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SHAPES AND COMPUTER GENERATION OF NUMERICAL RANGES OF KREIN SPACE OPERATORS*

CHI-KWONG LI† AND LEIBA RODMAN†

Dedicated to Hans Schneider on the occasion of his seventieth birthday.

Abstract. Let $(\mathcal{K}, \langle\cdot,\cdot\rangle)$ be a Hilbert space equipped with an indefinite inner product $[\cdot,\cdot]$. Then $(\mathcal{K}, [\cdot,\cdot])$ is a (complex) Krein space. One can define the Krein space numerical range of an operator A acting on $\mathcal{K}$ as the collection of complex numbers of the form $[Av, v]$ with $v \in \mathcal{K}$ satisfying $[v, v] = 1$. In this paper, the shapes of Krein space numerical ranges of operators in the complex plane using the joint numerical range of self-adjoint operators on $(\mathcal{K}, \langle\cdot,\cdot\rangle)$ are studied. Krein space numerical ranges of operators acting on a two-dimensional space are fully described. A Matlab program is developed to generate the sets in the finite dimensional case.

Key words. Indefinite inner product, Krein space, numerical range

AMS subject classifications. 15A60, 15A63.

1. Introduction. Let $(\mathcal{K}, \langle\cdot,\cdot\rangle)$ be a Hilbert space. Suppose S is an indefinite self-adjoint invertible operator acting on $(\mathcal{K}, \langle\cdot,\cdot\rangle)$. (All operators on $\mathcal{K}$ in our discussion are assumed to be linear and bounded with respect to $\langle\ \cdot\ ,\ \cdot\ \rangle$.) Then $\mathcal{K}$ can be viewed as a (complex) Krein space with respect to the indefinite inner product $[u, v] = \langle Su, v\rangle$. For any operator A acting on $\mathcal{K}$, the *Krein space numerical range* of A (with respect to $[\cdot,\cdot]$) is defined by

$$W_S^+(A) = \{[Av, v] :\ v \in \mathcal{K},\ [v, v] = 1\}.$$

This is a generalization of the (*classical*) *numerical range* of A defined by

$$W(A) = \{\langle Av, v\rangle :\ v \in \mathcal{K},\ \langle v, v\rangle = 1\}.$$

The classical numerical range has been studied extensively, and there are many results concerning the interplay between the algebraic and analytic properties of an operator and the geometrical properties of its numerical range. Likewise, there is substantial interest in studying these relations for Krein space operators; see, e.g., [B, LR, LTU, S]. It is worthwhile to mention that the more symmetrically defined set

$$W_S(A) = \{[Av, v]/[v, v] :\ v \in \mathcal{K},\ [v, v] \neq 0\},$$

has also been studied [LTU,S], especially in connection with the spectral containment property. One easily checks that

$$W_S(A) = W_S^+(A) \cup -W_{(-S)}^+(A).$$

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†Department of Mathematics, College of William and Mary, Williamsburg, P.O. Box 8795, VA 23187-8795 (ckli@math.wm.edu, lxrodm@math.wm.edu). Research of both authors was supported by NSF.

Thus, one can focus on $W_S^+(A)$ in studying the geometrical shape of $W_S(A)$.

In contrast with the classical numerical range $W(A)$, the set $W_S^+(A)$ is generally neither bounded nor closed, even when $\mathcal{K}$ is finite dimensional. Nonetheless, it is convex; see [B,LTU].

In this paper we use the approach of [LTU], namely, relate the Krein space numerical range of A and the *joint numerical range* of (H, G, S), where $H = (SA + A^*S)/2$ and $G = (SA - A^*S)/(2i)$, defined by

$$W(H, G, S) = \{(\langle Hv, v\rangle, \langle Gv, v\rangle, \langle Sv, v\rangle) \in \mathbb{R}^3 : \ v \in \mathcal{K}, \ \langle v, v\rangle = 1\}.$$

Here A^* denotes the adjoint operator of A, i.e., $\langle Au, v\rangle = \langle u, A^*v\rangle$ for all $u, v \in \mathcal{K}$. It is known [AT] that $W(H, G, S)$ is always convex if dim $\mathcal{K} > 2$, and is the surface of an (possibly degenerate) ellipsoid if dim $\mathcal{K} = 2$. Let

$$\begin{aligned} K(H, G, S) &= \bigcup_{\alpha \geq 0} \alpha W(H, G, S) \\ &= \{(\langle Hv, v\rangle, \langle Gv, v\rangle, \langle Sv, v\rangle) \in \mathbb{R}^3 : \ v \in \mathcal{K}\} \end{aligned}$$

be the convex cone generated by $W(H, G, S)$. The connection with Krein space numerical ranges is given by

Proposition 1.1. *Let $A : \mathcal{K} \to \mathcal{K}$ be an operator, and let $SA = H + iG$, where $H = (SA + A^*S)/2$ and $G = (SA - A^*S)/(2i)$. Then*

$$x + iy \in W_S^+(A) \Longleftrightarrow (x, y, 1) \in K(H, G, S).$$

For instance, one easily deduces from this proposition the result in [B] that $W_S^+(A)$ is always convex. Proposition 1.1 was used extensively in [LTU] and [S], and we shall further exploit it in this paper. In particular, we use it to determine the conditions on A so that $W_S^+(A)$ is a half space or contained in a line. A Matlab program is developed to generate Krein space numerical ranges for finite dimensional operators. Since the Krein space numerical range is not bounded in general, it is difficult to get an accurate computer plot. On the contrary, $W(H, G, S)$ is always compact for finite dimensional operators, and is easy to generate using computer programs (cf. Section 4). In view of this, many of our results include equivalent conditions stated in terms of $W(H, G, S)$. Furthermore, the results will be stated for both finite dimensional and infinite dimensional Krein spaces whenever possible. Also, we describe in full detail the Krein space numerical range of a 2×2 matrix in Section 3.

