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Computing c-numerical range of differential operator matrices

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Abstract. A linear operator on a Hilbert space may be approximated with finite matrices by choosing an orthonormal basis of the Hilbert space. In this paper, we establish an approximation of the *c-numerical range* of bounded and unbounded operator matrices by variational methods. Application to Schrödinger operator, and Hain-Lüst operator are given.

1. Introduction

Suppose $\mathcal{H}$ is a Hilbert space. For a bounded linear operators A, recall that the numerical range $W(A)$ of A is defined as

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

If c is a k-tuple of a non-zero real numbers $c_1, c_2, \ldots, c_k$, then the *c-numerical range* of A is

$$W_c(A) = \left\{ \sum_{j=1}^{k} c_j \langle Ae_j, e_j\rangle : (e_1, \ldots, e_k) \text{ is an orthonormal subset of } \mathcal{H} \right\} \tag{2}$$

Furthermore, if c consists of just one number c_1, $W_c(A)$ then we obtain the classical numerical range $W(A)$ (see [18].) Also, for $c_1 = c_2 = \cdots = c_k = 1$, the c-numerical range $W_c(A)$ turns into $W_k(A)$ – the so called *k-numerical range* introduced by Halmos, (see [6, 18].)

Originally, the *c-numerical range* was introduced for linear operators on $\mathbb{C}^n$ by Marcus [16]. Let A be an $n \times n$ complex matrix and $c = (c_1, c_2, \ldots, c_n)^t \in \mathbb{R}^n$. The c-numerical range of A is the set

$$W_c(A) = \left\{ \sum_{i=1}^{n} c_i x_i^* A x_i : \{x_1, \ldots, x_n\} \text{ is an orthonormal set} \right\}. \tag{3}$$

Westwick [2] has shown that $W_c(A)$ is convex for any $c \in \mathbb{R}^n$. Also he gave an example which shows that for complex vectors $c \in \mathbb{C}^n$ with $n \geq 3$, the range $W_c(A)$ may fail to be convex.

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By the famous Toeplitz-Hausdorff Theorem [10, 17] $W(A)$ is convex. Also $W_k(A)$ is convex (for a proof see [18]). The *c-numerical range* is not always convex. Westwick [22] proved that $W_c(A)$ is convex for any $c \in \mathbb{R}^n$.

The *c-numerical range* is unitary similarity invariant, $W_c(A) = W_c(UAU^*)$, for any unitary matrix U. It is also transpose invariant, $W_c(A) = W_c(A^T)$. Clearly, we have the basic property

$$W_c(aA + bI_n) = aW_c(A) + b\sum_{j=1}^{k} c_j, \tag{4}$$

for every $a, b \in \mathbb{C}$. A review of the properties of *c-numerical ranges* of operator matrices may be found in [24].

This set has been studied extensively see [23, 24] and has a lot of applications in functional analysis, operator theory, numerical analysis, perturbation theory, quantum mechanics see [13, 15, 18, 19], and the references therein. In recent years, several results about the *c-numerical range* of operators on finite-dimensional Hilbert spaces have been published see, [20, 23–27].

In this note we consider how to compute $W_c(A)$ by projection methods, which reduce the problem to that of computing the *c-numerical range* of a (finite) matrix and block matrix.

Projection methods always yield a subset of the *c-numerical range*, under hypotheses. Only when one wishes to be sure of generating the whole of $W_c(A)$, it is necessary to make some extra assumptions.

The paper is organized as follows. In Section 2, some theoretical results are investigated dealing with the approximation of *c-numerical range* for a (possibly) unbounded operators using projection method. In Section 3, applying these results to compute the *c-numerical range* of operators.

2. Convergence Theorems

In this section we will use finite matrices to approximate the numerical range of linear operators. However, the idea of approximating linear operators by finite matrices is an obvious one that must happen again and again. Suppose that one wishes to compute the *c-numerical range* of A by using the following projection method. Let $(\mathcal{L}_k)_{k=1}^{\infty}$ be a nested family of spaces in $\mathcal{H}$ given by $\mathcal{L}_k = span\{\phi_1, \phi_2, \ldots, \phi_k\}$, where $\{\mathcal{L}_k : k \in \mathbb{N}\}$ is orthonormal basis of a Hilbert space $\mathcal{H}$ whose element lie in $\mathcal{D}(A)$ and suppose that the corresponding orthogonal projections $P_k : \mathcal{H} \to \mathcal{L}_k$, converge strongly to the identity operator I. we identify A with its matrix representation with respect to $\{\phi_k : k \in \mathbb{N}\}$,

$$A = (A_{ij})_{i,j=1}^{\infty}, \quad A_{ij} := \langle A\phi_j, \phi_i\rangle \; i, j \in \mathbb{N}.$$

Then the compression of A to $\mathcal{L}_k$ is denoted by $\mathbb{A}_k := P_k A|_{\mathcal{L}_k}$, where

$$\mathbb{A}_k = \begin{pmatrix} \langle A\phi_1, \phi_1\rangle & \langle A\phi_1, \phi_2\rangle & \ldots & \langle A\phi_1, \phi_k\rangle \\ \langle A\phi_2, \phi_1\rangle & \langle A\phi_2, \phi_2\rangle & \ldots & \langle A\phi_2, \phi_k\rangle \\ \vdots & \vdots & & \vdots \\ \langle A\phi_k, \phi_1\rangle & \langle A\phi_l, \phi_2\rangle & \ldots & \langle A\phi_k, \phi_k\rangle \end{pmatrix}. \tag{5}$$

