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RESEARCH ARTICLE



Convergent spectral inclusion sets for banded matrices

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Abstract

We obtain sequences of inclusion sets for the spectrum, essential spectrum, and pseudospectrum of banded, in general non-normal, matrices of finite or infinite size. Each inclusion set is the union of the pseudospectra of certain submatrices of a chosen size n. Via the choice of n, one can balance accuracy of approximation against computational cost, and we show, in the case of infinite matrices, convergence as $n \to \infty$ of the respective inclusion set to the corresponding spectral set.

INTRODUCTION 1

In many finite difference schemes or in physical or social models, where interaction between objects is direct in a finite radius only (and is of course indirect on a global level), the corresponding matrix or operator is banded, also called of finite dispersion, meaning that the matrix is supported on finitely many diagonals only. In the case of finite matrices this is of course a tautology; in that context one assumes that the bandwidth is not only finite but small compared to the matrix size, where the bandwidth of a matrix A is the distance from the main diagonal in which nonzeros can occur. (Precisely: it is the largest |i-j| over all matrix positions (i,j) with $A_{i,j} \neq 0$.) So this is our setting: finite, semi-infinite or bi-infinite banded matrices.

We equip the underlying vector space with the Euclidian norm, so our operators act on an ℓ^2 space over $\{1, ..., N\}$ or $\mathbb{N} = \{1, 2, ...\}$ or $\mathbb{Z} = \{..., -1, 0, 1, ...\}$. In the two latter cases (semi- and bi-infinite matrices), we assume each diagonal to be a bounded sequence, whence the matrix acts as a bounded linear operator, again denoted by A, on the corresponding ℓ^2 space.

The exact computation of the spectrum by analytical means is in general impossible (by Abel-Ruffini) if the size of the matrix is larger than four. So one is forced to resort to approximations. But for non-normal matrices and operators, also the approximation of the spectrum is extremely delicate and unreliable, hence one often substitutes for the spectrum, spec A, the pseudospectrum,

$$\operatorname{spec}_{\varepsilon} A := \{ \lambda \in \mathbb{C} : \| (A - \lambda I)^{-1} \| > 1/\varepsilon \}, \qquad \varepsilon > 0,$$

that is much more stable to approximate, and then sends $\varepsilon \to 0$. Note that, by agreeing to say $||B^{-1}|| = \infty$ if B is not invertible, one has spec $A \subset \operatorname{spec}_{\varepsilon} A$ for all $\varepsilon > 0$. For an impressive account of pseudospectra and their applications, see the monograph [1].

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Our aim in this paper is to derive inclusion sets for spec A, spec_{ε}A as well as the essential spectrum, spec_{ess} A, in terms of unions of pseudospectra of moderately sized (but many) finite submatrices of A of column dimension n. Moreover, if the matrix is infinite, we prove convergence, as $n \to \infty$, of the respective inclusion set to each of spec A, spec_{ε}A, or spec_{ε}A.

2 | APPROXIMATING THE LOWER NORM ON $\ell^2(\mathbb{Z})$

Our arguments are, perhaps surprisingly, tailor-made for the case of bi-infinite vectors and matrices on them. In fact, instead of $\ell^2(\mathbb{Z})$, everything also works for $\ell^2(G)$ with a discrete group G, for example, $G = \mathbb{Z}^d$, subject to Yu's so-called Property A [2, 3]. Only later, in Section 6, we manage to work around the group structure and to transfer results to $\ell^2(\mathbb{N})$ and $\ell^2(\{1, ..., N\})$, hence: to semi-infinite and finite matrices.

