Operators
and
Matrices
Volume 17, Number 3 (2023), 583–598 doi:10.7153/oam-2023-17-39

COMPUTING THE S–NUMERICAL RANGES OF DIFFERENTIAL OPERATORS

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(*Communicated by N.-C. Wong*)

Abstract. Following a number of recent studies of *S-numerical range*, we study the problem of computing the *S-numerical range* numerically for differential operators and block differential operators, particularly these of Sturm-Liouville type, Hain-Lüst type and Stokes type.

1. Introduction and definitions

Let $\mathcal{H}$ be an infinite dimensional Hilbert space with scalar product $(.,.)$ and associated norm $\|.\|$. Let $B(\mathcal{H})$ denote the algebra of all bounded linear operators on $\mathcal{H}$, then the numerical range of A in $B(\mathcal{H})$ is defined by

$$W(A) = \{(Ax,x) : x \in \mathcal{H} \text{ with } \|x\| = 1\}. \tag{1}$$

Thus the numerical range of an operator, like the spectrum, is a subset of the complex plane whose geometrical properties should say something about the operator.

Previous research has established that the numerical range is a convex set (Toeplitz-Hausdorf theorem) [18, 19], and, the spectrum contained in the closure of its numerical range. A review of the properties of $W(A)$ of operator matrices may be found in the book of Gustafson and Rao [12]. The theory of numerical ranges and its variations is rich and varied. A lot of recent research has been focused on the numerical ranges of operators on indefinite inner product spaces. For $n\times n$ complex matrices A and an $n\times n$ Hermitian matrix S, Li, Tsing and Uhlig [17] introduced the concepts of the S-numerical range of A by

$$W_S(A) = \left\{ \frac{(Ax,x)_S}{(x,x)_S} : x \in \mathbb{C}^n \text{ with } (x,x)_S \neq 0 \right\}, \tag{2}$$

where $(x,x)_S := x^\star Sx$. $W_S(A)$ is the union of the positive S-numerical range $W_S^+(A)$ and negative S-numerical range $W_S^-(A)$ which are defined respectively as:

$$W_S^+(A) = \left\{ \frac{(Ax,x)_S}{(x,x)_S} : x \in \mathbb{C}^n \text{ with } (x,x)_S > 0 \right\}, \tag{3}$$

Mathematics subject classification (2020): 65L15, 65L12, 34L15, 15A22, 47A12.
Keywords and phrases: Operator matrices, block operator matrices, *S-numerical range*, finite difference, Sturm-Liouville operator, Hain-Lüst operator, Stokes operator.

Paper OaM-17-39

and

$$W_S^-(A) = \left\{ \frac{(Ax,x)_S}{(x,x)_S} : x \in \mathbb{C}^n \text{ with } (x,x)_S < 0 \right\}. \tag{4}$$

It is well-known that [10, 11] each of the sets $W_S^+(A)$ and $W_S^-(A)$ are convex and in [17] it is shown that the S-numerical range is pseudo-convex for a special class of matrices. A non-empty subset Q of $\mathbb{R}^n$ is said to be pseudo-convex [17] if for any distinct $u,v \in Q$, either $\{\alpha u + (1-\alpha)v : \alpha \in [0,1]\} \subset Q$. or $\{\alpha u + (1-\alpha)v : \alpha \leqslant 0 \text{ or } \alpha \geqslant 1\} \subset Q$. The S-numerical range, although sharing some analogous properties with the classical numerical range, has a quite different behavior. Unlike $W(A)$, the S-numerical range is neither closed nor bounded [17, Section 2]. On the other hand $W_S(A)$, may not be convex [17].

Extending the definition in (2) for bounded linear operator A on an infinte dimensional Hilbert space H with a sesquilinear form $(u,v) \mapsto (u,v)_S := (Su,v)$, $u,v \in H$, where S is self-adjoint, one may define

$$W_S(A) = \left\{ \frac{(Ax,Sx)}{(Sx,x)} : x \in H \text{ with } (Sx,x) \neq 0 \right\}, \tag{5}$$

and define $W_S^+(A)$ and $W_S^+(A)$ analogously. A review of the properties of $W_S(A)$ of bounded operator matrices may be found in [17, Section 4]. The numerical range and its generalization is a very useful tool in studying and understanding operators and matrices [12, 13, 14, 16] which has application in quantum theory. Many problems in quantum physics reduce to spectral theory of block operator matrices. It is a very useful tool in studying and understanding the spectral analysis of bounded and unbounded linear operators in Hilbert spaces as explained in most functional analysis and matrix analysis textbooks, for example, in [13, 14, 24]. The numerical computation of the boundary of S-numerical range remains a challenging task, and up to date not entirely satisfactory numerical algorithm has been found. The situation becomes even worse when dealing with unbounded operators as the 'random vector' method proposed in [15, 21].

