H}(\lambda)$.

REMARK. Lerer [5] gives an example of a 3×3 unitary matrix A with the property that $\mathscr{W}(A)$ is a proper subset of $\mathscr{H}(\lambda)$. Theorem 2.2 therefore implies that in general $\mathscr{W}(A)$ need not be convex.

THEOREM 2.3. *Let A be a normal matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, and for $\mu \in \mathbf{C}^n$ let $C(\mu)$ denote the convex hull of the set of normal matrices with spectrum the set of coordinates of μ. Then*

$$\{\operatorname{tr}(AB^*) : B \in C(\mu)\} = (\mathscr{H}(\lambda), \mu).$$

† A matrix with non-negative entries is doubly stochastic if the sum of the entries in each row and column is 1.

Proof. Let $[\mu]$ be the diagonal matrix whose main diagonal is μ. Then $(\text{diag}(T), \mu) = \text{tr}(T[\mu]^*)$ for any matrix T. Hence by Theorem 2.2,

$$\begin{aligned}(\mathscr{H}(\lambda), \mu) = \mathscr{C}(\mathscr{W}(A), \mu) &= \mathscr{C}\{(\text{diag}(U^{-1}AU), \mu): U \text{ unitary}\}\\ &= \mathscr{C}\{\text{tr}(U^{-1}AU[\mu]^*): U \text{ unitary}\}\\ &= \mathscr{C}\{\text{tr}(A(U[\mu]U^{-1})^*): U \text{ unitary}\}\\ &= \{\text{tr}(AB^*): B \in C(\mu)\}.\end{aligned}$$

Corollary 1 (F. John [4]). *For any subset σ of $\mathbf{R}^n$, let $C(\sigma)$ be the set of all Hermitian matrices A with $\mathscr{H}(\lambda) \subset \sigma$. If σ is compact and convex, so is $C(\sigma)$.*

Proof. If σ is the half-space $\{\xi \in \mathbf{R}^n : (\xi, \mu) \geqq r\}$, then by Theorem 2.3 a Hermitian matrix A belongs to $C(\sigma)$ if and only if $\text{tr}(AB^*) \geqq r$ for all matrices B that are unitarily equivalent to $[\mu]$. From this description it is clear that $C(\sigma)$ is closed and convex. If σ is compact and convex, it is an intersection of closed half-spaces, and $C(\sigma)$ is therefore an intersection of closed sets. Thus $C(\sigma)$ is closed and convex; because it is bounded it is compact.

Theorem 2.3 yields another proof of Theorem 1.5:

Corollary 2. *If A is normal with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then*

$$W_k(A) = \mathscr{C}\left\{\frac{1}{k}(\lambda_{i_1} + \lambda_{i_2} + \ldots + \lambda_{i_k})\right\} \qquad (k = 1, 2, \ldots, n).$$

Proof.
$$\begin{aligned} kW_k(A) &= \mathscr{C}\{\text{tr}(AP): P \text{ projection of rank } k\}\\ &= \{\text{tr}(AB^*): B \in C(\mu_k)\}\\ &= (\mathscr{H}(\lambda), \mu_k)\\ &= \mathscr{C}\{(\lambda_\pi, \mu_k): \pi \text{ permutation}\},\end{aligned}$$

where μ_k is the vector with the first k entries equal to 1 and the rest equal to 0.

The next theorem indicates a connection between k-numerical ranges and diagonals, and includes several results of [1].

Theorem 2.4. *If A is a matrix, then $\lambda \in W_k(A)$ if and only if $\mathscr{W}(A)$ contains a vector with at least k coordinates equal to λ.*

Proof. Without loss of generality we may suppose that $\lambda = 0$. If P is a projection, let $C_P(A) = PA|_{P(H)}$ be the compression of A to the range of P. A simple computation shows that $\text{tr}(PA) = \text{tr}(C_p(A))$.

Now if $0 \in W_k(A)$, then there is a projection P of rank k such that $\text{tr}(PA) = 0$. The operator $C_p(A)$ then has trace 0 and hence, using a result from [1], we can choose an orthonormal basis $f_1, \ldots, f_k$ of $P(H)$ such that $(Af_i, f_i) = (C_p(A)f_i, f_i) = 0$ for $i = 1, 2, \ldots, k$. If $f_{k+1}, \ldots, f_n$ form an orthonormal basis of $P(H)^\perp$, then the matrix of A relative to the basis $f_1, f_2, \ldots, f_n$ has at least k zeros on the main diagonal.

3. Diagonals of Hermitian matrices. For the remainder of the paper A will denote an $n\times n$ Hermitian matrix ($n\geqq 3$) with eigenvalues $\lambda_1\leqq\lambda_2\leqq\ldots\leqq\lambda_n$ and corresponding unit eigenvectors $e_1, e_2, \ldots, e_n$.

LEMMA 3.1. *If $\mu\in W(A)$, there is a unit vector f such that $(Af, f)=\mu$ and*

$$kW_k(A_1)=kW_k(A)\cap((k+1)W_{k+1}(A)-\mu),$$

where A_1 is the compression of A to the orthogonal complement of f, and $k=1, 2, \ldots, n-1$.

Proof. Choose the largest integer i such that $\mu\in[\lambda_i, \lambda_{i+1}]$. Since A is Hermitian there is a unit vector f in the span of e_i and e_{i+1} with $(Af, f)=\mu$. Define

$$\alpha_k=\max\left\{\sum_{j=1}^{k}\lambda_j, \sum_{j=1}^{k+1}\lambda_j-\mu\right\},$$

$$\beta_k=\min\left\{\sum_{j=n-k+1}^{n}\lambda_j, \sum_{j=n-k}^{n}\lambda_j-\mu\right\}.$$

It will be shown that each side of the above equation is $[\alpha_k, \beta_k]$.