As some sort of antagonist of the operator norm, $||A|| = \sup\{||Ax|| : ||x|| = 1\}$, we look at the so-called *lower norm*¹

$$\nu(A) := \inf\{||Ax|| : ||x|| = 1\}$$

of a banded and bounded operator on $\ell^2(\mathbb{Z})$. Fixing $n \in \mathbb{N}$ and limiting the selection of unit vectors x to those with a finite support of diameter less than n, further limits how small ||Ax|| can get. Precisely,

$$\nu_n(A) := \inf\{\|Ax\| : \|x\| = 1, \operatorname{diam}(\sup x) < n\}, \quad n \in \mathbb{N},$$
 (2.1)

is typically larger than $\nu(A)$ – but (and this is remarkable) only larger by at most the amount of a certain $\varepsilon_n \sim 1/n$ that we will quantify precisely below. Let us first write this important fact down:

$$\nu_n(A) - \varepsilon_n \le \nu(A) \le \nu_n(A). \tag{2.2}$$

This observation can be traced back to refs. [4, 5] and, for Schrödinger operators, even to refs. [6, 7]. Extensive use has been made of (2.2), for example, in refs. [8, 9]. The statement diam(supp x) < n in (2.1) translates to supp $x \subseteq k + \{1, ..., n\}$ for some $k \in \mathbb{Z}$. Hence,

$$\nu_n(A) = \inf\{\nu(A|_{\ell^2(k+\{1,\dots,n\}\}}) : k \in \mathbb{Z}\}.$$
(2.3)

Let us write $P_{n,k}$ for the operator of multiplication by the characteristic function of $k + \{1, ..., n\}$ and agree on writing

$$A|_{\ell^{2}(k+\{1,...,n\})} = : AP_{n,k} : \ell^{2}(k+\{1,...,n\}) \to \ell^{2}(\mathbb{Z}), \quad n \in \mathbb{N}, k \in \mathbb{Z}.$$

In matrix language, $AP_{n,k}$ corresponds to the matrix formed by columns number k+1 to k+n of A. By the band structure of A, that submatrix is supported in finitely many rows only, even reducing it to a finite $m \times n$ matrix, where m equals n plus two times the bandwidth of A. Then $\nu(AP_{n,k})$, as in (2.3), is the smallest singular value of this $m \times n$ matrix, making this a standard computation.

3 | ε_n AND THE REDUCTION TO TRIDIAGONAL FORM

Our analysis of ε_n is particularly optimized in the case of tridiagonal matrices, that is when A has bandwidth one, so that it is only supported on the main diagonal and its two adjacent diagonals. Let $\alpha, \beta, \gamma \in \ell^{\infty}(\mathbb{Z})$ denote, in this order, the sub-, main- and superdiagonal of A, with entries $\alpha_i = A_{i+1,i}$, $\beta_i = A_{i,i}$ and $\gamma_i = A_{i-1,i}$ with $i \in \mathbb{Z}$. In that case (see refs. [4, 12, 13]),

$$\varepsilon_n = 2(\|\alpha\|_{\infty} + \|\gamma\|_{\infty}) \sin \frac{\pi}{2(n+1)} < (\|\alpha\|_{\infty} + \|\gamma\|_{\infty}) \frac{\pi}{n+1} \sim \frac{1}{n}.$$
 (3.1)

¹ It is not a norm! Our terminology is that of refs. [10, 11].

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Although (2.2) holds with this choice of ε_n for the very general setting of all tridiagonal matrices, formula (3.1) turns out to be best possible in some nontrivial examples such as the shift operator [12].

To profit from these well-tuned parameters also in the case of larger bandwidths, note that (2.2) and (3.1) even work in the block case, that is when the entries in the ℓ^2 vectors are themselves elements of some Banach space X and the matrix entries of A are operators on X. So the trick with a band matrix B with a larger bandwidth b is to interpret B as block-tridiagonal with blocks of size b+1:

$$B = \begin{pmatrix} A_{1,1} & A_{1,2} & A_{1,3} & A_{1,4} \\ A_{2,1} & A_{2,2} & A_{2,3} & A_{2,4} \\ A_{3,1} & A_{3,2} & A_{3,3} & A_{3,4} \\ A_{4,1} & A_{4,2} & A_{4,3} & A_{4,4} \end{pmatrix} = A.$$

Here, a matrix *B* with bandwidth b = 2 is identified with a block-tridiagonal matrix *A* with 3×3 blocks, noting that 3 = b + 1.

Since the blocks of A can be operators on a Banach space X, one can even study spec B and spec_{ε}B by our techniques for bounded operators B on $L^2(\mathbb{R}) \cong \ell^2(\mathbb{Z}, X)$, where $X = L^2([0, 1])$, for example, for integral operators B with a banded kernel $k(\cdot, \cdot)$.