In this paper, we shall consider three particular special cases. In the first case L is the Sturm-Liouville operator. The underlying Hilbert space in this case is $H = L^2(0,1)$ and the operator is

$$L = -\frac{d^2}{dx^2},$$

and the domain of L is given by

$$\mathcal{D}(L) = \{y \in H^2(0,1) : y(0) = 0 = y(1)\}.$$

In the second case $\mathcal{A}$ is the Hain-Lüst operator, it is clear the underlying Hilbert space in this case is $H := L^2(0,1) \times L^2(0,1)$ and the operator is

$$\mathcal{A} = \mathcal{L} := \begin{pmatrix} L & w \\ \widetilde{w} & z \end{pmatrix}, \tag{6}$$

where $L = -\frac{d^2}{dx^2}$ while w, $\widetilde{w}$ and z are bounded multiplication operators. The domain of $\mathcal{L}$ is given by

$$\begin{aligned}\mathcal{D}(\mathcal{L}) &= H^2(0,1) \cap H_0^1(0,1) \times L^2(0,1) \\ &= \left\{ \begin{pmatrix} u \\ v \end{pmatrix} : u(0) = 0 = u(1), \int_0^1 (|u''|^2 + |u'|^2 + |u|^2 + |v|^2) < \infty \right\}.\end{aligned}$$

We shall be concerned with the effects of discretization, both of the unbounded second-order differential operator L and of the bounded multiplication operators which appear in the other entries. This operator was introduced by K. Hain and R. Lüst in application to problems of magnetohydrodynamics [7] and the problem of this type [12, 13, 14, 16] has been studied in [1, 2, 3, 4, 6, 8, 9, 23].

In the last case M is the Stokes type system of ordinary differential equations. The underlying Hilbert space in this case is also $H := L^2(0,1) \times L^2(0,1)$ and the operator is

$$M := \begin{pmatrix} -\frac{d^2}{dx^2} & -\frac{d}{dx} \\ \frac{d}{dx} & -\frac{3}{2}I \end{pmatrix}, \tag{7}$$

the domain of M is given by

$$\mathcal{D}(M) = \left\{ \begin{pmatrix} u \\ v \end{pmatrix} : u(0) = 0 = u(1),\ u \in H_0^1(0,1) \cap H^2(0,1) \text{ and } v \in H^1(0,1) \right\}.$$

Note that M is not closed; however M is closable and its closure is self-adjoint [1]. The paper is organized as follows. In section 3, some theoretical results are investigated dealing with the *S-numerical range* of operators using finite difference method. In section 4, we shall applying these results to compute the *S-numerical range* of differential operators.

2. An approximating discrete operator

We shall replace the Sturm-Liouville operator by a matrices Suppose $u \in \mathcal{D}(L)$. Pick $N+1$ points $x_0, x_1, \ldots, x_N$ in the interval $[0,1]$; for the sake of simplicity we assume equal spacing, so that $x_0 = 0,\ x_j = jh,\ x_N = 1 = Nh$ with $h = \frac{1}{N}$. We would like to form the vectors

$$\mathbf{u} = \begin{pmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{N-1}) \end{pmatrix} \in \mathbb{C}^{N-1}. \tag{8}$$

Moreover, if we are to use quadrature estimates we shall need more smoothness in u. We therefore observe that the set

$$\mathcal{C}(L) := C^4(0,1) \cap \mathcal{H}_0^1(0,1) \tag{9}$$

is a core of the operator L; for $u \in \mathcal{C}(L)$, equation (9) makes sense. Recall the second order divided difference approximation of the second derivative,

$$\frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2} = u''(x_j) + \frac{1}{4!}h^2(u^4(\xi_j) + u^4(\eta_j)). \tag{10}$$

Hence

$$\begin{pmatrix} u''(x_1) \\ u''(x_2) \\ \vdots \\ u''(x_{N-1}) \end{pmatrix} \simeq \frac{1}{h^2} T\mathbf{u},$$

where $T = \mathrm{tridiag}(1, -2, 1)$ is the tridiagonal matrix with entries $T_{jj} = -2$, $T_{j,j\pm 1} = 1$.

Our matrix replacement of the Sturm-Liouville operator is a matrix of dimension $(N-1) \times (N-1)$ given by

$$L_N := -\frac{1}{h^2} T. \tag{11}$$

Muhammad and Marletta [4] replaced the Hain-Lüst operator and Stokes operator by matrix. To discretize the Hain-Lüst operator, Suppose that $\begin{pmatrix} u \\ u \end{pmatrix} \in \mathcal{D}(A)$. Pick $N+1$ points $x_0, x_1, \ldots, x_N$ in the interval $[0,1]$; for the sake of simplicity we assume equal spacing, so that $x_0 = 0$, $x_j = jh$, $x_N = 1 = Nh$ with $h = \frac{1}{N}$. We would like to form the vectors

$$\mathbf{u} = \begin{pmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{N-1}) \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} v(x_1) \\ v(x_2) \\ \vdots \\ v(x_{N-1}) \end{pmatrix} \in \mathbb{C}^{N-1}; \tag{12}$$

however since we only have $v \in L^2(0,1)$, point values of v are meaningless. Moreover, we shall need more smoothness in u and v if we are to use the quadrature estimates we need. We therefore observe that the set

$$\mathcal{C}(A) := (C^4(0,1) \cap H_0^1(0,1)) \times C^1(0,1) \tag{13}$$

is a core of the operator $\mathcal{L}$, for $\begin{pmatrix} u \\ u \end{pmatrix} \in \mathcal{C}(\mathcal{L})$, Eq. (12) makes sense. We also define diagonal matrices:

$$B_N = \mathrm{diag}(w(x_1), w(x_2), \cdots, w(x_{N-1})),$$

$$C_N = \mathrm{diag}(\tilde{w}(x_1), \tilde{w}(x_2), \cdots, \tilde{w}(x_{N-1})),$$

$$D_N = \mathrm{diag}(z(x_1), z(x_2), \cdots, z(x_{N-1})),$$

Our matrix replacement of the Hain-Lüst operator is a matrix of dimension $2(N-1) \times 2(N-1)$ given by