Throughout our paper we fix an operator $A : \mathcal{K} \to \mathcal{K}$, and let $SA = H + iG$, where $H = (SA + A^*S)/2$ and $G = (SA - A^*S)/(2i)$.

In our subsequent discussion we often apply the following transformations that preserve the shape of Krein space numerical ranges.

Proposition 1.2.
(i) *If an operator T is invertible, then $W_{T^*ST}^+(T^{-1}AT) = W_S^+(A)$.*
(ii) *$W_S^+(A + \mu I) = W_S^+(A) + \mu$ for any $\mu \in \mathbb{C}$.*
(iii) *Let $H' = aH + bG$, $G' = cH + dG$, where the numbers a, b, c, d are real and the 2×2*

matrix $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$ *is invertible, and let* $A' = S^{-1}(H' + iG')$. *Then* $\tilde{x} + i\tilde{y} \in W_S^+(A')$ *if and only if* $\begin{bmatrix} \tilde{x} \\ \tilde{y} \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$ *for some* $x + iy \in W_S^+(A)$.

Proposition 1.2 can be easily verified with the help of Proposition 1.1. We remark that by Proposition 1.2, one can apply suitable affine transforms to $W_S^+(A)$ to simplify the statements of results and proofs substantially. In particular, if one identifies $\mathbb{C}$ with $\mathbb{R}^2$, then

$$W_S^+(A' + \mu I) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} W_S^+(A) + \begin{bmatrix} \operatorname{Re}\mu \\ \operatorname{Im}\mu \end{bmatrix},$$

where A', μ, etc. satisfy conditions (ii) and (iii) of Proposition 1.2, and $\operatorname{Re}\mu$ and $\operatorname{Im}\mu$ are the real and imaginary parts of μ.

2. Numerical Ranges with Special Shapes. It is well known that the classical numerical range $W(A)$ of an operator A is a singleton if and only if A is a scalar operator; $W(A) \subseteq \mathbb{R}$ if and only if A is self-adjoint. Similar studies have been carried out for the Krein space numerical range. We summarize and refine below some results in this direction. We start with the following proposition.

PROPOSITION 2.1. *Let A be an operator acting on $\mathcal{K}$. Then $W_S^+(A) = \{\lambda\}$ if and only if $A = \lambda I$. Moreover, if $W_S^+(A)$ is not a singleton, then $W_S^+(A)$ is unbounded.*

This is a particular case of Theorem 2.3 of [LR]; see also [LTU, Theorem 2.3]. It is known that $W_S^+(A) \subseteq \mathbb{R}$ if and only if A is S-self-adjoint, i.e., $SA = A^*S$. The case when $W_S^+(A)$ is a line under the assumption that $W_S^+(A)$ is the intersection of half spaces was discussed in [LR, Theorem 4.1]. More generally, we have the following result.

THEOREM 2.2. *Suppose $SA = H + iG$ and $A \neq \lambda I$ for any $\lambda \in \mathbb{C}$. The following conditions are equivalent.*
(a) *$W_S^+(A)$ is a subset of a line.*
(b) *$W(H, G, S)$ is contained in a two dimensional subspace.*
(c) *H, G, S are linearly dependent.*
(d) *There exist a nonzero $\mu \in \mathbb{C}$ and $\eta \in \{0, 1\}$ such that the matrix $B = \mu A - i\eta I$ is S-self-adjoint), i.e., $SB = B^*S$.*
Moreover, if one (and therefore all) of (a) - (d) *holds, then one of the two mutually exclusive alternatives occurs for the matrix B satisfying condition* (d)*:*
(i) *There exists $\nu \in \mathbb{R}$ such that $\nu S + SB$ is either positive semidefinite or negative semidefinite, and $W_S^+(A)$ is a half line, which may or may not contain its endpoint.*
(ii) *The operator $\nu S + SB$ is indefinite for any $\nu \in \mathbb{R}$, and $W_S^+(A)$ is a line.*

Proof. Since A is not a scalar operator, $H + iG$ is not a multiple of S. Clearly, $W_S^+(A)$ is a subset of a line if and only if $W(H, G, S)$ belongs to a two dimensional subspace of $\mathbb{R}^3$. The latter condition is equivalent to the fact that H, G, S are linearly dependent. Thus, (a), (b) and (c) are equivalent.

Evidently, condition (d) implies condition (a). Now, if (c) holds, then there exists a nonzero vector $(a, b, c) \in \mathbb{R}^3$ such that $ax + by + cz = 0$ for all $(x, y, z) \in W(H, G, S)$. It follows that $\langle (aH + bG + cS)v, v \rangle = 0$ for all unit vectors $v \in \mathcal{K}$, and hence

$aH + bG + cS = 0$. If $c = 0$, let $\mu = (b + ia)$, $\eta = 0$, and $B = S^{-1}(bH - aG)$. If $c \neq 0$, let $\mu = -c(b + ia) \neq 0$, $\eta = 1$, and $B = -S^{-1}(bH - aG)/c$. In both cases, we have $B = \mu A - i\eta I$ as asserted.

