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On the maximal numerical range

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H - Hilbert space

A - bounded linear operator on $\mathcal{H}$

$$W(A) = \{ (Ax, x) : \|x\| = 1 \}$$

So,

$$\text{cl}\, W(A) \ni \lambda \iff$$

$$\exists\ x_n \in \mathcal{H},\ \|x_n\| = 1$$

$$(Ax_n, x_n) \to \lambda$$

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$W_0(A) \ni \lambda \overset{\text{def}}{\Longleftrightarrow}$

$\exists\, x_n \in \mathcal{H},\ \|x_n\| = 1,$

$\|Ax_n\| \to \|A\|,$

$(Ax_n, x_n) \to \lambda$

(Stampfli, Pacific J. Math 1970)

So, $W_0(A) \subseteq \operatorname{cl} W(A)$

Also, closed, convex

What else?

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L1 $\mathcal{E}_A = \{z : |z| = \|A\|\}$

$W_0(A) \cap \mathcal{E}_A =$

$\operatorname{cl} W(A) \cap \mathcal{E}_A =$ } known

$\sigma(A) \cap \mathcal{E}_A$

Th1 $W_0(A) \cap \partial W(A) \neq \emptyset$

$\Leftrightarrow$ A normaloid

($\overset{\text{def}}{\Leftrightarrow}$ $\sigma(A) \cap \mathcal{E}_A \neq \emptyset$)

In particular,

normaloid $\Leftrightarrow w(A) = w_0(A)$

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Cor 1 $W_0(A) \cap \partial W(A) = (\sigma(A) \cap \mathcal{C}_A) \cup \mathcal{I}_A$

$\mathcal{I}_A$ = all chords of $\mathcal{C}_A$ lying on $\partial W(A)$

Th2 A normal $\Longrightarrow$

$W_0(A) \cap \partial W(A) = \operatorname{conv}(\sigma(A) \cap \mathcal{C}_A)$

Cor 2 A subnormal $\Longrightarrow$

ditto

Case $\dim \mathcal{H} < \infty$

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$W_0(A) = W(B)$, where

$B = A|$ e-space of A^*A

corr. its max e-value

Th3 $W_0(A) = W(A) \Leftrightarrow$

A unitarily similar to

$c\,U \oplus B$, where

U - unitary, $c > 0$,

$W(B) \subseteq c\,W(U)$.

On the maximal numerical range of some matrices.☆

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Abstract

The maximal numerical range $W_0(A)$ of a matrix A is the (regular) numerical range $W(B)$ of its compression B onto the eigenspace $\mathcal{L}$ of A^*A corresponding to its maximal eigenvalue. So, always $W_0(A) \subseteq W(A)$. We establish conditions under which $W_0(A)$ has a non-empty intersection with the boundary of $W(A)$, in particular, when $W_0(A) = W(A)$. We also describe $W_0(A)$ explicitly for matrices unitarily similar to direct sums of 2-by-2 blocks, and provide some insight into the behavior of $W_0(A)$ when $\mathcal{L}$ has codimension one.

Keywords: Numerical range, Maximal numerical range, Normaloid matrices

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1. Introduction

Let $\mathbb{C}^n$ stand for the standard n-dimensional inner product space over the complex field $\mathbb{C}$. Also, denote by $\mathbb{C}^{m\times n}$ the set (algebra, if $m = n$) of all m-by-n matrices with the entries in $\mathbb{C}$. We will think of $A \in \mathbb{C}^{n\times n}$ as a linear operator acting on $\mathbb{C}^n$.

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The *numerical range* (a.k.a. the *field of values*, or the *Hausdorff set*) of such A is defined as

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

It is well known that $W(A)$ is a convex compact subset of $\mathbb{C}$ invariant under unitary similarities of A; see e.g. [6] for this and other properties of $W(A)$ needed in what follows.

The notion of a *maximal* numerical range $W_0(A)$ was introduced in [14] in a general setting of A being a bounded linear operator acting on a Hilbert space $\mathcal{H}$. In the case we are interested in, $W_0(A)$ can be defined simply as the (usual) numerical range of the compression B of A onto the eigenspace $\mathcal{L}$ of A^*A corresponding to its largest eigenvalue:

$$W_0(A) = \{x^*Ax \colon x^*x = 1,\ x \in \mathcal{L}\}. \tag{1.1}$$

Consequently, $W_0(A)$ is a convex closed subset of $W(A)$, invariant under unitary similarities of A. Moreover, for A unitarily similar to a direct sum of several blocks A_j:

$$W_0(A) = \operatorname{conv}\{W_0(A_j) \colon j \text{ such that } \|A_j\| = \|A\|\}; \tag{1.2}$$

here and below we are using a standard notation $\operatorname{conv} X$ for the convex hull of the set X.

In the finite dimensional setting property (1.2) is rather trivial; the infinite dimensional version is in [7, Lemma 2].

Since $W_0(A) \subseteq W(A)$, two natural questions arise: (i) whether $W_0(A)$ intersects with the boundary $\partial W(A)$ of $W(A)$ or lies completely in its interior, and (ii) more specifically, for which A do the two sets coincide. We deal with these questions in Section 2. These results are illustrated in Section 3 by the case $n = 2$ in which a compete description of $W_0(A)$ is readily accessible. With the use of (1.2) we then (in Section 4) tackle the case of marices A unitarily reducible to 2-by-2 blocks. The last Section 5 is devoted to matrices with the norm attained on a hyperplane.