$$\mathbb{A}_N := \begin{pmatrix} L_N & B_N \\ C_N & D_N \end{pmatrix}, \tag{14}$$

where $L_N := -\frac{1}{h^2}T$. To discretize the Stokes operator observe that

$$-\left(\frac{u(x_{j+1})-2u(x_j)+u(x_{j-1})}{h^2}\right)-\left(\frac{u(x_j)-u(x_{j-1})}{2h}\right)=-\lambda u(x_j)+O(h^2), \quad (15)$$

and

$$-\left(\frac{u(x_j)-u(x_{j-1})}{2h}\right)-\frac{1}{2}u(x_{j-\frac{-3}{2}})=\lambda u(x_{j-\frac{-3}{2}})+O(h^2). \quad (16)$$

Hence our matrix replacement of the Stokes operator is a matrix of dimension $2(N-1)\times 2(N-1)$ given by

$$\mathbb{M}_N := \begin{pmatrix} E_N & W_N \\ W_N^T & Z_N \end{pmatrix}, \quad (17)$$

where $E_N := -\frac{1}{h^2}T$,

$$W_N = -\frac{1}{2h}\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix},$$

and $Z_N = \frac{-3}{2}I_{N\times N}$. We shall use this technique in this paper for computing S-numerical range.

3. S-numerical range inclusion

The definition of the S-numerical ranges for bounded linear operators in Equation(5) generalizes as follows to unbounded operator matrices A with dense domain $\mathcal{D}(A)\cap\mathcal{D}(S)$.

DEFINITION 3.1. For a linear operator A with $\mathcal{D}(A)\subset\mathcal{H}$ on an infinte dimensional Hilbert space H with a sesquilinear form (infinite inner product) $(u,v)\mapsto(u,v)_S := (Su,v)$, $u,v\in\mathcal{D}(S)$, where S is self-adjoint operator, we define S-numerical ranges of A by

$$W_S(A)=\left\{\frac{(Ax,Sx)}{(Sx,x)} : x\in\mathcal{D}(A)\cap D(S) \text{ with } (Sx,x)\neq 0\right\}. \quad (18)$$

$W_S(A)$ is the union of the positive S-numerical range $W_S^+(A)$ and negative S-numerical range $W_S^-(A)$ which are defined respectively as:

$$W_S^+(A)=\left\{\frac{(Ax,Sx)}{(Sx,x)} : x\in\mathcal{D}(A)\cap D(S) \text{ with } (Sx,x)>0\right\}. \quad (19)$$

and

$$W_S^-(A)=\left\{\frac{(Ax,Sx)}{(Sx,x)} : x\in\mathcal{D}(A)\cap D(S) \text{ with } (Sx,x)<0\right\}. \quad (20)$$

One may obtain result analogous to [17, Theorem 4.1]. The following theorem shows that every point of the S-numerical range of the Sturm-Liouville operator $L=-\frac{d^2}{dx^2}$ can be approximated to arbitrary accuracy.

THEOREM 3.2. *Suppose λ is a point of the S-numerical range of the Sturm-Liouville operator $L=-\frac{d^2}{dx^2}$. Then for any $\varepsilon>0$ there exists $\tilde{N}$ such that for all $N\geqslant\tilde{N}$ there is a point of the S-numerical range of L_N which is ε-close to λ.*

Proof. Fix $\varepsilon>0$ and $\lambda\in W_S(L)$. Then there exist $u\in\mathcal{C}(L)$ with $\langle Su,u\rangle\neq 0$ such that

$$\lambda=\frac{\langle Lu,Su\rangle_{L^2}}{\langle Su,u\rangle_{L^2}}.$$

Then we need two types of integrals which are estimated by quadrature.

Type 1: L^2 integrals of smooth functions u.

Let $u\in C^4(0,1)$ with Dirchlet boundary conditions at 0 and 1, also we observe that Su is Lipschitz because $u''\in C^2(0,1)$, then

$$\begin{aligned}\langle Su,u\rangle_{L^2}&=\int_0^1(Su)\overline{u}dx=\sum_{j=1}^{N}\int_{x_{j-1}}^{x_j}(Su)(x)\overline{u(x)}dx\\&=\sum_{j=1}^{N}\left[\frac{h}{2}\big((Su)(x_{j-1})\overline{u(x_{j-1})}+(Su)(x_j)\overline{u(x_j)}\big)+O(h^2)\right]\\&=\sum_{j=1}^{N-1}h((Su)(x_j)\overline{u(x_j)})+O(h)=\sum_{j=1}^{N-1}h(S_N\mathbf{u})_j\overline{\mathbf{u}_j}+O(h)\\&=h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}}+O(h).\end{aligned}\tag{21}$$

Type 2: The integrals $\langle Lu,Su\rangle_{L^2}$ for smooth u.