To prove that either (i) or (ii) holds, we may apply a suitable affine transformation to A (cf. Proposition 1.2) and assume that $A = B$, where B is S-self-adjoint. Then $W_S^+(A)$ is just the intersection of the sets

$$\{(x, 0, z) : x + iz \in \alpha W(SB + iS),\ \ \alpha \geq 0\} \cap \{(x, y, 1) : x, y \in \mathbb{R}\}.$$

It is then clear that (i) or (ii) holds depending on whether 0 belongs to the closure or to the exterior of $W(SB + iS)$, or equivalently, whether or not there exist $a, b \in \mathbb{R}$ such that $aS + bSB$ is semidefinite. Since S is indefinite, it suffices to check whether or not there exists an $a \in \mathbb{R}$ such that $aS + SB$ is semidefinite. □

If $W_S^+(A)$ is a subset of a line (and not a point), the line can be easily identified. Indeed, if μ, η and B are defined as in Theorem 2.2(d), then for every vector v such that $\langle Sv, v\rangle = 1$ we have

$$\langle Hv, v\rangle = (\operatorname{Re}\mu)\ \langle SBv, v\rangle\ -\ \eta(\operatorname{Im}\mu), \qquad \langle Gv, v\rangle = (\operatorname{Im}\mu)\langle SBv, v\rangle\ +\ \eta(\operatorname{Re}\mu).$$

Eliminating $\langle SBv, v\rangle$ from these equations, we obtain the equation of the line that contains $W_S^+(A)$, namely

$$(\operatorname{Im}\mu)x - (\operatorname{Re}\mu)y + \eta|\mu|^2 = 0.$$

Note that checking computationally whether there exists $\nu \in \mathbb{R}$ such that $\nu S + SB$ is positive semidefinite can be reduced to checking whether 0 is the solution of the following optimization problem.

$$\sup_{\nu \in \mathbb{R}} \inf \sigma(\nu S + SB),$$

where $\sigma(X)$ denotes the spectrum of X. In the finite dimensional case, there are standard optimization packages for solving this problem; see [FNO].

In case condition (i) in the above theorem holds, one may ask whether the endpoint of the half line belongs to $W_S^+(A)$. One easily sees from our proof that
(1) $W_S^+(A)$ is a half line without the endpoint if and only if $W(H, G, S)$ is properly contained in a 2-dimensional plane and no support line of the convex hull of $W(H, G, S)$ passing through the origin contains a point $(x, y, z) \in W(H, G, S)$ with $z > 0$.
(2) $W_S^+(A)$ is a half line with the endpoint if and only if $W(H, G, S)$ is properly contained in a 2-dimensional plane and there is a support line of the convex hull of $W(H, G, S)$ that passes through the origin and contains a point $(x, y, z) \in W(H, G, S)$ with $z > 0$.

For example, if $SA = H + iG$ are such that

$$S = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},\ H = 0_2,\ G = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

then $W_S^+(A) = \{iy : y > 0\}$; if $SA = H + iG$ are such that

$$S = [1] \oplus \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \; H = 0_3, \; G = [0] \oplus \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

then $W_S^+(A) = \{iy : y \geq 0\}$.

Holtz and Strauss [HS] raised the question of studying those A for which $W_S^+(A)$ is a half plane. We have the following answer.

THEOREM 2.3. *Suppose $SA = H + iG$. The following conditions are equivalent.*
(a) *$W_S^+(A)$ is a half plane, with or without some of its boundary points.*
(b) *The set $W(H, G, S)$ is not contained in a two dimensional subspace, the origin of $\mathbb{R}^3$ lies on its boundary, and there is a unique support plane of $W(H, G, S)$ passing through the origin.*
(c) *The operators H, G, S are linearly independent, and there is a unique unit vector $(a, b, c) \in \mathbb{R}^3$ satisfying the equation*

$$\sup_{\alpha,\beta,\gamma\in\mathbb{R}} \inf \sigma(\alpha H + \beta G + \gamma S) = \inf \sigma(aH + bG + cS) = 0.$$

If one (and therefore all) of (a) - (c) *holds, and if $(a, b, c) \in \mathbb{R}^3$ satisfies condition* (c)*, then the interior of $W_S^+(A)$ coincides with the open half plane $\{(x, y) \in \mathbb{R}^2 : ax + by + c > 0\}$.*

Proof. Clearly, (b) and (c) are equivalent, and each condition implies (a). Suppose (a) holds. Then $W(H, G, S)$ cannot lie in a two dimensional subspace. Otherwise, $W(H, G, S)$ will be a subset of a line by Theorem 2.2. Also, 0 cannot be in the interior of $W(H, G, S)$. Otherwise, $W_S^+(A) = \mathbb{C}$. Also, 0 cannot be in the exterior of $W(H, G, S)$. Otherwise, $K(H, G, S)$ will be a pointed cone in $\mathbb{R}^3$ and its intersection with $\{(x, y, 1) : x, y \in \mathbb{R}\}$ will not be a half plane. Suppose there are two support planes of $W(H, G, S)$ at 0. They must intersect at a line on the (x, y)-plane. Otherwise, the two planes and $\{(x, y, 1) : \; x, y \in \mathbb{R}\}$ will intersect at a sharp point, and $W_S^+(A)$ will not be a half plane. Apply a rotation to the (x, y)-plane, we may assume that the two support planes intersect at the x-axis. Then $W(G + iS)$ lies on the (y, z)-plane and has a sharp point at $(0, 0)$. In other words, there are infinitely many support lines of the convex set $W(G + iS)$ at 0. By a theorem of Hildebrandt [H], 0 belongs to the approximate spectrum of $G + iS$, i.e., there exists a sequence $\{w_n\}_{n=1}^\infty$ of unit vectors (in the sense of $\langle \cdot, \cdot \rangle$) of $\mathcal{K}$ such that $\lim_{n\to\infty}(G + iS)w_n = 0$. Since 0 is a boundary point of $W(G + iS)$, there is a non-trivial real linear combination $aG + bS$ of G and S such that the resulting operator is positive semidefinite. Now

$$2\langle Gw_n, w_n\rangle = \langle (G + iS)w_n, w_n\rangle + \langle (G + iS)^* w_n, w_n\rangle \to 0,$$

and similarly $\langle Sw_n, w_n\rangle \to 0$. By the positive semidefiniteness of $aG + bS$, it follows that $(aG + bS)w_n \to 0$, and combining with the property $(G + iS)w_n \to 0$, we obtain $Sw_n \to 0$, a contradiction with the invertibility of S. Thus, there can only be one support plane of $W(H, G, S)$ at 0. ▯