Theorem 2.1. *Let A be a bounded operator in $\mathcal{H}$. Let $\{\mathcal{L}_k : k \in \mathbb{N}\}$ be a nested family of spaces in $\mathcal{H}$ given by $\mathcal{L}_k = span\{\phi_1, \phi_2, \ldots, \phi_k\}$, where $\{\phi_k : k \in \mathbb{N}\}$ is orthonormal, and $\mathbb{A}_k$ be as in (5). Then $W_c(\mathbb{A}_k) \subseteq W_c(A)$, for $c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n$.*

Proof Define an isometry $i : \mathcal{L}_k \to \mathbb{C}^k$ by $i\left(\sum_{j=1}^{k} \alpha_{1j}\phi_j\right) := \overset{(r)}{\alpha}$, $r = 1, \cdots k$ where $\overset{(1)}{\alpha} := (\alpha_{11}, \alpha_{12}, \cdots, \alpha_{1k}) \in O_k(\mathbb{C}^k)$, $\overset{(2)}{\alpha} := (\alpha_{21}, \alpha_{22}, \cdots, \alpha_{2k}) \in O_k(\mathbb{C}^k), \cdots, \overset{(k)}{\alpha} := (\alpha_{k1}, \alpha_{k2}, \cdots, \alpha_{kk}) \in O_k(\mathbb{C}^k)$, where $O_k(\mathbb{C}^k)$ be the set of all orthonormal k-tuples of vectors in $\mathbb{C}^k$. Suppose that $\lambda \in W_c(\mathbb{A}_k)$. Then there exist an orthonormal vectors $(\overset{(1)}{\alpha}, \overset{(2)}{\alpha}, \cdots, \overset{(k)}{\alpha}) \in \mathbb{C}^k$, such that $\lambda = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k \overset{(j)}{\alpha}, \overset{(j)}{\alpha}\rangle$. Choose $\xi_1, \xi_2, \cdots, \xi_k \in \mathcal{L}_k$, such that $i(\xi_r) = \overset{(r)}{\alpha}$, $r = 1, \cdots k$

Then a direct computation shows that $\lambda = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k \xi_j, \xi_j \rangle$, where $\xi_r = \sum_{j=1}^{k} \phi_j \alpha_{rj}$, where $r = 1, \cdots, k$. Thus $\lambda \in W_c(A)$.

The next inclusion, which will be used in the proof of Theorem 2.3, asserts that $\{W_c(\mathbb{A}_k) : k \geq 2\}$ forms an increasing sequence of sets.

Proposition 2.2. *Let $\{\mathcal{L}_k : k \in \mathbb{N}\}$ and $\mathbb{A}_k$ be as in Theorem 2.1. Given $c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n$,, then $W_c(\mathbb{A}_k) \subseteq W_c(\mathbb{A}_{k+r})$, $r = 1, 2, \ldots$.*

Proof This is an immediate consequence of the fact that $\mathbb{C}^k$ is a subspace of $\mathbb{C}^{k+1}$. In detail: if λ is in $W_c(\mathbb{A}_k)$ then we can choose $(e_1, e_2, \cdots, e_k) \in O_k(\mathbb{C}^k)$, where $e_1, e_2, \cdots, e_k$, defined in Theorem 2.1 such that $\lambda = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k e_j, e_j \rangle$, so in this case $(e_1, e_2, \cdots, e_k) \in O_k(\mathbb{C}^k)$, can be extended to vectors in $\mathbb{C}^{k+1}$, say $(\hat{e_1}, \hat{e_2}, \cdots, \hat{e_k}$, whose $(k+1)$-th components are zero. It is easy to see that $\sum_{j=1}^{k} c_j \langle \mathbb{A}_k e_j, e_j \rangle = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k \hat{e_j}, \hat{e_j} \rangle$ and the result follows.

In the following theorem, the c-numerical range of bounded operator is presented as the infinity union of c-numerical ranges of the reduction operator in a matrix polynomial by finite dimension (smaller size of a firstly linear operator).

Theorem 2.3. *Let A, $\mathbb{A}_k$ and $(\mathcal{L}_k)_k^\infty$ be as in Theorem 2.1. Suppose that $(\phi_k)_{k=1}^\infty$ is orthnormal basis of H. Then, for $c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n$ holds $\overline{W_c(A)} = \overline{\bigcup_{j=1}^\infty W_c(\mathbb{A}_j)}$.*

Proof In view of Theorem 2.1 it therefore now suffices to show $W_c(A) \subseteq \overline{\cup_{j\in\mathbb{N}} W_c(\mathbb{A}_j)}$. Suppose $\lambda \in W_c(A)$. Choose an orthonormal vectors $(\overset{(1)}{x}, \overset{(2)}{x}, \cdots, \overset{(k)}{x}) \in H$, such that $\lambda = \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle$. Since $(\phi_k)_{k=1}^\infty$ is orthnormal basis of H, then there exist sequences $\left(\overset{(i)}{x_k}\right)_{k=1}^\infty \subset \mathbb{C}$, $i = 1, \cdots, k$ with each $\overset{(1)}{x_k}, \overset{(2)}{x_k}, \cdots, \overset{(k)}{x_k} \in \operatorname{Span}\{\phi_1, \ldots, \phi_{s_k}\}$ for some $s_k > 0$, such that $\sum_{j=1}^{k} \left\|\overset{(j)}{x} - \overset{(j)}{x_k}\right\| \to 0$ and $\sum_{j=1}^{k} \left\|A\overset{(j)}{x} - A\overset{(j)}{x_k}\right\| \to 0$. So this means that $\left\|\sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle\right\| \to 0$ as $k \to \infty$.