2. Position within the numerical range

In order to state the main result of this section, we need to introduce some additional notation and terminology. The *numerical radius* $w(A)$ of A is defined by the formula

$$w(A) = \max\{|z| : z \in W(A)\}.$$

The Cauchy-Schwarz inequality implies that $w(A) \le \|A\|$, and the equality $w(A) = \|A\|$ holds if and only if there is an eigenvalue λ of A with $|\lambda| = \|A\|$, i.e., the norm of A coincides with its spectral radius $\rho(A)$. If this is the case, A is called *normaloid* . In other words, A is normaloid if

$$\Lambda(A) := \{\lambda \in \sigma(A) \colon |\lambda| = \|A\|\} \,(= \{\lambda \in W(A) \colon |\lambda| = \|A\|\}) \neq \emptyset.$$

Theorem 1. *Let $A \in \mathbb{C}^{n\times n}$. Then the following statements are equivalent:*

(i) *A is normaloid;*
(ii) *$W_0(A) \cap \partial W(A) \neq \emptyset$;*
(iii) *$\{\lambda \in W_0(A) \colon |\lambda| = \|A\|\} \neq \emptyset$.*

Proof. (i) ⇒ (iii). As was shown in [5], $\rho(A) = \|A\|$ if and only if A is unitarily similar to a direct sum $cU \oplus B$, where U is unitary, c is a positive constant and the block B (which may or may not be actually present) is such that $\rho(B) < c$, $\|B\| \le c$.

For such A we have $\|A\| = \rho(A) = c$, and according to (1.2):

$$W_0(A) = \begin{cases} W(cU) = \operatorname{conv}\Lambda(A) & \text{if } \|B\| < c, \\ \operatorname{conv}(\Lambda(A) \cup W_0(B)) & \text{otherwise.} \end{cases} \tag{2.1}$$

Either way, $W_0(A) \supset \Lambda(A)$.

(iii) ⇒ (ii). Since $w(A) \le \|A\|$, the points of $W(A)$ (in particular, $W_0(A)$) having absolute value $\|A\|$ automatically belong to $\partial W(A)$.

(ii) ⇒ (i). Considering $A/\|A\|$ in place of A itself, we may without loss of generality suppose that $\|A\| = 1$. Pick a point $a \in W_0(A) \cap \partial W(A)$. By definition of $W_0(A)$, there exists a unit vector $x \in \mathbb{C}^n$ for which $\|Ax\| = 1$ and $x^*Ax = a$. Choose also a unit vector y orthogonal to x, requiring in addition that $y \in \operatorname{Span}\{x, Ax\}$ if x is not an eigenvector of A. Let C be the compression of A onto the 2-dimensional subspace $\operatorname{Span}\{x, y\}$. The matrix $A_0 := \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ of C with respect to the orthonormal basis $\{x, y\}$ then satisfies $|a|^2 + |c|^2 = 1$. From here:

$$A_0^* A_0 = \begin{bmatrix} 1 & \overline{a}b + \overline{c}d \\ a\overline{b} + c\overline{d} & |b|^2 + |d|^2 \end{bmatrix}. \tag{2.2}$$

But $\|A_0\| \le \|A\| = 1$. Comparing this with (2.2) we conclude that

$$\overline{a}b + \overline{c}d = 0. \tag{2.3}$$

Moreover, $W(A_0) \subset W(A)$, and so $a \in \partial W(A_0)$. This implies $|b| = |c|$, as was stated explicitly in [16, Corollary 4] (see also [4, Proposition 4.3]). Therefore, (2.3) is only possible if $b = c = 0$ or $|a| = |d|$.

In the former case $|a| = 1$, immediately implying $w(A) = 1 = \|A\|$.

In the latter case, some additional reasoning is needed. Namely, then $|b|^2 + |d|^2 = |c|^2 + |a|^2 = 1$ which in combination with (2.3) means that A_0 is unitary. Since $W(A) \supset \sigma(A_0)$, we see that $w(A) \geq 1$. On the other hand, $w(A) \leq \|A\| = 1$, and so again $w(A) = \|A\|$. □

Note that Theorem 1 actually holds in the infinite-dimensional setting. For this (more general) situation, the equivalence *(i)* ⇔ *(iii)* was established in [2, Corollary 1], while *(i)* ⇔ *(ii)* is from [13]. Moreover, the paper [2] prompted [13]. The proof in the finite-dimensional case is naturally somewhat simpler, and we provide it here for the sake of completeness.

If the matrix B introduced in the proof of Theorem 1 is itself normaloid, then $\|B\| < c$ and $W_0(A)$ is given by the first line of (2.1). This is true in particular for normal A, when B is also normal. On the other hand, if $\|B\| = c$, then Theorem 1 (applied to B) implies that $W_0(B)$ lies strictly in the interior of $W(B)$. In particular, there are no points in $W(B)$ with absolute value $c(= \|A\|)$. From here we immediately obtain

Corollary 1. *For any $A \in \mathbb{C}^{n\times n}$,*

$$\{\lambda \in W_0(A) \colon |\lambda| = \|A\|\} = \Lambda(A).$$

This is a slight refinement of condition (ii) in Theorem 1.

Theorem 2. *Given a matrix $A \in \mathbb{C}^{n\times n}$, its numerical range and maximal numerical range coincide if and only if A is unitarily similar to a direct sum $cU \oplus B$ where U is unitary, $c > 0$, and $W(B) \subseteq cW(U)$.*

Proof. Sufficiency. Under the condition imposed on B, $W(A) = cW(U)$. At the same time, $W_0(A) \supseteq W_0(cU) = cW(U)$.

Necessity. If $W(A) = W_0(A)$, then in particular $W_0(A)$ has to intersect $\partial W(A)$, and by Theorem 1 A is normaloid. As such, A is unitarily similar to $cU \oplus B$ with $\|B\| \leq c$, $\rho(B) < c$. It was observed in the proof of Theorem 1 that, if B itself is normaloid, then $W_0(A) = cW(U)$, and so we must have $W(A) = cW(U)$, implying $W(B) \subseteq cW(U)$.