There still remains a question concerning the situation when $W_S^+(A)$ is a half plane: What part of the boundary of the half plane belongs to $W_S^+(A)$? Denote by T

the set of boundary points of $W_S^+(A)$ lying in $W_S^+(A)$. Let $(a,b,c) \in \mathbb{R}^3$ be the unique unit vector of Theorem 2.3(c). Then $(x,y) \in T$ if and only if $(x,y) = (\langle Hv, v\rangle, \langle Gv, v\rangle)$ for some $v \in \mathcal{K}$ such that $\langle Sv, v\rangle = 1$ and $a\langle Hv, v\rangle + b\langle Gv, v\rangle + c\langle Sv, v\rangle = 0$. By Theorem 2.3(c), such vectors v necessarily belong to

$$\mathcal{L} \stackrel{\text{def}}{=} \text{Ker } (aH + bG + cS).$$

Now several situations are possible. If S is negative semidefinite on $\mathcal{L}$, then obviously $T = \emptyset$. If S is positive semidefinite and invertible on $\mathcal{L}$, then T is essentially the classical numerical range of $H + iG$ with respect to the positive definite scalar product induced by S on $\mathcal{L}$, and therefore T is a closed bounded line segment, perhaps degenerated to a point. If the restriction of S on $\mathcal{L}$ is indefinite but invertible, then by Theorem 2.2 T is either a line or a half line with or without the endpoint (unless $H + iG$ is a scalar multiple of S on $\mathcal{L}$). Finally, T being a convex subset of a straight line, it is possible for T to be a bounded segment without one or both endpoints. We illustrate in the following examples that all these cases can indeed occur.

Examples. In the seven examples below, the vector (a,b,c) of Theorem 2.3(c) is $(a,b,c) = (1,0,0)$. Let $X = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, $Y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$, and $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. Then

(1) $T = \emptyset$ if $S = Z$ and $SA = X + iY$;
(2) $T = \{0\}$ if $S = [1] \oplus Z$ and $SA = ([0] \oplus X) + i([0] \oplus Y)$;
(3) $T = \{0 + iy : y \in [0,1]\}$ if $S = I_2 \oplus Z$ and $SA = (0_2 \oplus X) + i(\text{diag}(0,1) \oplus Y)$;
(4) $T = \{0+iy : y \in (0,1]\}$ if $S = Z \oplus I$ and $SA = (X \oplus 0) + i(Y \oplus \text{diag}(1, 1/2, 1/3, \ldots))$;
(5) $T = \{0 + iy : y \geq 0\}$ if $S = Z \oplus Z$ and $SA = (X \oplus 0_2) + i(Y \oplus \text{diag}(0,1))$;
(6) $T = \{0 + iy : y > 0\}$ if $S = Z \oplus Z \oplus I$ and $SA = (X \oplus 0_2 \oplus 0) + i(Y \oplus Z \oplus \text{diag}(1, 1/2, 1/3, \ldots))$;
(7) $T = \{0+iy : y \in \mathbb{R}\}$ if $S = Z \oplus Z \oplus Z$ and $SA = (X \oplus 0_4) + i(Y \oplus \text{diag}(0,1,0,-1))$.

One can easily modify Example (4) so that T is a line segment without endpoints on both ends. Moreover, in each example one can apply a suitable affine transformation to A so that the boundary of $W_S^+(A)$ lies on any prescribed straight line.

We note also the following easily verified fact.

Proposition 2.4. *Let $A \in \mathcal{K}$. The following conditions are equivalent.*
(a) $W_S^+(A) = \mathbb{C}$.
(b) $\alpha H + \beta G + \gamma S$ *is indefinite for every unit vector* $(\alpha, \beta, \gamma) \in \mathbb{R}^3$.
(c) *The convex hull of* $W(H,G,S)$ *has non-empty interior containing the origin.*

Indeed, the indefiniteness of $\alpha H + \beta G + \gamma S$ for every unit vector $(\alpha,\beta,\gamma) \in \mathbb{R}^3$ means that no support plane of $W(H,G,S)$ passes through the origin, i.e., the origin is an interior point of the convex hull of $W(H,G,S)$. Then $W_S^+(A) = \mathbb{C}$ by Proposition 1.1. Conversely, if $W_S^+(A) = \mathbb{C}$, then $K(H,G,S) \supseteq \{(x,y,z) \in \mathbb{R}^3 : z > 0\}$. Since S is indefinite, there exists $(x_0, y_0, -1) \in K(H,G,S)$. Now the convexity of $K(H,G,S)$ guarantees that $K(H,G,S) = \mathbb{R}^3$ which implies the indefiniteness of $\alpha H + \beta G + \gamma S$ for every unit vector $(\alpha,\beta,\gamma) \in \mathbb{R}^3$.

It is known that $W(A)$ is closed and polygonal (the boundary of $W(A)$ is a convex polygon) if and only if A is unitarily similar to $B \oplus C$, where B is a normal operator whose spectrum is finite and consists of the vertices of the polygon, and where $W(C) \subseteq W(B) \setminus \sigma(B)$. In the infinite dimensional case this result is obtained by using the fact that the eigenvectors of A corresponding to a sharp point of the boundary of $W(A)$ form a subspace which is invariant for A^* as well (it was proved in [D] that sharp points of the boundary of $W(A)$ are indeed eigenvalues of A, see [LR] and [S] for a Krein space generalization of this fact). Finite dimensional accounts of the characterization of the polygonal property of $W(A)$ are found in [GL, Section III.10], [HJ]. Recently, [S] extended this result to the Krein space operators. Note that one has to use information on both $W_S^+(A)$ and $W_{(-S)}^+(A)$ to get the desired generalization.