Fix $k > 0$. Let $i : \operatorname{span}\{\phi_1, \ldots, \phi_{s_k}\} \to \mathbb{C}^{s_k}$, be the standard isometries as in the proof of Theorem 2.1. Define $\overset{(1)}{\eta_k}, \overset{(2)}{\eta_k}, \cdots, \overset{(k)}{\eta_k} \in \mathbb{C}^{s_k}$ by $\overset{(1)}{\eta_k} := i(\overset{(1)}{x_k}), \overset{(2)}{\eta_k} := i(\overset{(2)}{x_k}), \cdots, \overset{(k)}{\eta_k} := i(\overset{(k)}{x_k})$, Consider the $s_k \times s_k$ matrix $\mathbb{A}_{s_k}$ that is, the $(p, r)-$ element of $\mathbb{A}_{s_k}$ matrix is equal to $\langle A\phi_p, \phi_r \rangle$, for $p, r = 1, 2, \ldots, s_k$. Then for each $k \in \mathbb{N}$ choose $\lambda_k = \sum_{j=1}^{k} c_j \langle \mathbb{A}_{s_k} \overset{(j)}{\eta_k}, \overset{(j)}{\eta_k} \rangle$, thus a simple computation shows that $\lambda_k = \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle$. Since

$$\left\|\sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle\right\| \to 0$$

as $k \to \infty$ we have $\|\lambda_k - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle\| \to 0$. Hence there exist $\lambda_k \in W_c(\mathbb{A}_{s_k})$ such that $\lambda_k \longrightarrow \lambda$. In view of proposition 2.2 this immediately gives $\lambda \in \overline{\cup_{j\in\mathbb{N}} W_c(\mathbb{A}_j)}$.

Remark 2.4. *Let A and $(\mathcal{L}_k)_k^\infty$ be as in Theorem 2.1. Let P_k, denote orthogonal projection onto $\mathcal{L}_k$. If A is bounded then the hypotheses that $P_k \to I$,strongly as $k \to \infty$, is equivalent to the C is core of A. It is easy to construct an example to show that theses hypotheses is necessary.*

Example 2.5. *Let A be an operator matrix in $\mathcal{H} = \ell^2(\mathbb{N})$ where $A = diag\{\frac{1}{n}\}_{n=1}^\infty$ Let $(\mathcal{L}_k)_{k\in\mathbb{N}}$, be a nested family of subspace in $\ell^2(\mathbb{N})$, with $\mathcal{L}_k = Span\{e_2, ..., e_{k+1}\}$, where $e_j = j^{th}$ standard basis vector, Then performing an analysis analogous to the previous Theorem 2.3, we see that $\lambda_k = \sum_{j=1}^{k} c_j \langle \mathbb{A}_{s_k} \overset{(j)}{\eta_k}, \overset{(j)}{\eta_k} \rangle$, in the proof of Theorem 2.3 is not convergent to $\lambda = \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle$. unless $\overset{(1)}{x}$ is orthogonal to e_1.*

In what follow we assume readers familiar with basic notions, definitions and results on unbounded operators, as well as matrices of non necessarily bounded operators. useful references are [6] [7] and [8]. We call a few definitions though: A linear operator A with a domain $\mathcal{D}(A)$ contained in a Hilbert space $\mathcal{H}$ is said to be densely defined if $\mathcal{D}(A) = \mathcal{H}$. A linear operator A is closed if its graph Γ_A is closed in $\mathcal{H} \oplus \mathcal{H}$. A linear operator A is called closable if, the closure $\overline{\Gamma_A}$ of its graph is the graph of some operator. A subspace $\mathcal{D} \subset \mathcal{D}(A)$ is called a core of a closable operator A if $A|_D$ is closable with closure A. The definition of the *q-numerical range* for bounded linear operators in (2) generalizes as follows to unbounded operator matrices A with dense domain $\mathcal{D}(A)$.

Definition 2.6. *For a linear operator A with domain $\mathcal{D}(A) \subset \mathcal{H}$ we define the c-numerical range of A for $c = (c_1, c_2, \ldots, c_k)$, by*

$$W_c(A) = \left\{ \sum_{j=1}^{k} c_j \langle Ae_j, e_j \rangle : (e_1, \ldots, e_k) \text{ is an orthonormal subset of } \mathcal{D}(A)) \right\} \tag{6}$$

In the following result we describe that the closure of the range $W_c(A)$ is approximated by $W_c(\mathbb{A}_k)$ under the assumption that the linear span of $\{\phi_1, \phi_2, \ldots, \}$ is a core of A.