A real number x belongs to the interval $[\alpha_k, \beta_k]$ if and only if

$$\sum_{1}^{k}\lambda_j\leqq x\leqq\sum_{n-k+1}^{n}\lambda_j,$$

$$\sum_{1}^{k+1}\lambda_j\leqq x+\mu\leqq\sum_{n-k}^{n}\lambda_j.$$

Theorem 1.5 shows that these conditions are respectively equivalent to

$$x\in kW_k(A),\ x+\mu\in(k+1)W_{k+1}(A).$$

This proves that

$$[\alpha_k, \beta_k]=kW_k(A)\cap((k+1)W_{k+1}(A)-\mu).$$

Now $kW_k(A_1)$ is the set of all sums $\sum_{j=1}^{k}(Ag_j, g_j)$ where $g_1, g_2, \ldots, g_k$ are orthonormal vectors in $\{f\}^{\perp}$. Hence clearly $kW_k(A_1)\subset kW_k(A)$. It is also clear that $\sum_{j=1}^{k}(Ag_j, g_j)+(Af, f)$ belongs to $(k+1)W_{k+1}(A)$. Therefore

$$kW_k(A_1)\subset kW_k(A)\cap((k+1)W_{k+1}(A)-\mu).$$

To prove the reverse inclusion, it suffices to prove that the numbers α_k and β_k belong to $kW_k(A_1)$. Note first that α_k is $\sum_{j=1}^{k}\lambda_j$ or $\sum_{j=1}^{k+1}\lambda_j-\mu$ according as $\lambda_{k+1}\leqq\mu$ or $\lambda_{k+1}>\mu$. If $\lambda_{k+1}\leqq\mu$ then f is orthogonal to $e_1, \ldots, e_k$, and so $\alpha_k=\sum_{j=1}^{k}\lambda_j\in kW_k(A_1)$. If $\lambda_{k+1}>\mu$ then f is in the span of $e_1, \ldots, e_{k+1}$; let Q be the projection on this span and P the projection on the orthogonal complement of f in this span. Then $\mathrm{tr}(QA)=\mathrm{tr}(PA)+\mu$ and $\mathrm{tr}(QA)=\sum_{j=1}^{k+1}\lambda_j$, so

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that

$$\operatorname{tr}(PA_1) = \operatorname{tr}(PA) = \sum_{j=1}^{k+1} \lambda_j - \mu = \alpha_k$$

and $\alpha_k \in kW_k(A_1)$. The proof is completed by arguing similarly for β_k.

The last part of this proof can be based on the fact, proved in [7], that the spectrum of A_1 consists of $\lambda_i + \lambda_{i+1} - \mu$ and the points λ_j with $j \neq i, i+1$.

It is now easy to obtain Horn's characterization of $\mathscr{W}(A)$.

THEOREM 3.2. *Let A be an $n \times n$ Hermitian matrix with eigenvalues $\lambda = \langle \lambda_1, \lambda_2, \ldots, \lambda_n \rangle$, and let $\mu = \langle \mu_1, \mu_2, \ldots, \mu_n \rangle$. The following are equivalent.*

(i) $\mu \in \mathscr{H}(\lambda)$.
(ii) $\mu \in \mathscr{W}(A)$.
(iii) $\mu_{i_1} + \mu_{i_2} + \ldots + \mu_{i_k} \in kW_k(A)$

for each choice of subscripts and $k = 1, 2, \ldots, n$.

Proof. The equivalence of (i) and (ii) is an immediate consequence of Birkhoff's theorem (see [3]). Moreover, it is obvious that (ii) implies (iii). We show that (iii) implies (ii).

Choose a unit vector f_1 such that $(Af_1, f_1) = \mu_1$ as in Lemma 3.1, and let A_1 be the compression of A to the orthogonal complement of f_1. If $j \geqq 2$, then $\mu_1 + \mu_j \in 2W_2(A)$; hence $\mu_j \in W(A_1)$ by Lemma 3.1. Also, if $j \neq k$ and $j, k \geqq 2$, then

$$\mu_j + \mu_k \in (3W_3(A) - \mu_1) \cap 2W_2(A) = 2W_2(A_1).$$

The argument can now be repeated with A_1 replacing A. This gives a unit vector f_2 in $\{f_1\}^\perp$ such that $(Af_2, f_2) = (A_1 f_2, f_2) = \mu_2$. Also, if A_2 is the compression of A_1 to $\{f_1\}^\perp \cap \{f_2\}^\perp$, then as before

$$\mu_j \in W(A_2),$$

$$\mu_j + \mu_k \in 2W_2(A_2),$$

for $j, k \geqq 3$ and $j \neq k$.

The proof is completed by $n-1$ repetitions of the same argument.

REMARK. We observed earlier that in general $\mathscr{W}(A) \neq \mathscr{H}(\lambda)$ for normal matrices. The reason for this is that Lemma 3.1 fails. For example, let A be the 3×3 diagonal matrix with non-collinear eigenvalues $\lambda_1, \lambda_2, \lambda_3$, and let $\mu = \frac{2}{3}\lambda_1 + \frac{1}{3}\lambda_2$. Let f be any unit vector such that $(Af, f) = \mu$, and let A_1 be the compression of A to $\{f\}^\perp$. If $z = \frac{1}{3}\lambda_2 + \frac{2}{3}\lambda_3$, then z belongs to $W_1(A) \cap (2W_2(A) - \mu)$. However, it is easy to see that $W(A_1)$ is the line segment $[\frac{1}{3}\lambda_1 + \frac{2}{3}\lambda_2, \lambda_3]$ (see [7] for example) and this does not contain z.

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