3. Small Matrices. One important result in the classical numerical range is the elliptical range theorem asserting that the numerical range of a 2×2 matrix A with eigenvalues λ_1 and λ_2 is an elliptical disk with foci λ_1 and λ_2, and with the length of minor axis equal to $\sqrt{\operatorname{tr}(A^*A) - |\lambda_1|^2 - |\lambda_2|^2}$. In this section, we give a detailed description of Krein space numerical ranges of 2×2 matrices. In particular, it is shown that except for the degenerate cases when $W_S^+(A)$ is a subset of a line, the whole complex plane or a half plane, it is always bounded by a branch of a hyperbola. There has also been considerable interest (see [KRS] and its references) in studying the shape of $W(A)$ for A acting on higher dimensional space, but the description is more complicated. We expect that the results on $W_S^+(A)$ are complicated as well. In any event, using the algorithm and the program in the next two sections, one can get a computer plot for $W_S^+(A)$ for any matrix A of reasonable size.

Assume in this section that S and $A = S^{-1}(H + iG)$ are 2×2 matrices, and as before S is indefinite and invertible and S, H, G are Hermitian. Whenever convenient, we apply a suitable transformation described in Proposition 1.2.

Using Proposition 1.2(i), by applying simultaneous congruence

$$(S, H, G) \mapsto (T^*ST, T^*HT, T^*GT)$$

with a suitable invertible T, we can assume that one of the following three cases holds (here the canonical form of two Hermitian matrices under simultaneous similarity is used; see, e.g., [T]).

(α)

$$S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad H = \begin{bmatrix} 0 & \lambda \\ \lambda & \pm 1 \end{bmatrix},$$

where λ is a real number.

(β)

$$S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad H = \begin{bmatrix} 0 & \lambda + i\mu \\ \lambda - i\mu & 0 \end{bmatrix},$$

where λ and μ are real and $\mu \neq 0$.

(γ)

$$S = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad H = \begin{bmatrix} \lambda & 0 \\ 0 & \mu \end{bmatrix},$$

where λ and μ are real.

Consider the case (α). Applying a suitable affine transformation (described in Proposition 1.2(ii) and (iii)), we may assume that

$$S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad H = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \qquad G = \begin{bmatrix} g & i\lambda \\ -i\lambda & 0 \end{bmatrix},$$

for some real numbers g and λ. If $g = 0$, then Theorem 2.3(iii) holds, and $W_S^+(A)$ is a half plane. So assume $g \neq 0$, and then by scaling G we set $g = 1$. Every $v \in \mathbb{C}^2$ can be brought to the form

$$v = \begin{bmatrix} a + ib \\ c \end{bmatrix} \tag{1}$$

for some real a, b, c, using a multiplication by a unimodular complex number. We will therefore consider only vectors v in this form for constructing the set $W_S^+(A)$. A calculation shows that $\langle Sv, v\rangle = 1$ if and only if $2ac = 1$. Furthermore, assuming $\langle Sv, v\rangle = 1$, we have

$$(\langle Hv, v\rangle, \langle Gv, v\rangle) = (c^2, a^2 + b^2 + 2\lambda bc) = (c^2, \frac{1}{4c^2} + (b + \lambda c)^2 - \lambda^2 c^2). \tag{2}$$

It is clear from (2) that $W_S^+(A)$ is bounded by the branch of the hyperbola $\{(x, \frac{1}{4x} - \lambda^2 x) : x > 0\}$ (where we put $x = c^2$). The equation of this hyperbola in the (x, y)-coordinates is $\lambda^2 x^2 + xy = \frac{1}{4}$, and it has the asymptotes $x = 0$ and $y = -\lambda^2 x$.

Consider now the case (β). Applying a suitable affine transformation, we assume that $\lambda = 0$ and that G is of the form $G = \begin{bmatrix} p & 0 \\ 0 & q \end{bmatrix}$, where p, q are real. If $pq < 0$, then $W_S^+(A) = \mathbb{C}$ by Proposition 2.4. If $pq = 0$, then $W_S^+(A)$ is a half plane by Theorem 2.4. So we assume in the sequel that $pq > 0$, and then by scaling G we let $p = 1$ (and $q > 0$). Consider the vectors v of the form $v = \begin{bmatrix} c \\ a + bi \end{bmatrix}$, where a, b, c are real. The condition $\langle Sv, v\rangle = 1$ amounts to $2ac = 1$. A calculation gives

$$(\langle Hv, v\rangle, \langle Gv, v\rangle) = (-2\mu bc, c^2 + q(a^2 + b^2)).$$

Fix $x = -2\lambda bc$, and let $y = c^2 + q(a^2 + b^2)$. Then, by using the equality $2ac = 1$, we obtain:

$$y = c^2 + \frac{q}{4c^2} + \frac{qx^2}{4\lambda^2 c^2} = c^2 + \frac{(\lambda^2 + x^2)q}{4\lambda^2 c^2}. \tag{3}$$

When c varies over the set of nonzero real numbers, the right hand side of (3) is bounded below by $\sqrt{(\lambda^2 + x^2)q\lambda^{-2}}$; this value is achieved for

$$c^2 = \sqrt{\frac{(\lambda^2 + x^2)q}{4\lambda^2}}.$$

Thus, $W_S^+(A)$ is bounded by the branch of the hyperbola

$$\{(x,y) : y^2 = q + \lambda^{-2}qx^2,\ y > 0\}.$$

Finally, consider case (γ). We assume that H, S, G are linearly independent (otherwise Theorem 2.2 applies and $W_S^+(A)$ is contained in a line). Using the affine transformation of Proposition 1.2(i), we further assume that

$$S = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad H = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \qquad G = \begin{bmatrix} 0 & \lambda + i\mu \\ \lambda - i\mu & 0 \end{bmatrix},$$

where $\lambda, \mu \in \mathbb{R}$ and $\lambda^2 + \mu^2 = 1$. Consider vectors v of the form (1) such that $\langle Sv, v\rangle = 1$, i.e., $a^2 + b^2 - c^2 = 1$. For such vectors v,

$$(\langle Hv, v\rangle, \langle Gv, v\rangle) = (c^2, 2c(\lambda a + \mu b)). \tag{4}$$