Let $u\in C^4(0,1)$ with $u(0)=0=u(1)$, we observe that both Lu and Su are Lipschitz because $u''\in C^2(0,1)$ then

$$\begin{aligned}\langle Lu,Su\rangle_{L^2}&=\int_0^1(Lu)\overline{(Su)}dx=\sum_{j=1}^{N}\int_{x_{j-1}}^{x_j}(Lu)(x)\overline{(Su)(x)}dx\\&=\sum_{j=1}^{N}\left[\frac{h}{2}\big((Lu)(x_{j-1})\overline{(Su)(x_{j-1})}+(Lu)(x_j)\overline{(Su)(x_j)}\big)+O(h^2)\right]\\&=\sum_{j=1}^{N-1}h((Lu)(x_j)\overline{(Su)(x_j)})+O(h)=\sum_{j=1}^{N-1}h(L_N\mathbf{u})_j\overline{(S_N\mathbf{u})_j}+O(h)\\&=h\langle L_N\mathbf{u},S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}+O(h),\end{aligned}\tag{22}$$

also we have

$$\langle L_N\mathbf{u}-\lambda\mathbf{u}\rangle_j:=(Lu)(x_j)-\lambda u(x_j)-\frac{1}{4!}h^2r_j\tag{23}$$

where $r_j := u^4(\xi_j) + u^4(\eta_j)$, and $\xi_j, \eta_j \in (x_{j-1}, x_{j+1})$, for $j = 1, \ldots, N-1$. Then by taking inner products on both sides of equation (23) we get

$$\langle L_N\mathbf{u} - \lambda\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}} = \langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}} - \lambda\langle S_N\mathbf{u}, \mathbf{u}\rangle_{\mathbb{C}^{N-1}} - \frac{h^2}{4!}\langle \mathbf{r}, \mathbf{u}\rangle_{\mathbb{C}^{N-1}}. \tag{24}$$

Multiplying by h and adding $\langle Lu, Su\rangle_{L^2} - h\langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}$ to both sides of equation (24) we obtain

$$h\langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}} + O(h) := \langle Lu, Su\rangle_{L^2} - \frac{h^3}{4!}\langle r, \mathbf{u}\rangle, \tag{25}$$

thus dividing both sides of equation (25) by $\langle Su, u\rangle_{L^2}$ we get

$$\frac{h\langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}} + O(h) + O(h^3)}{h\langle S_N\mathbf{u}, \mathbf{u}\rangle_{\mathbb{C}^{N-1}} + O(h^2)} = \frac{\langle Lu, Su\rangle_{L^2}}{\langle Su, u\rangle_{L^2}}.$$

This implies that

$$\frac{\langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}{\langle S_N\mathbf{u}, \mathbf{u}\rangle_{\mathbb{C}^{N-1}}} = \lambda + O(h).$$

It follows that there exists $\lambda_N \in W_{S_N}(L_N)$ such that $|\lambda - \lambda_N| \leqslant \varepsilon$. $\square$

3.1. Main convergence result

In order to bound some crucial parts in our main Theorem 3.5. we require Definition 3.3, which has not been introduced before, and which we expect will be useful in many contexts when dealing with unbounded operator matrices.

Suppose that A is an unbounded linear operator $A : \mathcal{D}(A) \subset H \to H$. Consider a sesquilinear form,

$$a(x) := \frac{\langle Ax, x\rangle_S}{\langle x, x\rangle_S} \quad \text{for } x \in \big(\mathcal{D}(A) \cap \mathcal{D}(S)\big), \quad \text{and } \langle x, x\rangle_S \neq 0,$$

where S is an unbounded self-adjoint operator. We define R-partial S-numerical range for $R \in \mathbb{R}^+$, as follows:

DEFINITION 3.3. Let A be an unbounded operator with quadratic form $a(.)$. Then the set

$$W_{S,R}(A) = \left\{ a(x) : \ x \in (\mathcal{D}(A) \cap \mathcal{D}(S)), \ \text{with } \langle x, x\rangle_S \neq 0 \ \text{and } |a(x)| \leqslant R \right\}$$

is called the R-partial *S-numerical ranges* of A.

$W_{S,R}(A)$ is the union of the positive R-partial *S-numerical ranges* $W_{S^+,R}(A)$ and negative R-partial *S-numerical ranges* $W_{S^-,R}(A)$ which are defined respectively as:

$$W_{S^+,R(A)} = \left\{ a(x) : \ x \in (\mathcal{D}(A) \cap \mathcal{D}(S)), \langle x, x\rangle_S > 0 \ \text{and } |a(x)| \leqslant R \right\},$$

and

$$W_{S^-,R(A)} = \left\{ a(x) : \ x \in (\mathcal{D}(A) \cap \mathcal{D}(S)), \langle x,x \rangle_S < 0 \ \text{ and } \ |a(x)| \leqslant R \right\}.$$

LEMMA 3.4. *For A as in Definition 3.3,*

$$\overline{W_S(A)} = \overline{\bigcup_{R>0} W_{S,R}(A)}.$$

Proof. Suppose that $\lambda \in W_S(A)$, then there exist $x \in (\mathcal{D}(A) \cap \mathcal{D}(A))$, such that $\lambda = a(x)$ with $\langle x,x \rangle_S \neq 0$. Therefore, by Definition (3.3), $\lambda \in W_{S,R}(A)$ for any $|a(x)| \leqslant R$. Hence $\overline{W_S(A)} \subseteq \overline{\bigcup_{R>0} W_{S,R}(A)}$. In order to prove opposite inclusion, it is clear $W_{S,R}(A) \subseteq W_S(A)$ for all $R > 0$, so this immediately gives $\overline{W_S(A)} \subseteq \overline{\bigcup_{R>0} W_{S,R}(A)}$. $\square$

Our aim now is to start from a point in the R-partial *S-numerical range* of L_N is close to a point in the *S-numerical range* of the Sturm-Liouville operator.