4 | THE ROLE OF THE LOWER NORM IN SPECTRAL COMPUTATIONS

If A sends a unit vector x to a vector Ax with norm $\frac{1}{4}$ then, clearly, A^{-1} , bringing Ax back to x, has to have at least norm four. The lower norm, $\nu(A)$, is pushing this observation to the extreme. By minimizing $\frac{\|Ax\|}{\|x\|}$, it minimizes $\frac{\|y\|}{\|A^{-1}y\|}$ and hence computes the reciprocal of $\|A^{-1}\|$ – with one possible exception: non-invertibility of A due to $\nu(A) = 0$ or $\nu(A^*) = 0$. Properly: since $\nu(A) > 0$ iff A is injective and has a closed range (e.g., [10, Lemma 2.32]), A is invertible iff both $\nu(A)$ and $\nu(A^*)$ are nonzero². Keeping this symmetry of A and A^* in mind,

$$1/\|A^{-1}\| = \min\{\nu(A), \nu(A^*)\} =: \mu(A),$$

(see, e.g., [2]), where, again, $||A^{-1}|| = \infty$ signals non-invertibility and where $1/\infty := 0$. From here it is just a small step to

$$\operatorname{spec} A = \{\lambda \in \mathbb{C} : \|(A - \lambda I)^{-1}\| = \infty\} = \{\lambda \in \mathbb{C} : \mu(A - \lambda I) = 0\}$$

and

$$\operatorname{spec}_{\varepsilon} A = \{ \lambda \in \mathbb{C} : \| (A - \lambda I)^{-1} \| > 1/\varepsilon \} = \{ \lambda \in \mathbb{C} : \mu(A - \lambda I) < \varepsilon \}, \qquad \varepsilon > 0.$$
 (4.1)

Being able to approximate $\nu(A)$, up to $\varepsilon_n \sim \frac{1}{n}$, by $\nu_n(A)$, enables us to approximate spec A and spec $\varepsilon_n(A)$, with a controllable error, by sets built on $\nu_n(A-\lambda I)$ and $\nu_n(A^*-\lambda I)$.

5 | APPROXIMATING THE PSEUDOSPECTRUM IN THE BI-INFINITE CASE

Applying (2.2) to $A - \lambda I$ and $(A - \lambda I)^* = A^* - \lambda I$ in place of A, we see that

$$\mu_n(A - \lambda I) < \varepsilon \quad \Rightarrow \quad \mu(A - \lambda I) < \varepsilon \quad \Rightarrow \quad \mu_n(A - \lambda I) < \varepsilon + \varepsilon_n,$$

where $\mu_n(B) := \min\{\nu_n(B), \nu_n(B^*)\}$, noting that ε_n is independent of $\lambda \in \mathbb{C}$, by (3.1).

² By A^* we denote the Banach space adjoint of A. In particular, $(\lambda I)^* = \lambda I$, not $\overline{\lambda}I$.

Combining this with (2.3) and (4.1), we conclude (cf. [4, Thm. 4.3 & Cor. 4.4]):

Proposition 5.1 (Bi-infinite case). For bounded band operators A on $\ell^2(\mathbb{Z})$ and corresponding ε_n from $(3.1)^3$, one has

$$\bigcup_{k\in\mathbb{Z}}\operatorname{spec}_{\varepsilon}(AP_{n,k},A^*P_{n,k}) \subseteq \operatorname{spec}_{\varepsilon}A \subseteq \bigcup_{k\in\mathbb{Z}}\operatorname{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k},A^*P_{n,k}), \qquad \varepsilon>0, \ n\in\mathbb{N}, \tag{5.1}$$

where we abbreviate $\operatorname{spec}_{\mathfrak{c}}(A,B) := \operatorname{spec}_{\mathfrak{c}}A \cup \operatorname{spec}_{\mathfrak{c}}B$.