Moreover, the expression $(\lambda a + \mu b)^2$ is bounded above by $1 + c^2$ if a and b are variable real numbers subject to the condition $a^2 + b^2 - c^2 = 1$. Thus, letting $x = c^2$, formula (4) shows that $W_S^+(A)$ is bounded by the branch of the hyperbola

$$\{(x,y) \in \mathbb{R}^2 : y^2 = 4x(1+x),\ x \geq 0\}.$$

As mentioned before, for a 2×2 matrix A, as long as $W_S^+(A)$ is not contained in a line and is not the whole complex plane or a half plane, the set $W_S^+(A)$ is bounded by a branch of a hyperbola and contains its boundary. Also, for a 2×2 matrix A, if $W_S^+(A)$ is a half plane, it cannot contain any points on its boundary. (This explains why Krein spaces of dimensions bigger than two are needed in Examples (2)-(7).) Indeed, in this case for $W_S^+(A)$ to have points on the boundary it is necessary that

$$\mathcal{L} = \text{Ker } (aH + bG + cS) \neq \{0\}$$

for some unit vector $(a,b,c) \in \mathbb{R}$ such that $aH + bG + cS$ is positive semidefinite, and that S is not negative semidefinite on $\mathcal{L}$ (cf. the discussion after the proof of Theorem 2.3). Assuming these necessary conditions, and assuming $\mathcal{L} \neq \mathbb{R}^2$ (otherwise $W_S^+(A)$ is contained in a straight line by Theorem 2.2 contrary to the hypotheses), we see that $\mathcal{L}$ is one-dimensional. Now with respect to an orthonormal basis in $\mathbb{R}^2$ formed by vectors $v_1 \in \mathcal{L} \setminus \{0\}$ and v_2, we have

$$aH + bG + cS = \begin{bmatrix} 0 & 0 \\ 0 & x \end{bmatrix}, \qquad S = \begin{bmatrix} y & z \\ \overline{z} & w \end{bmatrix},$$

where x and y are positive. But then it is easy to see that $aH + bG + (c+\alpha)S$ is positive definite for small positive values of α, a contradiction with Theorem 2.3(c).

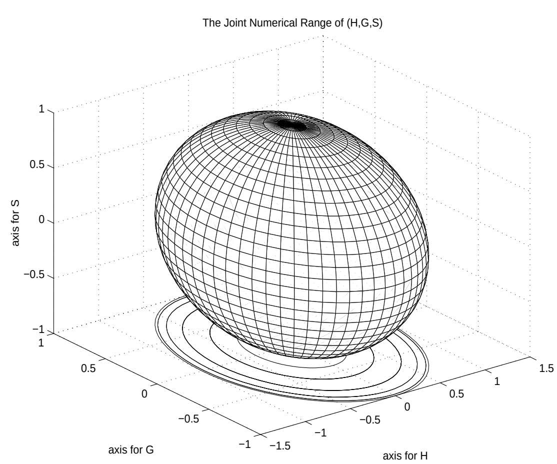
Here we describe a more geometric approach to the problem of Krein space numerical ranges for 2×2 matrices, without relying so much on the canonical forms. Assume that H, G, S are not linearly dependent. Then, by Theorem 2.2, $W_S^+(A)$ is not contained in a line. We focus on the case when 0 is in the exterior of $W(H,G,S)$ (otherwise, $W_S^+(A)$ is either a half plane or the whole plane). Then, there exist

$a, b, c \in \mathbb{R}$ with $a^2 + b^2 \neq 0$ such that $\tilde{H} = aH + bG + cS > 0$. Apply a suitable affine transform as described in Proposition 1.2 (ii) and (iii) and consider $W_S^+(A')$ instead of the original problem, where $SA' = \tilde{H} + i\tilde{G}$. Now, applying a suitable simultaneous congruence $X \mapsto \tilde{H}^{-1/2} X \tilde{H}^{-1/2}$ to the triple $(\tilde{H}, \tilde{G}, S)$, we get (I, G', S'). One can then compute the elliptical disk $W(I, G', S') = \{(1, y, z) : y + iz \in W(G' + iS')\}$. It is now easy to generate the set $K(I, G', S')$ and intersect it with $\{(x, y, 1) : x, y \in \mathbb{R}\}$ to obtain $W_S^+(A')$. Once we get $W_S^+(A')$, the set $W_S^+(A)$ can be easily obtained by using Proposition 1.2.

4. Algorithm and Examples. Algorithms and computer programs for generating the classical numerical range and its generalizations have been extensively studied in the literature; see, e.g., [J,MP,LN,LST,V]. In this section, we describe an algorithm for generating the Krein space numerical range.

For the classical numerical range (or a certain convex generalized numerical range), it is not difficult to find equations of its supporting lines. As a result, one can try to plot supporting lines in different directions, and use the intersection of the half spaces defined by these lines to approximate the (generalized) numerical range; see [J, LST]. Although the Krein space numerical range $W_S^+(A)$ is convex, it is not easy to determine its supporting lines. Thus, it is difficult to use this approach.

FIGURE 1



Another approach (see [MP]) is to generate certain subsets of the numerical range and show that these subsets can fill up the interior of the numerical range “efficiently”. However, since $W_S^+(A)$ is very often unbounded, it is difficult to fill up the its interior efficiently.

In our study, we connect the Krein space numerical range of A with the joint numerical range of (H, G, S) with $SA = H + iG$. We take the same approach to develop an algorithm for plotting the Krein space numerical range.