THEOREM 3.5. *Consider the $(N-1) \times (N-1)$ matrix L_N given in (11). For each $R > 0$, there exist a constant K_R independent of N such that $W_{S,R}(L_N)$ is contained in a $K_R N^{-1/2}-$neighborhood of $W_{S,R}(L)$.*

Proof. Suppose that $\lambda_N \in W_{S_N,R}(L_N)$; then

$$\lambda_N = \frac{\langle L_N \mathbf{u}, S_N \mathbf{u} \rangle_{\mathbb{C}^{N-1}}}{\langle S_N \mathbf{u}, \mathbf{u} \rangle_{\mathbb{C}^{N-1}}}.$$

for some $\mathbf{u} \in \mathbb{C}^{N-1}$ with $\|\mathbf{u}\| = 1$. let $u \in (H_0^1(0,1) \cap H^2(0,1))$ be the piecewise quadratic function given by $u(x) = u_j \frac{(x-x_{j-1})^2}{2(x_j - x_{j-1})} - u_{j-1} \frac{(x_j - x)^2}{2(x_j - x_{j-1})}$ for $x_{j-1} \leqslant x \leqslant x_j$ for $j = 1, 2, \ldots, N$, where $u_0 = 0 = u_N$. We simply note that the quadratic form associated with L is the usual Dirichlet form

$$\ell(u,u) := \int_0^1 |u''|^2 dx$$

so we need to estimate the difference

$$\left| \frac{\langle L_N \mathbf{u}, S_N \mathbf{u} \rangle_{\mathbb{C}^{N-1}}}{\langle S_N \mathbf{u}, \mathbf{u} \rangle_{\mathbb{C}^{N-1}}} - \frac{\ell(u,u)}{\langle Su, u \rangle_{L^2}} \right|. \tag{26}$$

By summation by parts

$$\int_0^1 |u''|^2 dx = \frac{1}{h} \sum_{j=1}^{N} |u_j - u_{j-1}|^2 = h^3 \left\langle -\frac{1}{h^2} T\mathbf{u}, -\frac{1}{h^2} T\mathbf{u} \right\rangle_{\mathbb{C}^{N-1}}. \tag{27}$$

Here $\|u'\|_2$ and $\|u''\|_2$ can be bounded in a way which depends only on R and not on h. In order to see this, recall that since $\lambda \in W_R(L_N)$, and by Definition (3.3),

$$\left| h \left\langle -\frac{1}{h^2} T\mathbf{u}, -\frac{1}{h^2} T\mathbf{u} \right\rangle_{\mathbb{C}^{N-1}} \right| \leqslant Rh \, \langle S_N \mathbf{u}, \mathbf{u} \rangle_{\mathbb{C}^{N-1}};$$

this yields, in light of (27),

$$\frac{\|u''\|_2^2}{h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}}} \leqslant R.$$

On the other hand since by assumption, $u \in (H_0^1(0,1)\cap H^2(0,1))$ be the piecewise quadratic function so for $-h/2 \leqslant x \leqslant h/2$ thus

$$\begin{aligned}
\int_{-h/2}^{h/2}(u'(x))^2dx &= \int_{-h/2}^{h/2}\left[\frac{1}{4}(u_j^2+u_{j-1}^2+2u_ju_{j-1})+\frac{x^2}{h^2}(u_j-u_{j-1})^2\right]dx\\
&= \int_{-h/2}^{h/2}\frac{1}{4}(u_j^2+u_{j-1}^2-(u_j-u_{j-1})^2+u_j^2+u_{j-1}^2)\,dx\\
&\quad+\int_{-h/2}^{h/2}\frac{x^2}{h^2}(u_j-u_{j-1})^2dx\\
&= \frac{h}{2}((u_j^2+u_{j-1}^2)-\frac{h}{6}(u_j-u_{j-1})^2,
\end{aligned}$$

thus

$$\int_0^1 |u'|^2 = \sum_{j=1}^N h|(S_Nu)_j|^2 - \frac{h}{6}\int_0^1 |u''|^2dx.$$

Rearranging gives

$$h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}} = \|u'\|^2+\frac{h^2}{6}\|u''\|^2 \tag{28}$$

$$h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}} = \int_0^1 |u'|^2+\frac{h^2}{6}\|u''\|_2^2 \geqslant \|u'\|_2^2. \tag{29}$$

Thus

$$\frac{\|u''\|_2^2}{\|u'\|_2^2} \leqslant R. \tag{30}$$

Now we estimate

$$\left|\frac{h\langle\frac{-1}{h^2}T_N\mathbf{u},\frac{-1}{h^2}T_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}{h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}-\frac{l(u,u)}{\langle Su,u\rangle_{L^2}}\right|. \tag{31}$$

From equations (27) and (29) we have

$$\begin{aligned}
\frac{h\langle\frac{-1}{h^2}T_N\mathbf{u},\frac{-1}{h^2}T_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}{h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}}} &= \frac{l(u,u)}{(\int_0^1|u'|^2)\left(1+\frac{h^2}{6}\frac{\|u''\|_2^2}{\|u'\|_2^2}\right)}\\
&\geqslant \frac{l(u,u)\left(1-\frac{h^2}{6}\frac{\|u''\|_2^2}{\|u'\|_2^2}\right)}{\int_0^1|u|^2}.
\end{aligned} \tag{32}$$