Consider now the case when B is not normaloid. If $W(B) \subseteq cW(U)$ does not hold, draw a support line ℓ of $W(B)$ such that $cW(U)$ lies to the same side of it as $W(B)$ but at a positive distance from it. Since $W(A) = \text{conv}(cW(U) \cup W(B))$, ℓ is also a support line of $W(A)$. Meanwhile $W_0(B)$ is contained in the interior of $W(B)$, making the distance between $W_0(B)$ and ℓ positive, and implying that ℓ is not a support line of $\text{conv}(cW(U) \cup W_0(B))$. According to (2.1), the latter set is the same as $W_0(A)$. Thus, $W_0(A) \neq W(A)$, which is a contradiction. □

3. 2-by-2 matrices

A 2-by-2 matrix A is normaloid if and only if it is normal. The situation is then rather trivial: denoting $\sigma(A) = \{\lambda_1, \lambda_2\}$ with $|\lambda_1| \leq |\lambda_2|$, we have $W(A) = [\lambda_1, \lambda_2]$ (the line segment connecting λ_1 with λ_2), and

$$W_0(A) = \begin{cases} \{\lambda_2\} \quad \neq W(A) & \text{if } |\lambda_1| < |\lambda_2|, \\ [\lambda_1, \lambda_2] = W(A) & \text{otherwise.} \end{cases}$$

So, the only interesting case is that of a non-normal A. The eigenvalues of A^*A are then simple, and $W_0(A)$ is therefore a point. According to Theorem 1, this point lies inside the ellipse $W(A)$. Our next result is the formula for its exact location.

Theorem 3. *Let $A \in \mathbb{C}^{2\times 2}$ be not normal but otherwise arbitrary. Then $W_0(A) = \{z_0\}$, where*

$$z_0 = \frac{(t_0 - |\lambda_2|^2)\lambda_1 + (t_0 - |\lambda_1|^2)\lambda_2}{2t_0 - \text{trace}(A^*A)}, \tag{3.1}$$

λ_1, λ_2 are the eigenvalues of A, and

$$t_0 = \frac{1}{2}\left(\text{trace}(A^*A) + \sqrt{(\text{trace}(A^*A))^2 - 4\,|\det A|^2}\right). \tag{3.2}$$

Note that an alternative form of (3.1),

$$z_0 = \frac{t_0 \cdot \text{trace}\, A - (\det A) \cdot \overline{\text{trace}\, A}}{2t_0 - \text{trace}(A^*A)}, \tag{3.3}$$

without λ_j explicitly present, is sometimes more convenient.

Proof. Since both the value of z_0 and the right-hand sides of formulas (3.1)–(3.3) are invariant under unitary similarities, it suffices to consider A in the upper triangular form

$$A = \begin{bmatrix} \lambda_1 & c \\ 0 & \lambda_2 \end{bmatrix}, \quad c > 0.$$

Then

$$1A^*A - tI = \begin{bmatrix} |\lambda_1|^2 - t & c\overline{\lambda_1} \\ c\lambda_1 & c^2 + |\lambda_2|^2 - t \end{bmatrix},$$

so the maximal eigenvalue t_0 of A^*A satisfies

$$c^2 |\lambda_1|^2 = (t_0 - |\lambda_1|^2)(t_0 - |\lambda_2|^2 - c^2) \tag{3.4}$$

and is thus given by formula (3.2). Choosing a respective eigenvector as

$$x = \left[c\overline{\lambda_1},\ t_0 - |\lambda_1|^2\right]^T,$$

we obtain successively

$$\|x\|^2 = c^2 |\lambda_1|^2 + (t_0 - |\lambda_1|^2)^2,$$

$$Ax = \left[ct_0,\ (t_0 - |\lambda_1|^2)\lambda_2\right]^T,$$

$$x^*Ax = c^2 t_0 \lambda_1 + (t_0 - |\lambda_1|^2)^2 \lambda_2,$$

and so finally

$$z_0 = \frac{x^*Ax}{\|x\|^2} = \frac{c^2 t_0 \lambda_1 + (t_0 - |\lambda_1|^2)^2 \lambda_2}{c^2 |\lambda_1|^2 + (t_0 - |\lambda_1|^2)^2}. \tag{3.5}$$

To put this expression for z_0 in form (3.1), we proceed as follows. Due to (3.4), the denominator in the right-hand side of (3.5) is nothing but

$$\begin{aligned}(t_0 - |\lambda_1|^2)\left((t_0 - |\lambda_2|^2 - c^2) + (t_0 - |\lambda_1|^2)\right)& \\ = (t_0 - |\lambda_1|^2)(2t_0 - \operatorname{trace}(A^*A)).&\end{aligned} \tag{3.6}$$

On the other hand, also from (3.4),

$$c^2 t_0 = (t_0 - |\lambda_1|^2)(t_0 - |\lambda_2|^2),$$

and the numerator in the right-hand side of (3.5) can be rewritten as

$$(t_0 - |\lambda_1|^2)(t_0 - |\lambda_2|^2)\lambda_1 + (t_0 - |\lambda_1|^2)\lambda_2 \\ = (t_0 - |\lambda_1|^2)\left((t_0 - |\lambda_2|^2)\lambda_1 + (t_0 - |\lambda_1|^2)\lambda_2\right). \quad (3.7)$$

It remains to divide (3.7) by (3.6). □

To interpret formula (3.1) geometrically, let us rewrite it as

$$z_0 = t_1\lambda_1 + t_2\lambda_2,$$

where

$$t_1 = \frac{t_0 - |\lambda_2|^2}{2t_0 - \mathrm{trace}(A^*A)}, \quad t_2 = \frac{t_0 - |\lambda_1|^2}{2t_0 - \mathrm{trace}(A^*A)}.$$