By iterated application of (5.1), one can extend (5.1) to the left and right as follows:

$$\operatorname{spec}_{\varepsilon-\varepsilon_n}A\subseteq\bigcup_{k\in\mathbb{Z}}\operatorname{spec}_\varepsilon(AP_{n,k},A^*P_{n,k})\subseteq\operatorname{spec}_\varepsilon A\subseteq\bigcup_{k\in\mathbb{Z}}\operatorname{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k},A^*P_{n,k})\subseteq\operatorname{spec}_{\varepsilon+\varepsilon_n}A.$$

And now, sending $n \to \infty$, we have $\varepsilon_n \to 0$, by (3.1), and then Hausdorff-convergence $\operatorname{spec}_{\varepsilon + \varepsilon_n} A \to \operatorname{spec}_{\varepsilon} A$ as well as $\operatorname{spec}_{\varepsilon - \varepsilon_n} A \to \operatorname{spec}_{\varepsilon} A$, see for example, [14]⁴. We conclude (cf. [4, Sec. 4.3]):

Proposition 5.2. The subsets and supersets of spec_sA in (5.1) both Hausdorff-converge to spec_sA as $n \to \infty$.

6 | APPROXIMATING THE PSEUDOSPECTRA OF SEMI-INFINITE AND FINITE MATRICES

Now take a bounded and banded operator A on $\ell^2(\mathbb{N})$. In ref. [13] we show how to reduce this case (via embedding A into a bi-infinite matrix plus some further arguments) to the bi-infinite result:

Proposition 6.1 (Semi-infinite case). For bounded band operators A on $\ell^2(\mathbb{N})$ and corresponding ε_n from (3.1), one has

$$\bigcup_{k\in\mathbb{N}_0}\operatorname{spec}_\varepsilon(AP_{n,k},A^*P_{n,k}) \quad \subseteq \quad \operatorname{spec}_\varepsilon A \quad \subseteq \quad \bigcup_{k\in\mathbb{N}_0}\operatorname{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k},A^*P_{n,k}), \qquad \varepsilon>0, \ n\in\mathbb{N},$$

where again spec_e $(A, B) := \operatorname{spec}_{\varepsilon} A \cup \operatorname{spec}_{\varepsilon} B$. Also here the sub- and supersets Hausdorff-converge to $\operatorname{spec}_{\varepsilon} A$ as $n \to \infty$.

The technique that helps to deal with one endpoint on the axis can essentially be repeated for a second endpoint:

Proposition 6.2 (Finite case). For finite band matrices A on $\ell^2(\{1,...,N\})$ with some $N \in \mathbb{N}$, one has

$$\bigcup_{k=0}^{N-n}\operatorname{spec}_{\varepsilon}(AP_{n,k},A^*P_{n,k}) \quad \subseteq \quad \operatorname{spec}_{\varepsilon}A \quad \subseteq \quad \bigcup_{k=0}^{N-n}\operatorname{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k},A^*P_{n,k}), \qquad \varepsilon>0, \ \ 1\leq n\leq N,$$

where again $\operatorname{spec}_{\varepsilon}(A, B) := \operatorname{spec}_{\varepsilon} A \cup \operatorname{spec}_{\varepsilon} B$.

This time, of course, there is no way of sending $n \to \infty$, hence no Hausdorff-convergence result.

7 | APPROXIMATING SPECTRA

So far we have convergent subsets and supersets of spec $_{\varepsilon}A$ for $\varepsilon > 0$. The spectrum, spec A, can now be Hausdorff-approximated via sending $\varepsilon \to 0$. However, there is a more direct approach: introducing closed-set versions of

³ Note that ε_n , if using (3.1), has to be computed for the block-tridiagonal representation of A, see Section 3.