Thus we get

$$\left|\frac{h\langle\frac{-1}{h^2}T_N\mathbf{u},\frac{-1}{h^2}T_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}{h\langle S_N\mathbf{u},\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}-\frac{l(u,u)}{\langle Su,u\rangle}\right| \leqslant \frac{l(u,u)}{\int_0^1|u'|^2}\frac{h^2}{6}\frac{\|u''\|_2^2}{\|u'\|_2^2} \leqslant C\Big(\frac{\|u''\|_2}{\|u'\|_2}\Big)^4h^2.$$

Using equation (30) we get

$$\left|\frac{\langle L_N\mathbf{u}, S_N\mathbf{u}\rangle_{\mathbb{C}^{N-1}}}{\langle S_N\mathbf{u}, \mathbf{u}\rangle_{\mathbb{C}^{N-1}}} - \frac{\ell(u,u)}{\langle Su, u\rangle_{L^2}}\right| \leqslant C\Big(\frac{\|u'\|_2^2}{\|u\|_2^2}\Big)^2 h^2 \leqslant Ch^2R^2. \quad \square \tag{33}$$

4. Numerical examples of matrix differential operators

In this section we study some specific examples and demonstrate that, despite of the results obtained in the previous section, practical calculation of the *S-numerical range* is very far from being straight forward. We shall show that the discretization techniques may often yield misleading results, and that a good knowledge of existing analytical estimates of *S-numerical ranges* is often needed in order to understand the results. The computation were carried out in MATLAB.

4.1. Application to Sturm-Liouville operator

In this subsection we will examine the Sturm-Liouville operator which fits into the framework of Sect. 3. See [5] for results on the Computing the q-numerical range of such operators.

In the Hilbert space $H := L^2(0,1)$, we introduce the Sturm-Liouville operators

$$L = S := -\frac{d^2}{dx^2}, \tag{34}$$

and the The domain of L and S are given by

$$\mathcal{D}(L) = \mathcal{D}(S) = \{u \in H^2(0,1) : u(0) = 0 = u(1)\}.$$

REMARK 1. Because S is uniformly positive operator then it is not difficult to show that $W_S(L) = W(S^{1/2}LS^{-1/2})$.

REMARK 2.

(i) By Remark 1 and Toeplitz-Hausdorf theorem [19], $W_S(L)$ is a convex set and it is inclusion regions for the eigenvalues of L.

(ii) Consider the Sturm-Liouville operator

$$Ly = -y'',$$

Because L is self-adjoint and bounded below with purely discrete spectrum, the eigenvalues of L is given by

$$\lambda_k := \inf_{\substack{F\subset(\mathcal{D}(L)\cap\mathcal{D}(S))\\ dim F=k}} \sup_{\substack{y\in F\\ y\neq 0}} q(y)$$

where q is the Rayleigh functional

$$q(y) := \frac{\langle Ly, Sy\rangle}{\langle Sy, y\rangle}, \quad y \in (\mathcal{D}(L) \cap \mathcal{D}(S)),\ y \neq 0.$$

Hence

$$\pi^2 = \lambda_1 := \inf_{\substack{y \in (\mathcal{D}(L) \cap \mathcal{D}(S)) \\ y \neq 0}} g(y),$$

and $\lambda_n = n^2\pi^2$ for $n = 1,2,3,4,\cdots$ so this implies that $\langle Ly, Sy\rangle \geqslant \langle Sy, y\rangle$ then $\Re\left(\frac{\langle Ly,Sy\rangle}{\langle Sy,y\rangle}\right) > 0$, so in this case $\overline{W_S(L)} = [\pi^2, \infty)$.

(iii) if we use Definition 3.3, we will see that the $R-$ partial *S-numerical range* of the Sturm-Liouville operator L is

$$W_{S,R}(L) = [\pi^2, \infty) \cap \{z \in \mathbb{C} |\ |z| \leqslant R\}. \tag{35}$$

(v) On the other hand the finite difference approximation to the Sturm-Liouville operator is given by a real symmetric $(N-1) \times (N-1)$ matrix

$$L_N := -\frac{1}{h^2} T,$$

with some real eigenvalues $\{\lambda_1, \lambda_2, \cdots, \lambda_N\}$.

Figure 1 show attempts to calculate approximations to the *S-numerical range* of the Sturm-Liouville operator using matrices (24) for different values of N.

4.2. Application to Hain-Lüst operator

In this subsection we will examine the Hain-Lüst operator which fits into the framework of Sect. 3. See [1, 2, 3, 4] for results on the approximation of the numerical range of polynomial and quadratic numerical range of such block operators. Assume that $w : [0,1] \to [0,\infty)$, $\widetilde{w} : [0,1] \to [0,\infty)$, and $z : [0,1] \to \mathbb{C}$ are such that $w(x) = 1$, $\widetilde{w}(x) = 1$,

$$z(x) = \begin{cases} 28e^{4\pi i x} - 30, & \text{for } 0 \leqslant x < 1/2; \\ 28e^{4\pi i x} - 100, & \text{for } 1/2 < x \leqslant 1. \end{cases}$$

for each $x \in [0,1]$. We introduce the differential expression

$$\tau_{\widetilde{A}} := -\frac{d^2}{dx^2}, \quad \tau_{\widetilde{B}} := w(x), \quad \tau_{\widetilde{C}} := \widetilde{w}(x), \quad \tau_{\widetilde{D}} := z(x). \tag{36}$$