According to (3.2), the denominator of these formulas can be rewritten as

$$\sqrt{(\mathrm{trace}(A^*A))^2 - 4\,|\det A|^2} = \sqrt{(|\lambda_1|^2 + |\lambda_2|^2 + c^2)^2 - 4\,|\lambda_1\lambda_2|^2} \\ = \sqrt{(|\lambda_1|^2 - |\lambda_2|^2)^2 + 2c^2(|\lambda_1|^2 + |\lambda_2|^2) + c^4} > 0.$$

Also, $t_0 \geq c^2 + \max\{|\lambda_1|^2, |\lambda_2|^2\}$, and

$$(t_0 - |\lambda_1|^2) + (t_0 - |\lambda_2|^2) = 2t_0 - \mathrm{trace}(A^*A) + c^2 > 2t_0 - \mathrm{trace}(A^*A).$$

Consequently, $t_1, t_2 > 0$ and $t_1 + t_2 > 1$, implying that in case of non-collinear λ_1, λ_2 (equivalently, $\lambda_1\overline{\lambda_2} \notin \mathbb{R}$) z_0 lies in the sector spanned by λ_1, λ_2 and is separated from the origin by the line passing through λ_1, λ_2.

If, on the other hand, λ_1 and λ_2 lie on the line passing through the origin, the point z_0 also lies on this line. More specifically, the following statement holds.

Corollary 2. *Let A be a non-normal 2-by-2 matrix, with the maximal numerical range $W_0(A) = \{z_0\}$. Then the point z_0:*

(i) *is collinear with the spectrum $\sigma(A) = \{\lambda_1, \lambda_2\}$ if and only if $\lambda_1\overline{\lambda_2} \in \mathbb{R}$;*

(ii) *coincides with one of the eigenvalues of A if and only if the other one is zero;*

(iii) *lies in the open interval with the endpoints λ_1, λ_2 if and only if $\lambda_1\overline{\lambda_2} < 0$;*

(iv) *is the midpoint of the above interval if and only if* trace $A = 0$*;*

(v) *lies on the line passing through* λ_1 *and* λ_2 *but outside of the interval* $[\lambda_1, \lambda_2]$ *if and only if* $\lambda_1\overline{\lambda_2} > 0$.

Proof. Part (i) follows from the discussion preceding the statement. When proving (ii)–(v) we may therefore suppose that $\lambda_1\overline{\lambda_2} \in \mathbb{R}$ holds. Since all the statements in question are invariant under rotations of A, without loss of generality even $\lambda_1, \lambda_2 \in \mathbb{R}$. Then $z_0 \in \mathbb{R}$ as well. Using formula (3.5) for z_0:

$$z_0 - \lambda_2 = \frac{c^2\lambda_1(t_0 - \lambda_1\lambda_2)}{c^2\lambda_1^2 + (t_0 - \lambda_1^2)^2},$$

and so the signs of $z_0 - \lambda_2$ and λ_1 are the same. Relabeling the eigenvalues of A (which of course does not change z_0) we thus also have that the signs of $z_0 - \lambda_1$ and λ_2 are the same. Statements (ii)–(v) follow immediately. □

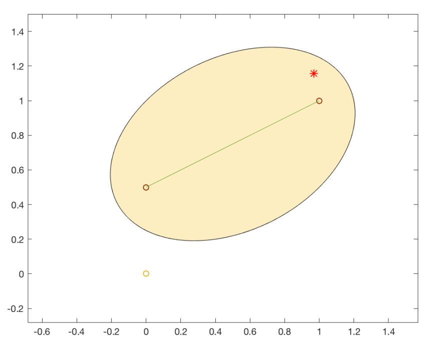

Figure 1: $A = \begin{bmatrix} 0.5i & -1 \\ 0 & 1+i \end{bmatrix}$; z_0 is not collinear with the spectrum.

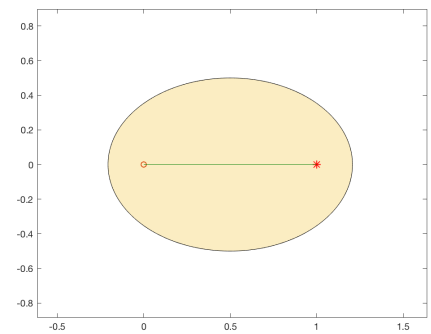

Figure 2: $A = \begin{bmatrix} 1 & i \\ 0 & 0 \end{bmatrix}$; z_0 coincides with one of the eigenvalues since the other is zero.

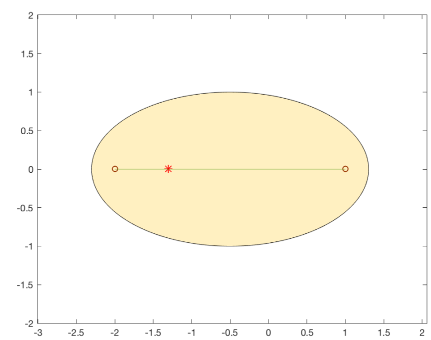

Figure 3: $A = \begin{bmatrix} -2 & 2 \\ 0 & 1 \end{bmatrix}$; z_0 is collinear with the spectrum and lies inside the interval connecting it.

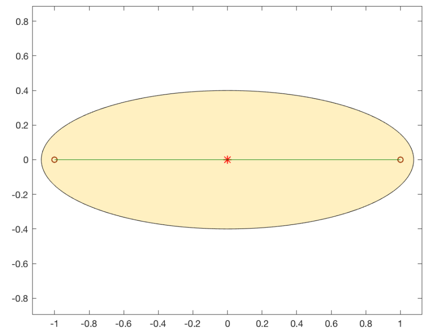

Figure 4: $A = \begin{bmatrix} 1 & 0.8 \\ 0 & -1 \end{bmatrix}$; z_0 is the midpoint of the line connecting the eigenvalues.