Theorem 2.7. *Let A be an unbounded operator in $\mathcal{H}$. Let $\{\mathcal{L}_k : k \in \mathbb{N}\}$ be a nested family of spaces in $\mathcal{D}(A)$ given by $\mathcal{L}_k = span\{\phi_1, \phi_2, \ldots, \phi_k\}$, where $\{\phi_k : k \in \mathbb{N}\}$ is orthonormal, and $\mathbb{A}_k$ be as in (5). Then $W_c(\mathbb{A}_k) \subseteq W_c(A)$, for $c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n$.*

Proof Define an isometry $i : \mathcal{L}_k \to \mathbb{C}^k$ by $i\left(\sum_{j=1}^{k} \alpha_{1j}\phi_j\right) := \overset{(r)}{\alpha}$, $r = 1, \cdots k$ where $\overset{(1)}{\alpha} := (\alpha_{11}, \alpha_{12}, \cdots, \alpha_{1k}) \in O_k(\mathbb{C}^k)$, $\overset{(2)}{\alpha} := (\alpha_{21}, \alpha_{22}, \cdots, \alpha_{2k}) \in O_k(\mathbb{C}^k), \cdots, \overset{(k)}{\alpha} := (\alpha_{k1}, \alpha_{k2}, \cdots, \alpha_{kk}) \in O_k(\mathbb{C}^k)$. Suppose that $\lambda \in W_c(\mathbb{A}_k)$. Then there exist an orthonormal vectors $(\overset{(1)}{\alpha}, \overset{(2)}{\alpha}, \cdots, \overset{(k)}{\alpha}) \in \mathbb{C}^k$, such that $\lambda = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k \overset{(j)}{\alpha}, \overset{(j)}{\alpha} \rangle$. Choose $\xi_1, \xi_2, \cdots, \xi_k \in l_k$, such that $i(\xi_r) = \overset{(r)}{\alpha}$, $r = 1, \cdots k$ Then a direct computation shows that $\lambda = \sum_{j=1}^{k} c_j \langle \mathbb{A}_k \xi_j, \xi_j \rangle$, where $\xi_r = \sum_{j=1}^{k} \phi_j \alpha_{rj}$, where $r = 1, \cdots, k$. Thus $\lambda \in W_c(A)$.

The following Proposition can be proof in a similar fashion as Proposition 2.2

Proposition 2.8. *Let $\{\mathcal{L}_k : k \in \mathbb{N}\}$ be a nested family of spaces in $\mathcal{D}(A)$ given by $\mathcal{L}_k = span\{\phi_1, \phi_2, \ldots, \phi_k\}$, where $\{\phi_k : k \in \mathbb{N}\}$ is orthonormal, and $\mathbb{A}_k$ be as in Theorem 2.1. Then $W_c(\mathbb{A}_k) \subseteq W_c(\mathbb{A}_{k+r})$, $r = 1, 2, \ldots$, for $c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n$.*

In the following theorem, the c-numerical range of unbounded operator is presented as the infinity union of c-numerical ranges of the reduction operator in a matrix by finite dimension (smaller size of a firstly linear operator).

Theorem 2.9. *Let A, $\mathbb{A}_k$ and $(\mathcal{L}_k)_k^\infty$ be as in Theorem 2.7. Suppose that A is closable operators with dense domains and $\mathbb{C} = span\{\phi_1, \phi_2, \ldots\}$ is a core of A. Then, for $c = (c_1, c_2, \ldots, c_n)$ holds $\overline{W_c(A)} = \overline{\bigcup_{j=1}^{\infty} W_c(\mathbb{A}_j)}$.*

Proof In view of Theorem 2.7 it therefore now suffices to show $W_c(A) \subseteq \overline{\cup_{j\in\mathbb{N}} W_c(\mathbb{A}_j)}$. Suppose $\lambda \in W_c(A)$. Choose an orthonormal vectors $(\overset{(1)}{x}, \overset{(2)}{x}, \cdots, \overset{(k)}{x}) \in \mathcal{D}(A)$, such that $\lambda = \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle$. Since $\mathbb{C} = \text{span}\{\phi_1, \phi_2, \ldots\}$ is a core of A, then there exist sequences $\left(\overset{(i)}{x_k}\right)_{k=1}^{\infty} \subset \mathbb{C}$, $i = 1, \cdots, k$ with each $\overset{(1)}{x_k}, \overset{(2)}{x_k}, \cdots, \overset{(k)}{x_k} \in \text{Span}\{\phi_1, \ldots, \phi_{t_k}\}$ for some $t_k > 0$, such that $\sum_{j=1}^{k} \left\| \overset{(j)}{x} - \overset{(j)}{x_k} \right\| \to 0$ and $\sum_{j=1}^{k} \left\| A\overset{(j)}{x} - A\overset{(j)}{x_k} \right\| \to 0$. So this means that

$$\left\| \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle \right\| \to 0$$

as $k \to \infty$.