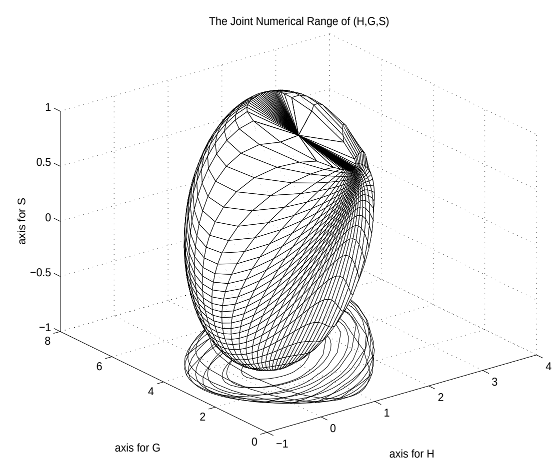
An algorithm for generating $W(H, G, S)$ has been described in [LN]. The basic idea was to compute the boundary point of the compact set $W(H, G, S)$ in each direction determined by a grid point on the unit sphere in $\mathbb{R}^3$. One then joints all these boundary points to form a polyhedron inside $W(H, G, S)$. After generating $W(H, G, S)$, one can collect the points $(x/z, y/z)$, where $(x, y, z) \in W(H, G, S)$ with $z > 0$. The collection of these points will be an approximation for $W_S^+(A)$. This approach allows us to get around the problem of computing supporting lines of $W_S^+(A)$. However, since the process involve the computations x/z and y/z, where z may be very small, the algorithm is not stable numerically. There is definitely room for improvement.

We describe the algorithm below. Matlab programs have been written to generate the joint numerical range and the Krein space numerical range. The programs are listed in the next section, and are also available at the following websites.

http://www.math.wm.edu/˜ckli/wjoint.html and

http://www.math.wm.edu/˜ckli/krein.html, respectively.

FIGURE 2



We first present an algorithm developed in [LN] for generating the *joint numerical range* of the hermitian matrix triple (H, G, S):

Step 1. Construct a grid on the unit sphere in $\mathbb{R}^3$ using the spherical coordinates

$$(\sin r \cos t, \sin r \sin t, \cos r),$$

with

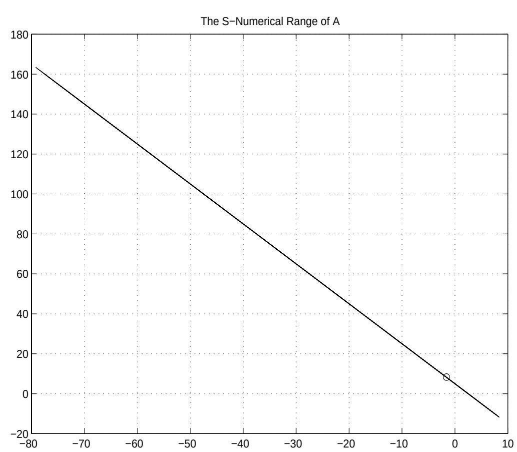
$$r = \pi/m, 2\pi/m, 3\pi/m, \ldots, \pi, \quad \text{and} \quad t = \pi/m, 2\pi/m, 3\pi/m, \ldots, 2\pi,$$

for some positive integer m.
Step 2. For each choice of $(\alpha, \beta, \gamma) = (\sin r \cos t, \sin r \sin t, \cos r)$, compute the largest eigenvalue d of of the matrix $\alpha H + \beta G + \gamma S$. Then for any $(a, b, c) \in W(H, G, S)$, we have $\alpha a + \beta b + \gamma c \le d$, i.e.,

$$P = \{(a, b, c) : \alpha a + \beta b + \gamma c = d\}$$

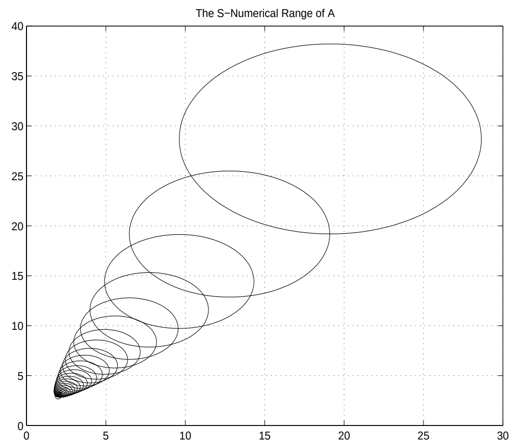
is a support plane for $W(H, G, S)$.
Step 3. For each triple (α, β, γ) in Step 2, compute a unit eigenvector v corresponding to the eigenvalue d of the matrix $\alpha H + \beta G + \gamma S$, and use $(\langle Hv, v\rangle, \langle Gv, v\rangle, \langle Sv, v\rangle)$ as a vertex. The convex hull of these vertices will be an inner polygonal region contained in $W(H, G, S)$.

FIGURE 3



We generated the pictures of $W(H, G, S)$ for
(1) $(H, G, S) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$; see Figure 1, and

FIGURE 4



(2) $(H,G,S) = (\operatorname{Re} A, \operatorname{Im} A, D)$ for some randomly generated 3×3 matrix A and $D = \operatorname{diag}(1,1,-1)$; see Figure 2.

We remark that if the largest or the smallest eiganvalue of any one of the three hermitian matrices has multiplicity larger than one, then the boundary of their joint numerical range has a flat surface parallel to a coordinate plane. For example, the top part of the picture of (2) is flat because S has a repeated largest eigenvalue.

Now to compute an approximation of $W_S^+(A)$, set $SA = H + iG$ and modify Step 3 to the following.