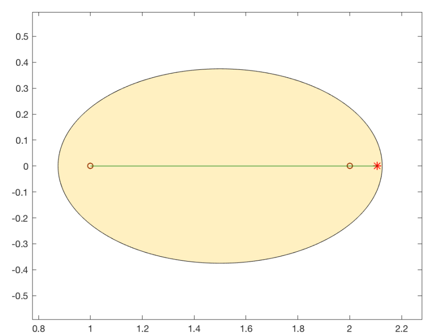

Figure 5: $A = \begin{bmatrix} 2 & 0.75 \\ 0 & 1 \end{bmatrix}$; z_0 is collinear with the spectrum and lies outside the interval connecting it.

4. Matrices decomposing into small blocks

A straightforward generalization of Theorem 3, based on Property (1.2), is the description of $W_0(A)$ for matrices A unitarily similar to direct sums of 2-by-2 and 1-by-1 blocks.

Theorem 4. *Let A be unitarily similar to*

$$\operatorname{diag}[\lambda_1, \dots, \lambda_k] \oplus A_1 \oplus \cdots \oplus A_m,$$

with $A_j \in \mathbb{C}^{2\times 2}$*,* $j = 1, \ldots, m$*. Denote*

$$t_j = \frac{1}{2}\left(\operatorname{trace}(A_j^* A_j) + \sqrt{(\operatorname{trace}(A_j^* A_j))^2 - 4\left|\det A_j\right|^2}\right), \tag{4.1}$$

$$z_j = \frac{t_j \cdot \operatorname{trace} A_j - (\det A_j)\cdot \overline{\operatorname{trace} A_j}}{2t_j - \operatorname{trace}(A^* A)}, \quad j = 1, \ldots, m, \tag{4.2}$$

$$t_0 = \max\{t_j, \left|\lambda_i\right|^2 : i = 1, \ldots, k;\ j = 1, \ldots, m\},$$

and let I *(resp.* J*) stand for the set of all* i *(resp.* j*) for which* $\left|\lambda_i\right|^2$ *(resp.* t_j*) equals* t_0*. Then*

$$W_0(A) = \operatorname{conv}\{\lambda_i, z_j \colon i \in I,\ j \in J\}. \tag{4.3}$$

According to (4.3), in the setting of Theorem 4, $W_0(A)$ is always a polygon.

Consider in particular A unitarily similar to

$$\begin{bmatrix} a_1 I_{n_1} & X \\ Y & a_2 I_{n_2} \end{bmatrix}, \tag{4.4}$$

with $X \in \mathbb{C}^{n_1 \times n_2}$ and $Y \in \mathbb{C}^{n_2 \times n_1}$ such that XY and YX are both normal. As was shown in the proof of [1, Theorem 2.1], yet another unitary similarity can be used to rewrite A as the direct sum of $\min\{n_1, n_2\}$ two-dimensional blocks

$$A_j = \begin{bmatrix} a_1 & \sigma_j \\ \delta_j & a_2 \end{bmatrix} \tag{4.5}$$

and $\max\{n_1, n_2\} - \min\{n_1, n_2\}$ one-dimensional blocks equal either a_1 or a_2.

Here σ_j are the s-numbers of X, read from the diagonal of the middle term in its singular value decomposition $X = U_1 \Sigma U_2^*$, while δ_j are the respective diagonal entries of the matrix $\Delta = U_2^* Y U_1$, which can also be made diagonal due to the conditions imposed on X, Y.

Since $\|A_j\| \geq \max\{|a_1|, |a_2|\}$, for matrices (4.4) (or unitarily similar to them) formula (4.3) implies that $W_0(A)$ is the convex hull of z_j given by (4.2) taken over those j only which deliver the maximal value of $\|A_j\|$.

Here are some particular cases in which all z_j, λ_i contributing to $W_0(A)$ happen to coincide. Then $W_0(A)$ is a singleton, as it was the case for 2-by-2 matrices A different from scalar multiples of a unitary matrix.

Proposition 1. *Let, in* (4.4), $a_1 = -a_2$. *Then* $W_0(A) = \{0\}$.

Proof. Indeed, in this case trace $A_j = 0$, and formula (4.2) implies that $z_j = 0$ for all j, in particular for those with maximal $\|A_j\|$ is attained. ☐

Recall that a *continuant* matrix is by definition a tridiagonal matrix $A \in \mathbb{C}^{n\times n}$ such that its off-diagonal entries satisfy the requirement

$$a_{k,k+1} = -\overline{a_{k+1,k}}, \quad k = 1, \dots, n-1.$$

Such a matrix can be written as

$$C = \begin{bmatrix} a_1 & b_1 & 0 & \dots & 0 \\ -\overline{b_1} & a_2 & b_2 & \ddots & \vdots \\ 0 & -\overline{b_2} & a_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & b_{n-1} \\ 0 & \dots & 0 & -\overline{b_{n-1}} & a_n \end{bmatrix}. \tag{4.6}$$

Proposition 2. *Let C be the continuant matrix* (4.6) *with a* 2*-periodic main diagonal:* $a_1 = a_3 = \dots$, $a_2 = a_4 = \dots$. *Then* $W_0(C)$ *is a singleton.*

Proof. Let T be the matrix with the columns $e_1, e_3, \dots, e_2, e_4, \dots$, where $\{e_1, \dots, e_n\}$ is the standard basis of $\mathbb{C}^n$. It is easy to see that a unitary similarity performed by T transforms the continuant matrix (4.6) with the 2-periodic main diagonal into the matrix (4.4) for which

$$X = \begin{bmatrix} b_1 & & & \\ b_2 & b_3 & & \\ & b_4 & b_5 & \\ & & \ddots & \ddots \end{bmatrix}, \quad Y = -X^*.$$

So, in (4.5) we have $\delta_j = -\sigma_j$, and thus $\|A_j\|$ depends monotonically on σ_j. The block on which the maximal norm is attained is therefore uniquely defined (though might appear repeatedly), and the respective maximal value of σ_j is nothing but $\|X\|$. ☐

It is clear from the proof of Proposition 2 how to determine the location of $W_0(C)$: it is given by formulas (4.1), (4.2) with trace A_j, trace$(A_j^* A_j)$ and det A_j replaced by a_1+a_2, $|a_1|^2+|a_2|^2+2\,\|X\|^2$, and $a_1a_2+\|X\|^2$, respectively.