 $^{^4}$ In the case of a Banach space-valued ℓ^2 , that Banach space should be finite-dimensional or subject to the conditions in Theorem 2.5 of ref. [14].

$$\operatorname{Spec}_{\varepsilon} A := \{ \lambda \in \mathbb{C} : \| (A - \lambda I)^{-1} \| \ge 1/\varepsilon \} = \{ \lambda \in \mathbb{C} : \mu(A - \lambda I) \le \varepsilon \}, \qquad \varepsilon \ge 0,$$

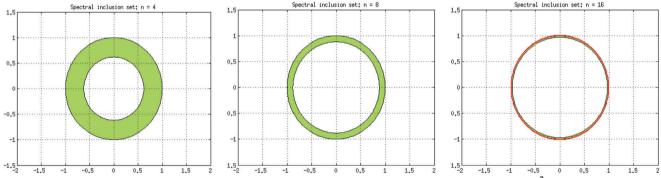
we can prove identical copies of Propositions 5.1, 6.1 and 6.2 with upper-case (i.e., closed) instead of lower-case (i.e., open) pseudospectra everywhere – and including the case $\varepsilon = 0$, see ref. [13]. The latter brings convergent supersets for spec $A = \operatorname{Spec}_0 A$ right away, without the need for a further limit $\varepsilon \to 0$. Here is the new formula for the bi-infinite case, evaluated for $\varepsilon = 0$.

$$\bigcup_{k\in\mathbb{Z}}\operatorname{spec}\left(AP_{n,k},A^*P_{n,k}\right)\subseteq\operatorname{spec}A\subseteq\bigcup_{k\in\mathbb{Z}}\operatorname{Spec}_{\varepsilon_n}(AP_{n,k},A^*P_{n,k}),\qquad n\in\mathbb{N}.\tag{7.1}$$

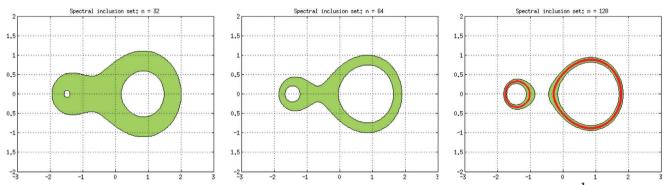
8 | EXAMPLES

For three selected operator examples, we show the Hausdorff-convergent (as $n \to \infty$) superset bounds on spec A from (7.1). All three operators are given by tridiagonal bi-infinite matrices. Moreover, all three matrices are periodic, so that we can analytically compute the spectrum by Floquet-Bloch; that is, treating the 3-periodic matrix as a 3×3 -block convolution on $\ell^2(\mathbb{Z}, \mathbb{C}^3)$ and turning that, via the corresponding block-valued Fourier-transform, into a 3×3 -block multiplication on $L^2(\mathbb{T}, \mathbb{C}^3)$, whose spectrum is obvious, see, for example, Theorem 4.4.9 in ref. [15]. For comparison, the exact spectrum is superimposed in each example as a red curve in the last column.

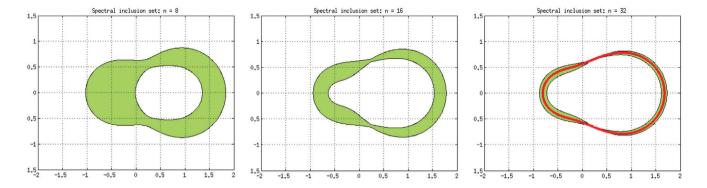
a) We start with the right shift, where the subdiagonal is $\alpha = (..., 1, 1, 1, ...)$ and the main and superdigonal are $\beta = \gamma = (..., 0, 0, 0, ...)$. The spectrum is the unit circle, and here are our supersets for $n \in \{4, 8, 16\}$:



b) Our next example is 3-periodic with subdiagonal $\alpha = (..., \mathbf{0}, 0, 0, ...)$, main diagonal $\beta = (..., -\frac{3}{2}, 1, 1, ...)$ and super-diagonal $\gamma = (..., \mathbf{1}, 2, 1, ...)$, where α_0 , β_0 and γ_0 are highlighted in boldface. The spectrum consists of two disjoint loops, and we depict our supersets for $n \in \{32, 64, 128\}$:



c) Our third example is also 3-periodic with subdiagonal $\alpha = (..., \mathbf{0}, 0, 0, ...)$, main diagonal $\beta = (..., -\frac{1}{2}, 1, 1, ...)$ and superdiagonal $\gamma = (..., \mathbf{1}, 2, 1, ...)$, where α_0 , β_0 and γ_0 are highlighted in boldface. The spectrum consists of one loop, and we depict our supersets for $n \in \{8, 16, 32\}$:



Another effect of the 3-periodicity of the diagonals in A is that there are only three distinct submatrices $AP_{n,k}$ and $A^*P_{n,k}$ each for $k \in \mathbb{Z}$. In fact, for many operator classes, the infinite unions in (5.1), (7.1) and so on, reduce to finite unions. For example, for a $\{0,1\}$ -valued aperiodic diagonal [16], there are only n+1 different subwords of length n, and for a $\{0,1\}$ -valued random diagonal, there are 2^n (again, finitely many) different subwords of length n. Also, for non-discrete diagonal alphabets, the infinite union can be reduced to a finite one via compactness arguments, see our discussion in ref. [12].

9 | APPROXIMATING ESSENTIAL SPECTRA

In the case where A is an infinite matrix there is large interest also in the approximation of the *essential spectrum*, spec_{ess} A, which is the spectrum in the Calkin algebra, that is, the set of all $\lambda \in \mathbb{C}$ where $A - \lambda I$ is not a Fredholm operator, that is, is not invertible modulo compact operators.

Our results in this section apply when each $A_{i,j} \in \mathbb{C}$, but also when each $A_{i,j}$ is a bounded linear operator on a Banach space X, as long as X is finite-dimensional or the operators $\{A_{i,j}\}$ are collectively compact in the sense of refs. [17, 18].

As for the spectrum (see Section 3) it is enough to consider the case when *A* is tridiagonal. The bi-infinite case is easily reduced to the semi-infinite case: Indeed, modulo compact operators,

so that

$$\operatorname{spec}_{\operatorname{ess}} A = \operatorname{spec}_{\operatorname{ess}} A_{-} \cup \operatorname{spec}_{\operatorname{ess}} A_{+}.$$

It remains to look at semi-infinite banded matrices A. Modulo compact operators, for every $m \in \mathbb{N}$,

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} & \ddots \\ & \ddots & \ddots \end{pmatrix} \cong \begin{pmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & & \\ & & & A_{m+1,m+1} & A_{m+1,m+2} \\ & & & & A_{m+2,m+1} & A_{m+2,m+2} & \ddots \\ & & & & \ddots & \ddots \end{pmatrix},$$

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so that, with

$$\begin{pmatrix} A_{m+1,m+1} & A_{m+1,m+2} \\ A_{m+2,m+1} & A_{m+2,m+2} & \ddots \\ & \ddots & \ddots \end{pmatrix} = \colon A_{>m} \,,$$

we have

$$\operatorname{spec}_{\operatorname{ess}} A \ = \ \operatorname{spec}_{\operatorname{ess}} A_{>m} \ \subseteq \ \operatorname{spec} A_{>m} \ \subseteq \ \bigcup_{k \ge m} \operatorname{Spec}_{\varepsilon_n} (A P_{n,k}, A^* P_{n,k}), \qquad m,n \in \mathbb{N},$$

using the semi-infinite version of (7.1) in the last step. Taking the intersection over all $m, n \in \mathbb{N}$ gives

$$\operatorname{spec}_{\operatorname{ess}} A \subseteq \bigcap_{n \in \mathbb{N}} \bigcap_{m \in \mathbb{N}} \bigcup_{k \geq m} \operatorname{Spec}_{\varepsilon_n} (AP_{n,k}, A^* P_{n,k}). \tag{9.1}$$

In ref. [13], using results from ref. [2], we prove the following:

Proposition 9.1 (Semi-infinite). For bounded band operators A on $\ell^2(\mathbb{N})$, formula (9.1) holds in fact with " \subseteq " replaced by equality. In addition, after this replacement,

- a) the intersection sign " $\cap_{n\in\mathbb{N}}$ " in (9.1) can be replaced by a Hausdorff-limit $\lim_{n\to\infty}$;
- b) the two intersection signs " $\cap_{n\in\mathbb{N}}\cap_{m\in\mathbb{N}}$ " in (9.1) can be replaced by a single Hausdorff-limit $\lim_{m=n\to\infty}$.

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