Fix $k > 0$. Let $\pi : \operatorname{span}\{\phi_1, \dots, \phi_{t_k}\} \to \mathbb{C}^{t_k}$, be the standard isometries as in the proof of Theorem 2.1. Define $\overset{(1)}{\zeta_k}, \overset{(2)}{\zeta_k}, \cdots, \overset{(k)}{\zeta_k} \in \mathbb{C}^{t_k}$ by $\overset{(1)}{\zeta_k} := \pi(\overset{(1)}{x_k}), \overset{(2)}{\zeta_k} := \pi(\overset{(2)}{x_k}), \cdots, \overset{(k)}{\zeta_k} := \pi(\overset{(k)}{x_k})$, Consider the $t_k \times t_k$ matrix $\mathbb{A}_{t_k}$ that is, the $(p,r)-$ element of $\mathbb{A}_{t_k}$ matrix is equal to $\langle A\phi_p, \phi_r \rangle$, for $p, r = 1, 2, \dots, t_k$. Then for each $k \in \mathbb{N}$ choose $\lambda_k = \sum_{j=1}^{k} c_j \langle \mathbb{A}_{s_k} \overset{(j)}{\eta_k}, \overset{(j)}{\eta_k} \rangle$, thus a simple computation shows that $\lambda_k = \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle$. Since

$$\left\| \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x_k}, \overset{(j)}{x_k} \rangle \right\| \to 0$$

as $k \to \infty$ we have $\|\lambda_k - \sum_{j=1}^{k} c_j \langle A\overset{(j)}{x}, \overset{(j)}{x} \rangle\| \to 0$. Hence there exist $\lambda_k \in W_c(\mathbb{A}_{t_k})$ such that $\lambda_k \longrightarrow \lambda$. In view of proposition 2.8 this immediately gives $\lambda \in \overline{\cup_{j\in\mathbb{N}} W_c(\mathbb{A}_j)}$.

3. Numerical experiments on differential operator

In this section we study some concrete examples and demonstrate that, in spite of the results obtained in the previous section, practical computation of the *c-numerical range* of differential operator is very far from being straightforward. We define the inner product $\langle u, v \rangle$ to be linear in the first parameter and conjugate linear in the second parameter, and we consider the space of square-integrable functions, $L^2(\Omega, dx)$, where Ω is an interval in $\mathbb{R}$, a Hilbert space with inner product

$$\langle u, v \rangle = \int_{\Omega} u\bar{v}dx. \tag{7}$$

The computations were performed in Matlab.

3.1. Application to Schrödinger operator.

In this subsection, we will examine the Schrödinger operator, which fits into the framework of Sect.2. See [5] for results on computing the q-numerical range of such operators. In the Hilbert space $\mathcal{H} := L^2(0,1)$, we introduce the Schrödinger operator

$$A = -\frac{d^2}{dx^2} + q, \tag{8}$$

(with bounded potential q) and the domain of A is given by

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

Remark 3.1.

(i) Because A is self-adjoint and bounded below with purely discrete spectrum, the eigenvalues of A are given by

$$\lambda_k := \inf_{\substack{F\subset\mathcal{D}(A)\\ \dim F = k}} \sup_{\substack{y\in F\\ y\neq 0}} p(y)$$

where p is the Rayleigh functional

$$p(y) := \frac{\langle Ay, y \rangle}{\langle y, y \rangle}, \quad y \in \mathcal{D}(A),\ y \neq 0.$$

(ii) It is clear the operator A in $L^2(0,1)$ has a sequence of eigenvalues and normalized eigenfunctions for the operator A in $L^2(0,1)$ are

$$\lambda_n = n^2\pi^2,\ \phi_n(x) = \sqrt{2}\sin(n\pi x) \text{ for } n = 1,2,3,\cdots \tag{9}$$

under the setting $q(x) = 0$.

(iii) Because Eq. (8) is closed operator, then it is not difficult to see that, the subspace $C_A = span\{\phi_1,\phi_2,\ldots\} \subset \mathcal{D}(A)$ is a core of A, so in this case the main Theorem 2.9 is applicable to this example.

(iv) We may use these eigenfunctions in (9) as basis elements for a discretization of the type discussed in Section 2, form the matrix elements $\langle -\phi_k'', \phi_j\rangle$, using the inner product in Eq.(7) with respect to the orthonormal basis in equation (9) and consider the (infinite) operator matrix

$$Q := \langle -\phi_k'', \phi_j\rangle \tag{10}$$

The matrix $\mathbb{A}_k$ in (5) is obtained by taking the leading sub-matrices of the (infinite) operator matrix in (10), with appropriate dimensions. Observe that, $\langle -\phi_k'', \phi_j\rangle = \text{diag}\{\pi^2, 4\pi^2, 9\pi^2, \ldots\}$ which can be evaluated explicitly. The following figure shows attempts to calculate $W_c(\mathbb{A}_k)$ for various k and c and also some attempts to estimate these sets by qualitative means, using existing theorems from the literature as well as the theorems proved above.