Finally, let A be *quadratic*, i.e., having the minimal polynomial of degree two. As is well known (and easy to show), A is then unitarily similar to a matrix

$$\begin{bmatrix} \lambda_1 I_{n_1} & X \\ 0 & \lambda_2 I_{n_2} \end{bmatrix}. \tag{4.7}$$

This fact was used e.g. in [15] to prove that for such matrices $W(A)$ is the same as $W(A_0)$, where $A_0 \in \mathbb{C}^{2\times 2}$ is defined as

$$A_0 = \begin{bmatrix} \lambda_1 & \|X\| \\ 0 & \lambda_2 \end{bmatrix},$$

and thus $W(A)$ is an elliptical disk.

The next statement shows that the relation between A unitarily similar to (4.7) and A_0 persists when maximal numerical ranges are considered.

Proposition 3. *Let $A \in \mathbb{C}^{n\times n}$ be quadratic and thus unitarily similar to (4.7). Then $W_0(A)$ is a singleton $\{z_0\}$, where*

$$z_0 = \frac{(\|A_0\|^2 - |\lambda_2|^2)\lambda_1 + (\|A_0\|^2 - |\lambda_1|^2)\lambda_2}{2\|A_0\|^2 - (|\lambda_1|^2 + |\lambda_2|^2 + \|X\|^2)}.$$

Proof. Observe that (4.7) is a particular case of (4.4) in which $Y = 0$ and $a_j = \lambda_j$, $j = 1,2$. So, the normality of XY and YX holds in a trivial way and, moreover, $\delta_j = 0$ for all the blocks A_j appearing in the unitary reduction of A. Similarly to the situation in Proposition 2, the norms of A_j depend monotonically on σ_j, and thus the maximum is attained on the blocks (of which there is at least one) coinciding with A_0. It remains only to invoke formula (3.1), keeping in mind that $t_0 = \|A_0\|^2$ and $\operatorname{trace}(A_0^* A_0) = |\lambda_1|^2 + |\lambda_2|^2 + \|X\|^2$. □

In general, however, there is no reason for the set (4.3) to be a singleton. To illustrate, let $A = A_1 \oplus A_2 \oplus A_3$, where

$$A_1 = \begin{bmatrix} -1 & 1 \\ 1-i & 2 \end{bmatrix}, \; A_2 = \begin{bmatrix} -1 & 1+i \\ 1 & 2 \end{bmatrix}, \; A_3 = \begin{bmatrix} -1 & \sqrt{\frac{3+3\sqrt{6}}{5}} \\ 0 & 2 \end{bmatrix}. \tag{4.8}$$

Then $\|A_j\| = \sqrt{4+\sqrt{6}}$ for each $j = 1,2,3$, while $W_0(A_j) = \{z_j\}$, with

$$z_{1,2} \approx 1.93 \mp 0.20i, \quad z_3 \approx 1.45. \tag{4.9}$$

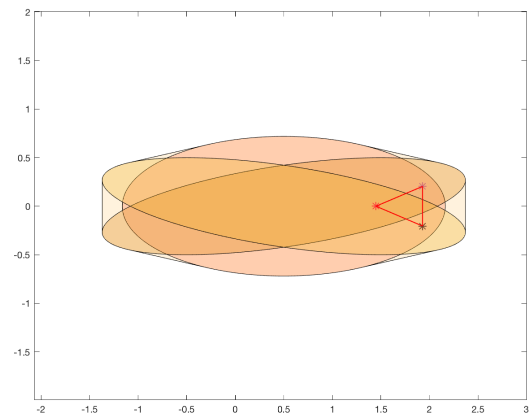

Figure 6: A is the direct sum of A_j given by (4.8). The maximal numerical range is the triangle with the vertices z_j given by (4.9).

5. Matrices with the norm attained on a hyperplane

Generically, the eigenvalues of A^*A are all distinct, and $W_0(A)$ is therefore a singleton. In more rigorous terms, the set of n-by-n matrices A with $W_0(A)$ being a point has the interior dense in $\mathbb{C}^{n\times n}$.

An opposite extreme is the case when A^*A has just one eigenvalue. This happens if and only if A is a scalar multiple of a unitary matrix — a simple situation, covered by Theorem 2.

If $n = 2$, these are the only options, which is of course in agreement with the description of $W_0(A)$ provided for this case in Section 3. Starting with $n = 3$, however, the situation when the maximal eigenvalue of A^*A has multiplicity $n-1$ becomes non-trivial. We here provide some additional information about the shapes of $W(A), W_0(A)$ in this case.

The only way in which such matrices A can be unitarily reducible is if they are unitarily similar to $cU \oplus B$, with U unitary and $\|B\| = c$ attained on a subspace of codimension one. Therefore, it suffices to consider the case of unitarily irreducible A only.