Step 3'. For each (α,β,γ) triple in Step 2, compute the unit eigenvector v corresponding to the eigenvalue d of the matrix $\alpha H + \beta G + \gamma S$, and evaluate

$$(\langle Hv,v\rangle, \langle Gv,v\rangle)/\langle Sv,v\rangle,$$

if $\langle Sv,v\rangle > 0$.

Note that our algorithm and Matlab program actually work for singular S as well. Also, in our Matlab program, for each grid point in Step 2, we compute

$$(\langle Hv,v\rangle, \langle Gv,v\rangle)/\langle Sv,v\rangle,$$

whenever $\langle Sv,v\rangle > tol$, for some positive number tol that depends on the machine precision and how much of the unbounded region one wants to see. Our program is very good in testing whether the $W_S^+(A)$ is part of a straight line. For example, we use our program to generate $W_S^+(A)$ for

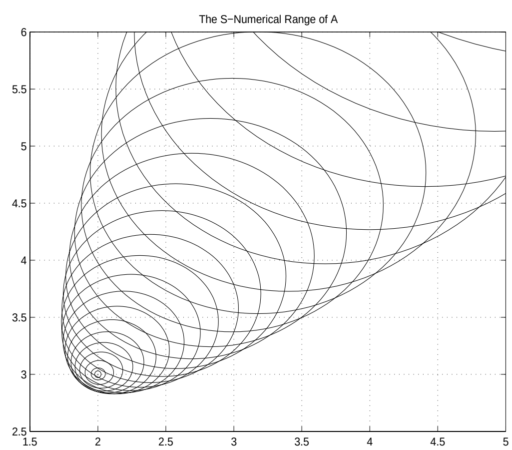
(3) $S = \text{diag}(1, 1, -1)$ and $A = (2 + i)(I + iSH)$, where H is a randomly generated 3×3 hermitian matrix; see Figure 3. The output is a straight line as expected (cf. Theorem 2.2).

If $W_S^+(A)$ is the whole complex plane, the picture $W_S^+(A)$ generated by our program can be quite chaotic. In such case one should check the corresponding joint numerical range $W(H, G, S)$ to see whether its convex hull has interior containing the origin. If this is teh case, then one can conclude that $W_S^+(A) = \mathbb{C}$ (cf. Proposition 2.4).

We also generated $W_S^+(A)$ for

(4) $S = \text{diag}(1, -1)$ and $A = S * B$ with $B = \begin{bmatrix} 2+3i & 2 \\ 0 & 2+3i \end{bmatrix}$; see Figure 4. It is an unbounded region bounded by a branch of hyperbola (cf. Section 3). One may also manually determine the ranges of the x and y axes to get more details of a certain part of the picture; see Figure 5.

FIGURE 5



5. Matlab Programs. We include the two Matlab programs for plotting the joint numerical range and the Krein space numerical range in what follows.

Matlab Program for plotting the joint numerical range of three Hermitian matrices.

```
%
% W(H,G,K,m), where H,G,K should be hermitian matrices of the same
%        size, and the program will evaluate 4m^2 boundary points
%        of the joint numerical range.
%
% This is used to plot the inside convex polytope of the joint
% numerical range of 3 hermitian matrices H, G, K.
%
function L = wjoint(H,G,K,m)
%
%
%
for r=1:(4*m+1)
              T = cos( (r-1)*pi/(2*m) )*H + sin( (r-1)*pi/(2*m) )*G;
   for s=1:(m+1)
     [U,D] = eig(sin( (s-1)*pi/(2*m) )*T + cos( (s-1)*pi/(2*m) )*K);
     [d1,t1] = max(real(diag(D)));
     u = U(:,t1);
     X(r,s)=real(u'*H*u);
     Y(r,s)=real(u'*G*u);
     Z(r,s)=real(u'*K*u);
     [d2,t2] = max(real(diag(-D)));
     v = U(:,t2);
     X(r,m+1+s)=real(v'*H*v);
     Y(r,m+1+s)=real(v'*G*v);
     Z(r,m+1+s)=real(v'*K*v);
   end
end
%
%
    meshc(X,Y,Z);
    title('The Joint Numerical Range of (H,G,K)');
    xlabel('axis for H');
    ylabel('axis for G');
    zlabel('axis for K');
%
```

Matlab Program for plotting the Krein space numerical range of a complex matrix.

```
%
% krein(S,A,m,tol), where S is the hermitian matrix that defines
%    the indefinite inner product, A is the Krein space operator,
%    4*m^2 is the number of boundary points (x,y,z) on W(H,G,S)
%    that the program evaluates, and tol > 0 is the lower limit
%    under which the program will compute a point (x/z, y/z) in the
%    Krein space numerical range.
%
%
function L = krein(K,A,m,d)
%
R = (K*A)/2;
H = R'+R;
G = (R-R')/i;
%
     [UU,DD] = eig(K);
     [dd,tt] = max(real(diag(DD)));
     uu = UU(:,tt);
     xx = real(uu'*H*uu)/dd;
     yy = real(uu'*G*uu)/dd;
%
% number of iterations and tolerance for the size of the z-coordinate
% are recorded as m and d, respectively
%
for r=1:(4*m+1)
              T = (cos((r-1)*pi/(2*m)))*H + (sin((r-1)*pi/(2*m)))*G;
 for s=1:(2*m)
  [U,D] = eig(sin( ((s-1)*pi)/(2*m) )*T + cos( ((s-1)*pi)/(2*m) )*K);
  [d1,t1] = max(real(diag(D)));
  u = U(:,t1);
  z1 = real(u'*K*u);  Z(r,s) = z1;
                  if z1 > d,
                      X(r,s)=real(u'*H*u)/z1;
                      Y(r,s)=real(u'*G*u)/z1;
                    else
                      X(r,s) = xx;
                      Y(r,s) = yy;
                    end
   end
end
%
%
      plot(xx,yy,'o',X,Y);
```

```
    title('The S-Numerical Range of A');
    grid;
%
```

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