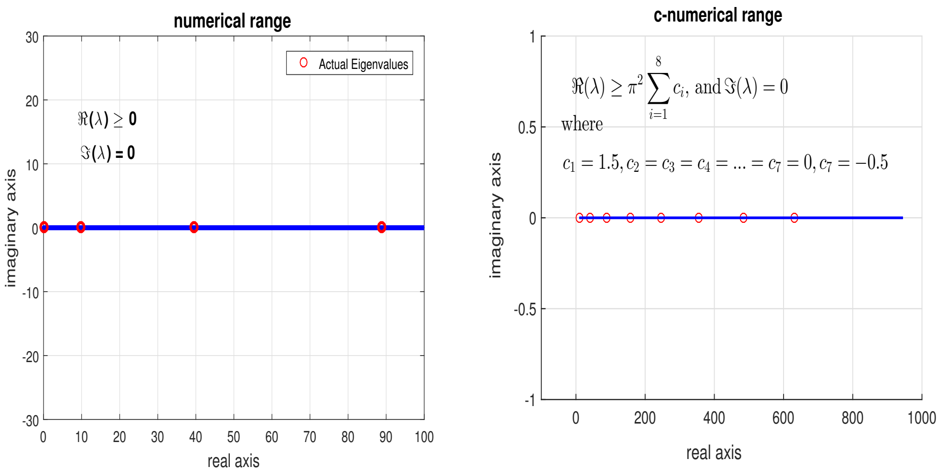

Figure 1: On the left-hand side, variational method approximation to the Schrödinger operator. The approximation $\mathbb{A}_k$ is given by a self-adjoint matrix with some real eigenvalues $\{\lambda_1, \lambda_2, \cdots, \lambda_k\}$ with $\lambda_1 \leq \lambda_2 \leq \cdots \lambda_k$. The *c-numerical range* $W_c(\mathbb{A}_8)$ of $\mathbb{A}_8$ for $c = (1,0,0,0,0,0,0,0)$ is the line segment $[\lambda_1, \lambda_8]$, the red dots are $\sigma(\mathbb{A}_8)$. On the right-hand side, the *c-numerical range* $W_c(\mathbb{A}_8)$ of $\mathbb{A}_8$ for $c = (1.5,0,0,0,0,0,0,-0.5)$ is the union of the closed circular discs. The small red circles on the real axis in side circular disk are $\sigma(\mathbb{A}_8)$.

3.2. *Analytical estimates for Schrödinger operator.*

In order to understand to what extent the Figure 1 is qualitatively correct, we now analyze the c-numerical range of the Schrödinger operator.
Suppose $\lambda \in W_c(A)$. Choose an orthonormal vectors $(\zeta_1, \zeta_2, \cdots, \zeta_k) \in \mathcal{D}(A)$ such that $\lambda = \sum_{j=1}^{k} c_j \langle A\zeta_j, \zeta_j\rangle$. In Remark 3.1 part(i), it is obvious $\sum_{j=1}^{k} c_j \langle A\zeta_j, \zeta_j\rangle \geq \pi^2 \sum_{j=1}^{k} c_j \langle \zeta_j, \zeta_j\rangle$. Thus the *c-numerical range* of Schrödinger operator is $[\pi^2 \sum_{j=1}^{k} c_j, \infty)$.

3.3. Application to Hain-Lüst operator

In this subsection we apply Theorem 2.9 to compute c-numerical range of Hain-Lüst-type operators.This operator was introduced by Hain and Lüst in application to problems of magnetohydrodynamics [14], and the problems of this type were studied in [1–4, 11, 12, 21]. Assume that $w : [0,1] \to [0,\infty)$, $\widetilde{w} : [0,1] \to [0,\infty)$, and $u : [0,1] \to \mathbb{C}$ are such that $w(x) = 1$, $\widetilde{w}(x) = 1$,

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

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

$$\tau_{\widetilde{A}} := -\tfrac{d^2}{dx^2}, \quad \tau_{\widetilde{B}} := w(x), \tag{11}$$

$$\tau_{\widetilde{C}} := \widetilde{w}(x), \quad \tau_{\widetilde{D}} := u(x). \tag{12}$$

Let A, 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

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

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

$$\mathcal{A} := \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} -\frac{d^2}{dx^2} & w(x) \\ \widetilde{w}(x) & u(x) \end{pmatrix}, \tag{13}$$

on the domain

$$\mathcal{D}(\mathcal{A}) := (H^2(0,1) \cap H_0^1(0,1)) \oplus L^2(0,1). \tag{14}$$

Remark 3.2.

(i) By [9, Corollary VII.2.7], the operator $A := -\frac{d^2}{dx^2}$ with domain $\mathcal{D}(A) := (H^2(0,1) \cap H_0^1(0,1))$ is closed. Moreover, because $\mathcal{D}(A) \subset \mathcal{D}(C)$, then the operator C is A-bounded with relative bound 0. This follows since, there is a $\gamma > 0$ such that, for every $\epsilon > 0$

$$\|Cf\|^2 \le \gamma \|\langle Af, f\rangle\| \le \gamma(\epsilon\|Af\|^2 + \epsilon^{-1}\|f\|^2).$$

On the other hand $\mathcal{D}(D) \subset \mathcal{D}(B)$, then the operator B is D-bounded we conclude that the operator matrix $\mathcal{D}(\mathcal{A})$ is diagonally dominant of order 0; it is closed by [7, Corollary 2.2.9 (i)].

(ii) In Eq.(13), since A is self-adjoint with purely discrete spectrum, then the linear span $C_A = \operatorname{span}\{\phi_1, \phi_2, \ldots\}$ is a core of A, where $\{\phi_k : \ k \in \mathbb{N}\}$ is an orthonormal basis in $L^2(0,1)$, and by the same argument because D in Eq. (13) is bounded then the linear span $C_D = \operatorname{span}\{\phi_1, \phi_2, \ldots\}$ is a core of D. Hence it is not difficult to see that the subspace $C := C_A \oplus C_D \subset \mathcal{D}(\mathcal{A}) = (\mathcal{D}(A) \cap \mathcal{D}(C)) \oplus (\mathcal{D}(B) \cap \mathcal{D}(D))$ is a core of $\mathcal{A}$. So the main Theorem 2.8 is applicable to this example.