To state the pertinent result, we need to recall one more notion. Namely, Γ is a *Poncelet curve* (of rank m with respect to a circle $\mathcal{C}$) if it is a closed convex curve lying inside $\mathcal{C}$ and such that for any point $z \in \mathcal{C}$ there is an m-gon inscribed in $\mathcal{C}$, circumscribed around Γ, and having z as one of its vertices.

Theorem 5. *Let $A \in \mathbb{C}^{n\times n}$ be unitarily irreducible, with the norm of A attained on an $(n-1)$-dimensional subspace. Then $\partial W(A)$ and $\partial W_0(A)$ both are Poncelet curves (of rank $n+1$ and n, respectively) with respect to the circle $\{z\colon\ |z| = \|A\|\}$.*

Proof. Considering $A/\|A\|$ in place of A, we may without loss of generality suppose that $\mathcal{C}$ is the unit circle $\mathbb{T}$, the matrix in question is a contraction with $\|A\| = 1$ and $\operatorname{rank}(I - A^*A) = 1$. Also, $\rho(A) < 1$ since otherwise A would be normaloid and thus unitarily reducible. In the notation of [3] (adopted in later publications), $A \in S_n$, and the result follows directly from [3, Theorem 2.1].

Moving to $W_0(A)$, consider the polar form UR of A. Since the statement in question is invariant under unitary similarities, we may suppose that the positive semi-definite factor R is diagonalized. Condition $\operatorname{rank}(I - A^*A) = 1$ then implies that $R = \operatorname{diag}[1, \dots, 1, c]$, where $0 \le c < 1$. In agreement with (1.1), $W_0(A) = W(U_0)$, where U_0 is the matrix obtained from U by deleting its last row and column. Note that U has no eigenvectors with the last coordinate equal to zero, since otherwise they would also be eigenvectors of R, implying unitary reducibility of A. In particular, the eigenvalues of U are distinct. The statement now follows by applying [11, Theorem 1] to $W(U_0)$. □

Note that the matrix U_0 constructed in the second part of the proof actually belongs to S_{n-1}. The properties of $W(T)$ for $T \in S_n$ stated in [3, Lemma 2.2] thus yield

Corollary 3. *In the setting of Theorem 5, both $\partial W(A)$ and $\partial W_0(A)$ are smooth curves, with each point generated by exactly one (up to a unimodular scalar multiple) vector.*

The above mentioned uniqueness of the generating vectors implies in particular that $\partial W(A)$, $\partial W_0(A)$ contain no flat portions.

To illustrate, consider the Jordan block $J_n \in \mathbb{C}^{n\times n}$ corresponding to the zero eigenvalue. Then $J_n \in S_n$, with the norm of J_n attained on the span $\mathcal{L}$ of the elements $e_2, \dots, e_n$ of the standard basis of $\mathbb{C}^n$. Consequently, the compression of J_n onto $\mathcal{L}$ is J_{n-1}, and $W_0(J_n) = W(J_{n-1})$ is the circular disk $\{z\colon\ |z| \le \cos\frac{\pi}{n}\}$, while $W(J_n)$ is the (concentric but strictly larger) circular disk $\{z\colon\ |z| \le \cos\frac{\pi}{n+1}\}$.

Finally, let us concentrate on the smallest size for which the situation of this Section is non-trivial, namely $n = 3$.

Proposition 4. *A matrix $A \in \mathbb{C}^{3\times 3}$ is unitarily irreducible with the norm attained on a 2-dimensional subspace if and only if it is unitarily similar to*

$$\omega \begin{bmatrix} \lambda_1 & \sqrt{(1-|\lambda_1|^2)(1-|\lambda_2|^2)} & -\lambda_2\sqrt{(1-|\lambda_1|^2)(1-|\lambda_3|^2)} \\ 0 & \lambda_2 & \sqrt{(1-|\lambda_2|^2)(1-|\lambda_3|^2)} \\ 0 & 0 & \lambda_3 \end{bmatrix}, \tag{5.1}$$

where $\omega \in \mathbb{C}\setminus\{0\}$, $-1 < \lambda_2 \le 0$, and $|\lambda_j| < 1$, $j = 1, 3$.

Proof. According to Schur's lemma, we can put any $A \in \mathbb{C}^{3\times 3}$ in an upper triangular form

$$A_0 = \begin{bmatrix} \lambda_1 & x & y \\ 0 & \lambda_2 & z \\ 0 & 0 & \lambda_3 \end{bmatrix}. \tag{5.2}$$

Further multiplication by an appropriate non-zero complex number w allows us without loss of generality to suppose that $\|A\| = 1$ and $x\overline{y}z \ge 0$. An additional (diagonal) unitary similarity can then be used to arrange for x, y, z all to be non-negative. Being an irreducible contraction, the matrix (5.2) has to satisfy $|\lambda_j| < 1$ $(j = 1, 2, 3)$ and $xz \neq 0$. Rewriting the rank-one condition for $I - A_0^*A_0$ as the collinearity of its columns and solving the resulting system of equations for x, y, z yields

$$\begin{aligned} x =& \sqrt{(1-|\lambda_1|^2)(1-|\lambda_2|^2)}, \\ y =& -\lambda_2\sqrt{(1-|\lambda_1|^2)(1-|\lambda_3|^2)}, \\ z =& \sqrt{(1-|\lambda_2|^2)(1-|\lambda_3|^2)}. \end{aligned} \tag{5.3}$$

In particular, λ_2 has to be non-positive, due to the non-negativity of y.

Setting $\omega = w^{-1}$, we arrive at representation (5.1).

A straightforward verification shows that the converse is also true, i.e., any matrix of the form (5.1) is unitarily irreducible with a norm attained on a 2-dimensional subspace. □

Note that the form (5.1) can also be established by invoking [11, Theorem 4], instead of solving for x, y, z in terms of λ_j straightforwardly.