Let L, B, C, D be the operators in the Hilbert space $L^2(0,1)$ induced by the differential expressions $\tau_{\widetilde{A}}$, $\tau_{\widetilde{B}}$, $\tau_{\widetilde{C}}$, $\tau_{\widetilde{D}}$ with domain

$$\mathcal{D}(L) := H^2(0,1) \cap H_0^1(0,1), \quad \mathcal{D}(B) = \mathcal{D}(C) = \mathcal{D}(D) := L^2(0,1).$$

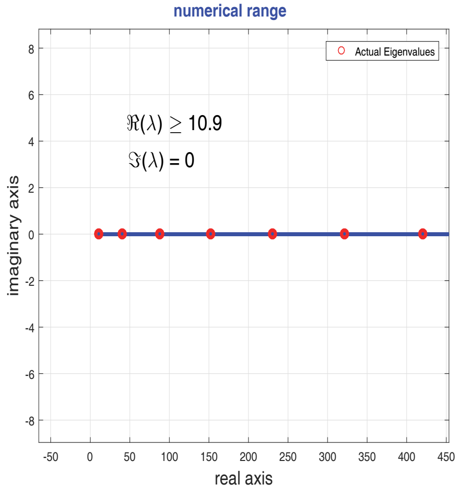

Figure 1: *The approximation L_N in equation (24) is given by a self-adjoint matrix with some real eigenvalues $\{\lambda_1, \lambda_2, \cdots, \lambda_N\}$ with $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \lambda_N$. The S-numerical range $W_{S_{24}}(L_{24})$ of L_{24} for $S_{24} = L_{24}$ is the line segment $[10.9, 2491.1]$, the red dots are $\sigma(L_{24}) = \{10.9, 40.3, \cdots, 2491.1\}$.*

In the Hilbert space $L_2^2(0,1) := L^2(0,1) \oplus L^2(0,1)$, we introduce the matrix differential operator

$$\mathcal{A} = \begin{pmatrix} L & B \\ C & D \end{pmatrix} = \begin{pmatrix} -\frac{d^2}{dx^2} & w(x) \\ \widetilde{w}(x) & z(x) \end{pmatrix}, \tag{37}$$

on the domain

$$\mathcal{D}(\mathcal{A}) := \left\{ \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} : y_1 \in H^2(0,1) : y_1(0) = 0 = y_1(1) \text{ and } y_2 \in L_2(0,1) \right\}.$$

The finite difference approximation to the Hain-Lüst operator is given by a non self-adjoint $2(N-1) \times 2(N-1)$ matrix

$$\mathcal{A}_N := \begin{pmatrix} L_N & B_N \\ C_N & D_N \end{pmatrix},$$

given in Equation (14). On the other hand, in the Hilbert space $L_2^2(0,1) := L^2(0,1) \oplus L^2(0,1)$, we introduce the self-adjoint matrix differential operator

$$\widetilde{S} = \begin{pmatrix} L & B \\ C & \widetilde{D} \end{pmatrix} = \begin{pmatrix} -\frac{d^2}{dx^2} & w(x) \\ \widetilde{w}(x) & u(x) \end{pmatrix}, \tag{38}$$

where $u(x) = e^{-x^2}$ on the domain

$$\mathcal{D}(\widetilde{S}) := \left\{ \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} : y_1 \in H^2(0,1) : y_1(0) = 0 = y_1(1) \text{ and } y_2 \in L_2(0,1) \right\}.$$

The finite difference approximation to the matrix differential operator in Eq. (38) is given by a self-adjoint $2(N-1)\times 2(N-1)$ matrix

$$\widetilde{\mathbb{S}}_N := \begin{pmatrix} L_N & B_N \\ C_N & \widetilde{D_N} \end{pmatrix}, \tag{39}$$

where $\widetilde{D_N} = \mathrm{diag}(u(x_1), u(x_2), \cdots, u(x_{N-1}))$.

Figure 2 show attempts to calculate approximations to the $\widetilde{S}-$numerical range of the Hain-Lüst operator using matrices (14) and (39) for different values of N.

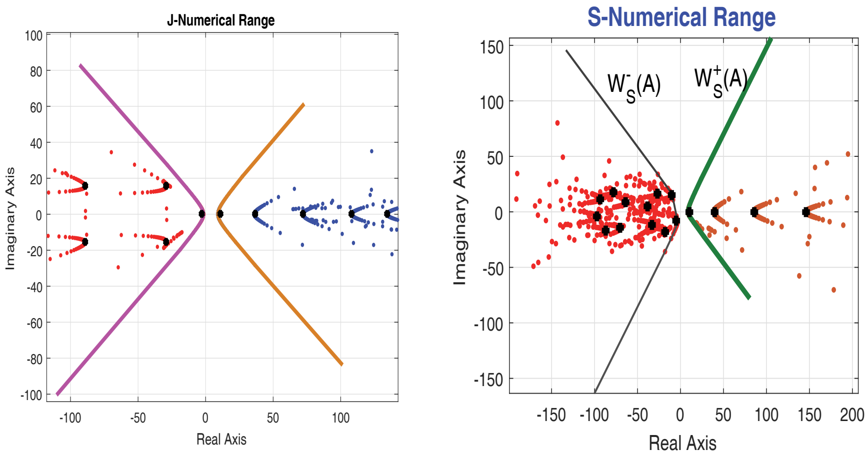

Figure 2: *On the left-hand side, for $k=3$, $W_{\mathbb{S}_k}(\mathbb{A}_k)$ is bounded by the hyperbola centered at $(0,0)$ and the foci of the hyperbola are the eigenvalues of $\mathbb{A}_k$. While for the right-hand side, for $k=10$, $W_{\mathbb{S}_k}(\mathbb{A}_k)$ is bounded by the hyperbola centered at $(0,0)$ and and the foci of the hyperbola are the eigenvalues of $\mathbb{A}_k$.*

REMARK 3.