(iii) We may use the eigenfunctions in Eq.(9) as basis elements for a discretization of the type discussed in Section 2, forming the matrix elements $\langle A\phi_k, \phi_j\rangle$, $\langle w\phi_k, \phi_j\rangle$, $\langle \widetilde{w}\phi_k, \phi_j\rangle$, $\langle u\phi_k, \phi_j\rangle$, with respect to the inner product in (7) and considering the infinite block matrix

$$Q := \begin{pmatrix} \langle A\phi_k, \phi_j\rangle & \langle w\phi_k, \phi_j\rangle \\ \langle \widetilde{w}\phi_k, \phi_j\rangle & \langle u\phi_k, \phi_j\rangle \end{pmatrix}.$$

The defined matrix $\mathbb{A}_k$ in (5) is obtained by taking the leading sub-matrices of the block Q, with appropriate dimensions. Observe that
$\langle A\phi_k, \phi_j\rangle = \mathrm{diag}\{\pi^2, 4\pi^2, 9\pi^2, \ldots\}$, $\langle w\phi_k, \phi_j\rangle = \mathrm{diag}\{1, 1, 1, \ldots\}$, $\langle \widetilde{w}\phi_k, \phi_j\rangle = \mathrm{diag}\{1, 1, 1, \ldots\}$, and $\langle u\phi_k, \phi_j\rangle = 56\int_0^{1/2} e^{4\pi ix}\sin(k\pi x)\sin(j\pi x)dx + 56\int_1^{1/2} e^{4\pi ix}\sin(k\pi x)\sin(j\pi x)dx - 65\delta_{k,j}$, which can be evaluated explicitly. If the operator A included a potential, for instance, then its eigenfunctions would not generally be explicitly computable. We could still use the functions ϕ_j in (9) as basis functions, but the matrix elements $\langle A\phi_k, \phi_j\rangle$ would have to be computed by quadrature and the corresponding matrix would no longer diagonal. The following figure show attempts to compute the numerical approximation of the boundary of $W_c(\mathbb{A}_k)$ for various k, and c also some attempts to estimate these sets by qualitative means, using existing theorems from the literature as well as the theorems proved above.

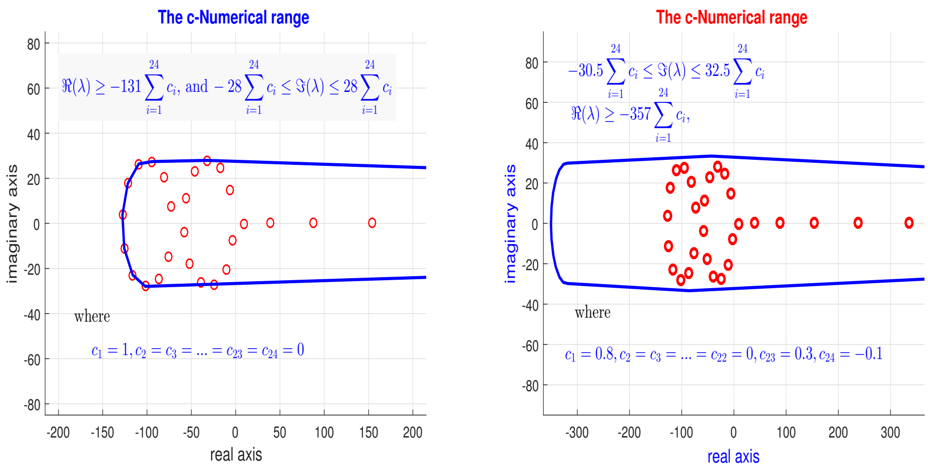

Figure 2: On the left-hand side, Variational method approximation to the Hain-Lüst operator for computing *c-numerical range* $W_c(\mathbb{A}_{24})$ of $\mathbb{A}_{24}$ for $c = (c_1, c_2, \cdots, c_{24})$ where $c_1 = 1$, $c_2 = c_3 = \cdots, c_{24} = 0$ The red dots are $\sigma(\mathbb{A}_{24})$. On the right-hand side, for $c_1 = 0.8$, $c_2 = c_3 = \cdots, c_{22} = 0$, $c_{23} = 0.3$ and $c_{24} = -0.1$. Variational method approximation for computing $W_c(\mathbb{A}_{24})$ of $\mathbb{A}_{24}$. The red dots are $\sigma(\mathbb{A}_{24})$.

3.4. *Analytical estimates for non self-adjoint Hain-L¨ust operator*

In order to understand the results in Figure 2 it is useful to find an analytical estimate for $W_c(\mathcal{A})$. Let $\underline{\eta}_1, \underline{\eta}_2, \cdots, \underline{\eta}_k$ be an orthonormal vectors in $\mathcal{D}(\mathcal{A})$ where

$$\underline{\eta}_1 = \begin{pmatrix} \eta_{11} \\ \eta_{12} \end{pmatrix}, \ \underline{y}_2 = \begin{pmatrix} \eta_{21} \\ \eta_{22} \end{pmatrix}, \cdots, \ \underline{\eta}_k = \begin{pmatrix} \eta_{k1} \\ \eta_{k2} \end{pmatrix}$$

and let

$$\begin{aligned} \lambda &= \sum_{j=1}^{k} c_j \langle \mathcal{A}\underline{\eta}_j, \underline{\eta}_j \rangle \\ &= \sum_{j=1}^{k} c_j \langle -\eta_{j1}'', \eta_{j1} \rangle_{L^2(0,1)} + 2\sum_{j=1}^{k} c_j \Re\langle \eta_{j1}, \eta_{j2} \rangle_{L^2(0,1)} + \sum_{j=1}^{k} c_j \langle \eta_{j2}, \eta_{j1} \rangle_{L^2(0,1)} \end{aligned} \tag{15}$$