In the setting of Proposition 4 the set $W_0(A)$ is the numerical range of a 2-by-2 matrix, and in agreement with Corollary 3 is an elliptical disk. By the same Corollary 3, $W(A)$ also cannot have flat portions on its boundary (this of course can also be established by applying the respective criteria for 3-by-3 matrices from [8, Section 3] or [12]). According to Kippenhahn's classification of the shapes of numerical ranges in the $n = 3$ case [9] (see also the English translation [10]), $W(A)$ can a priori be either an elliptical disk or an ovular figure bounded by a convex algebraic curve of degree 6. As it happens, both options materialize. The next result singles out the case in which $W(A)$ is elliptical; in all other cases it is therefore ovular.

Theorem 6. *Let A be given by formula* (5.1)*, with λ_j as described by Proposition 4. Then $W(A)$ is an elliptical disk if and only if*

$$\lambda_i = \lambda_j \frac{1 - |\lambda_k|^2}{1 - |\lambda_j \lambda_k|^2} + \lambda_k \frac{1 - |\lambda_j|^2}{1 - |\lambda_j \lambda_k|^2} \tag{5.4}$$

for some reordering (i, j, k) of the triple $(1, 2, 3)$*.*

Proof. According to [8, Section 2], for a unitarily irreducible matrix (5.2) to have an elliptical numerical range it is necessary and sufficient that

$$\lambda = \frac{\lambda_3 |x|^2 + \lambda_2 |y|^2 + \lambda_1 |z|^2 - x\overline{y}z}{|x|^2 + |y|^2 + |z|^2}$$

coincides with one of the eigenvalues λ_j. Plugging in the values of x, y, z from (5.3), we may rewrite λ as

$$\frac{\lambda_1(1 - |\lambda_2|^2)(1 - |\lambda_3|^2) + \lambda_2(1 - |\lambda_1|^2)(1 - |\lambda_3|^2) + \lambda_3(1 - |\lambda_1|^2)(1 - |\lambda_2|^2)}{2 - |\lambda_1|^2 - |\lambda_2|^2 - |\lambda_3|^2 + |\lambda_1 \lambda_2 \lambda_3|^2}.$$

Now it is straightforward to check that $\lambda = \lambda_i$ if and only if (5.4) holds. $\square$

Proposition 4 and Theorem 6 both simplify greatly if A is singular.

Theorem 7. *A singular 3-by-3 matrix A is unitarily irreducible with the norm attained on a 2-dimensional subspace if and only if it is unitarily similar to*

$$B = \omega \begin{bmatrix} 0 & \sqrt{1 - |\lambda|^2} & -\lambda\sqrt{1 - |\mu|^2} \\ 0 & \lambda & \sqrt{(1 - |\lambda|^2)(1 - |\mu|^2)} \\ 0 & 0 & \mu \end{bmatrix}, \tag{5.5}$$

where $\omega \neq 0$, $-1 < \lambda \leq 0$ and $|\mu| < 1$. Its numerical range $W(A)$ is an elliptical disk if and only if $\mu = \pm\lambda$, and has an ovular shape otherwise.

Note that for matrices (5.5) $\mathcal{L} = \text{Span}\{e_2, e_3\}$, and so $W_0(B)$ is nothing but the numerical range of the right lower 2-by-2 block of B. The next three figures show the shape of $W_0(B)$ and $W(B)$ for B given by (5.5) with $\omega = 1$ for several choices of λ, μ.

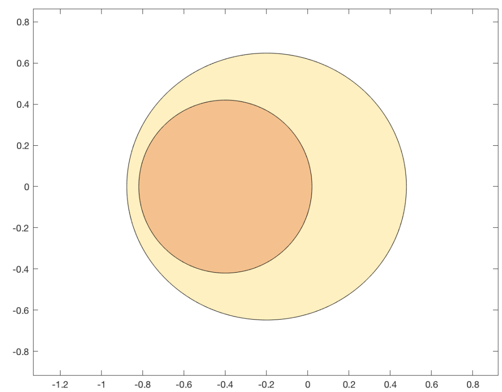

Figure 7: $\mu = \lambda = -2/5$. The numerical range and maximal numerical range are both circular discs.

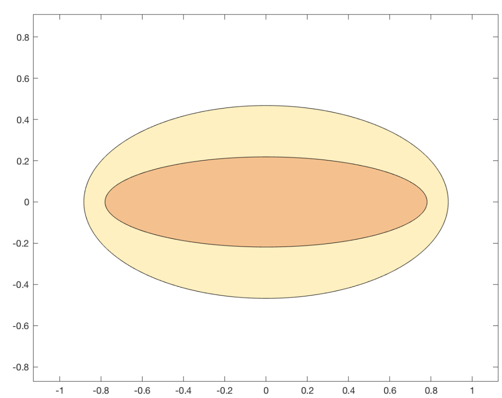

Figure 8: $\mu = -\lambda = 3/4$. The numerical range and maximal numerical range are both elliptical discs.

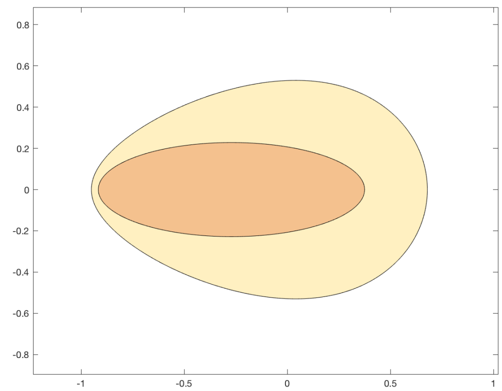

Figure 9: $\mu = 1/3, \lambda = -7/8$. The numerical range is an ovular disc, and the maximal numerical range is an elliptical disc.

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