(i) The Hermitian matrix $\widetilde{\mathbb{S}}_N$ in Eq. (37) is indefinite matrix, according to the [22, Theorem 3.2]. We obtain hyperbolical discs.

(ii) The Hermitian matrix $\widetilde{\mathbb{S}}_N$ in (39) is nonsingular it is not restriction to consider the matrix J instead of S in the definition of S-numerical range [22].

4.3. Application to Stokes operator

In this subsection we will examine the Stoke operator which fits into the framework of Sect. 3. See [1, 2, 3, 4] for results on the approximation of the numerical range of polynomial and quadratic numerical range of such a block operators. We consider the Stokes operator introduced in Section 1, Equation (7), and it is discrete approximation equations (15) and (16) with N = 100. The finite difference approximation to the Stokes operator is the $((2N-1)\times(2N-1)$ matrix M_N given in Equation (17).

On the other hand Let $\mathcal{S}$ be a self-adjoint operator in the space $\mathcal{H} = [L^2((-\pi,\pi))]^2$ and consider a 2×2 block operator matrix

$$\mathcal{S} = \begin{pmatrix} -\frac{d^2}{dx^2}+4 & 1 \\ 1 & \psi \end{pmatrix} \tag{40}$$

where

$$\psi(x) = \begin{cases} 0, & \text{for } -\pi \leqslant x < 0; \\ 2, & \text{for } 0 \leqslant x < \pi. \end{cases}$$

on the domain

$$\mathcal{D}(\mathcal{S}) := \left\{ \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} : y_1 \in H^2(0,1) : y_1(-\pi) = 0 = y_1(\pi) \ \text{ and } \ y_2 \in L_2(0,1) \right\}.$$

The finite difference approximation to the matrix differential operator in Eq. (40) is given by a self-adjoint $2(N-1)\times 2(N-1)$ matrix

$$\mathcal{S}_N := \begin{pmatrix} L_N & B_N \\ C_N & \widehat{D_N} \end{pmatrix}, \tag{41}$$

where $\widehat{D_N} = \operatorname{diag}(\psi(x_1), \psi(x_2), \cdots, \psi(x_{N-1}))$.

Figure 3 show attempts to calculate approximations to the $\mathcal{S}$-numerical range of the Stokes operator using matrices (17) and (41) for different values of N.

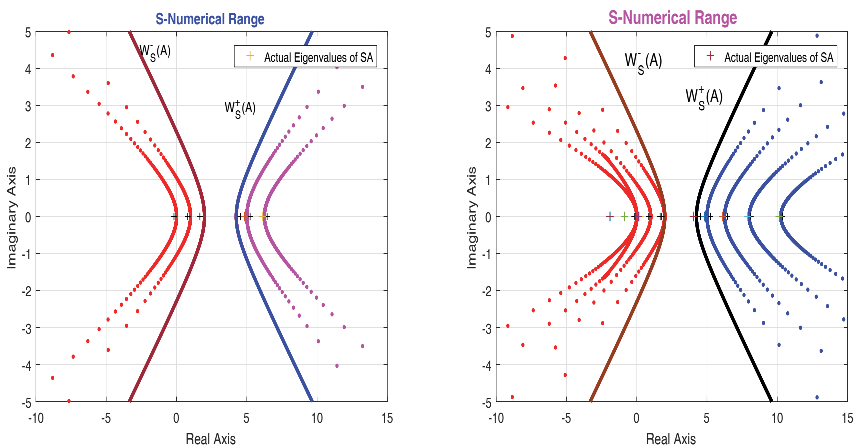

Figure 3: *On the left-hand side, for* $k=3$, $W_{\mathbb{S}_k}(\mathbb{A}_k)$ *is bounded by the hyperbola centered at* $(0,0)$ *and the foci of the hyperbola are the eigenvalues of* $\mathbb{A}_k$. *While for the right-hand side, for* $k=10$, $W_{\mathbb{S}_k}(\mathbb{A}_k)$ *is bounded by the hyperbola centered at* $(0,0)$ *and and the foci of the hyperbola are the eigenvalues of* $\mathbb{A}_k$.

REMARK 4. **(i)** The Hermitian matrix $\mathcal{S}_N$ in Eq. (41) is indefinite matrix, according to the theorem 3.2 [22]. We obtain hyperbolical discs.

(ii) The Hermitian matrix $\mathcal{S}_N$ in Eq. (41) is nonsingular it is not restriction to consider the matrix J instead of S in the definition of S-numerical range [22].

5. Conclusions

The calculation of *S-numerical range* of differential operators by finite difference techniques is easier to implement than Galerkin discretization methods, but the theoretical analysis is more involved and the results obtained are less aesthetically satisfactory. In the case of Galerkin discretizations, the *S-numerical range* are nested:

$$W_S(\mathbb{A}_{N+1}) \supseteq W_S(\mathbb{A}_N) \quad \text{for all } N \in \mathbb{N}.$$

This is not guaranteed for finite differences, where only have Theorem 3.5.

Acknowledgement. The authors are very grateful for the comments and corrections of the referee, whose detailed attention allowed us to make very worthwhile improvements.

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(Received March 20, 2022)

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