The first term of Eq.(15) gives, as an estimate;

$$\sum_{j=1}^{k} c_j \langle -\eta_{j1}'', \eta_{j1} \rangle_{L^2(0,1)} \geq \pi^2 \sum_{j=1}^{k} c_j \langle \eta_{j1}, \eta_{j1} \rangle_{L^2(0,1)} \tag{16}$$

For the second term on the right hand side of Eq.(15), the Cauchy Schwarz inequality and Youngs inequality yield

$$2\sum_{j=1}^{k} c_j \Re\langle \eta_{j1}, \eta_{j2}\rangle_{L^2(0,1)} \geq -\sum_{j=1}^{k} c_j. \tag{17}$$

The third term of the right hand side of Eq. (15) satisfies

$$\sum_{j=1}^{k} c_j \langle u\eta_{j2}, \eta_{j1}\rangle_{L^2(0,1)} \geq \inf_{x\in[0,1]} \Re(u) \sum_{j=1}^{k} c_j (1 - \langle \eta_{j1}, \eta_{j1}\rangle_{L^2(0,1)}). \tag{18}$$

Hence from equations (16),(17) and (18) we get that

$$\Re(\lambda) \geq (\pi^2 - \inf_{x\in[0,1]} \Re(u)) \sum_{j=1}^{k} c_j \langle \eta_{j1}, \eta_{j1}\rangle_{L^2(0,1)} + (\inf_{x\in[0,1]} \Re(u) - 1) \sum_{j=1}^{k} c_j. \tag{19}$$

This yields

$$\Re(\lambda) \geq \begin{cases} (\inf\limits_{x\in[0,1]} \Re(u) - 1) \sum_{j=1}^{k} c_j, & \text{if } \pi^2 - \inf\limits_{x\in[0,1]} \Re(u) \geq 0; \\ (\pi^2 - 1) \sum_{j=1}^{k} c_j, & \text{if } \pi^2 - \inf\limits_{x\in[0,1]} \Re(u) < 0. \end{cases}$$

For our example these yield $\Re(\lambda) \geq -131 \sum_{j=1}^{k} c_j$. To estimate $\Im(\lambda)$ observe that

$$\begin{aligned} \Im(\lambda) &= \sum_{j=1}^{k} c_j \langle u\eta_{j2}, \eta_{j1}\rangle_{L^2(0,1)} \\ &\leq \sup_{x\in[0,1]} \Im(u) \sum_{j=1}^{k} c_j \langle \eta_{j2}, \eta_{j2}\rangle_{L^2(0,1)}) \leq 18 \sum_{j=1}^{k} c_j \langle \eta_{j2}, \eta_{j2}\rangle_{L^2(0,1)}) \end{aligned} \tag{20}$$

and

$$\begin{aligned} \Im(\lambda) &= \sum_{j=1}^{k} c_j \langle u\eta_{j2}, \eta_{j1}\rangle_{L^2(0,1)} \\ &\geq \inf_{x\in[0,1]} \Im(u) \sum_{j=1}^{k} c_j \langle \eta_{j2}, \eta_{j2}\rangle_{L^2(0,1)}) \geq -18 \sum_{j=1}^{k} c_j \langle \eta_{j2}, \eta_{j2}\rangle_{L^2(0,1)}) \end{aligned} \tag{21}$$

hence

$$-28 \sum_{j=1}^{k} c_j \leq \Im(\lambda) \leq 28 \sum_{j=1}^{k} c_j.$$

This completes the estimates on $W_c(\mathcal{A})$.

The following result shows that the *c-numerical range* of Hain-L¨ust operator, is unbounded.

Remark 3.3. *Let $\eta_1, \eta_2, \cdots, \eta_k$ be an orthonormal vectors in $\mathcal{D}(\mathcal{A})$, where*

$$\eta_1 = \begin{pmatrix} \sqrt{2}sin(l\pi x) \\ 0 \end{pmatrix}, \eta_2 = \begin{pmatrix} \sqrt{2}sin(k\pi x) \\ 0 \end{pmatrix}, \cdots, \eta_k = \begin{pmatrix} \sqrt{2}sin(k\pi x) \\ 0 \end{pmatrix}$$

then

$$\sum_{j=1}^{k} c_j \langle A\eta_j, \eta_j\rangle_{L^2(0,1)} = l^2\pi^2 \sum_{j=1}^{k} c_j.$$

But $l \in \mathbb{Z}$ can be arbitrary large. This means that $\Re(\lambda)$ is unbounded above.

4. Conclusions

This paper illustrates the practical difficulties associated with the computation of *c-numerical ranges* of operator matrices and block operator matrices of differential operators, even when good theoretical results are available to underpin the approximation procedure. Purely analytic approaches are still needed to understand when the numerical results are deceptive, and even apparently convincing numerical results should be treated with skepticism.

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