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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.

1 | INTRODUCTION

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 $\{1,\dots,N\}$ or $\mathbb{N} = \{1,2,\dots\}$ or $\mathbb{Z} = \{\dots,-1,0,1,\dots\}$. 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*,

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

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 $\mathrm{spec}\, A \subset \mathrm{spec}_\varepsilon A$ for all $\varepsilon > 0$. For an impressive account of pseudospectra and their applications, see the monograph [1].

Our aim in this paper is to derive inclusion sets for $\operatorname{spec} A$, $\operatorname{spec}_\varepsilon A$ as well as the essential spectrum, $\operatorname{spec}_{\mathrm{ess}} A$, 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 $\operatorname{spec} A$, $\operatorname{spec}_\varepsilon A$, or $\operatorname{spec}_{\mathrm{ess}} A$.

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 $\ell^2(\{1, \dots, N\})$, 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,

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

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 $\operatorname{diam}(\operatorname{supp} x) < n$ in (2.1) translates to $\operatorname{supp} x \subseteq k + \{1, \dots, n\}$ for some $k \in \mathbb{Z}$. Hence,

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

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

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

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

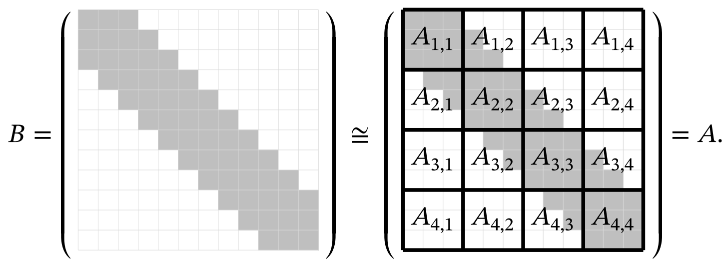
Our analysis of ε_n is particularly optimized in the case of tridiagonal matrices, that is when A has bandwidth one, so that it is only supported on the main diagonal and its two adjacent diagonals. Let $\alpha, \beta, \gamma \in \ell^\infty(\mathbb{Z})$ denote, in this order, the sub-, main- and superdiagonal 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]),

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

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

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 $b+1$:



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 $\operatorname{spec} B$ and $\operatorname{spec}_\varepsilon B$ 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 nonzero[2]. 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

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

Being able to approximate $\nu(A)$, up to $\varepsilon_n \sim \frac{1}{n}$, by $\nu_n(A)$, enables us to approximate $\operatorname{spec} A$ and $\operatorname{spec}_\varepsilon A$, 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*

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

where we abbreviate $\mathrm{spec}_\varepsilon(A,B) := \mathrm{spec}_\varepsilon A \cup \mathrm{spec}_\varepsilon B$.

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

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

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

Proposition 5.2. *The subsets and supersets of* $\mathrm{spec}_\varepsilon A$ *in (5.1) both Hausdorff-converge to* $\mathrm{spec}_\varepsilon A$ *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*

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

where again $\mathrm{spec}_\varepsilon(A,B) := \mathrm{spec}_\varepsilon A \cup \mathrm{spec}_\varepsilon B$. *Also here the sub- and supersets Hausdorff-converge to* $\mathrm{spec}_\varepsilon A$ *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 $\ell^2(\{1,\dots,N\})$ with some $N\in\mathbb{N}$, one has*

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

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

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 $\mathrm{spec}_\varepsilon A$ for $\varepsilon>0$. The spectrum, $\mathrm{spec}\, A$, 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].

pseudospectra,

$$\mathrm{Spec}_\varepsilon A \;:=\; \{\lambda \in \mathbb{C} : \|(A-\lambda I)^{-1}\| \geq 1/\varepsilon\} \;=\; \{\lambda \in \mathbb{C} : \mu(A-\lambda I) \leq \varepsilon\}, \qquad \varepsilon \geq 0,$$

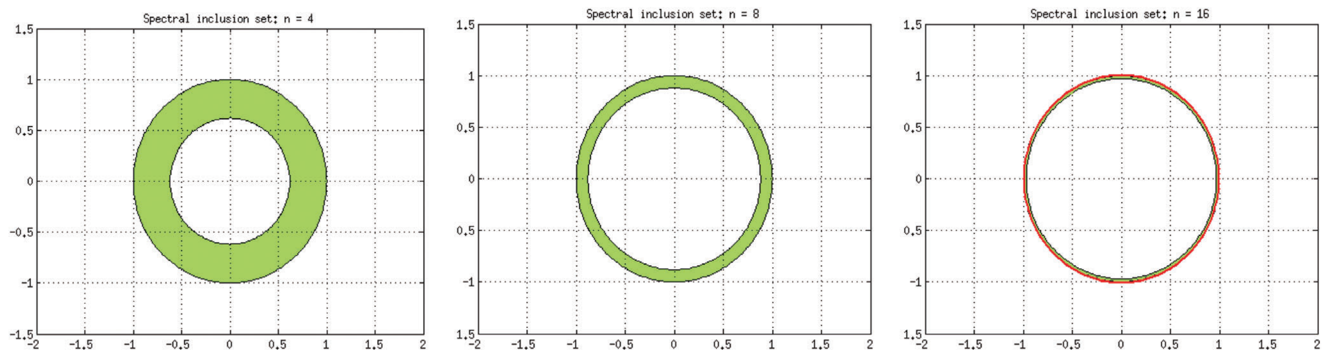
we can prove identical copies of Propositions 5.1, 6.1 and 6.2 with upper-case (i.e., closed) instead of lower-case (i.e., open) pseudospectra everywhere – and including the case $\varepsilon = 0$, see ref. [13]. The latter brings convergent supersets for spec $A = \mathrm{Spec}_0 A$ right away, without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

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

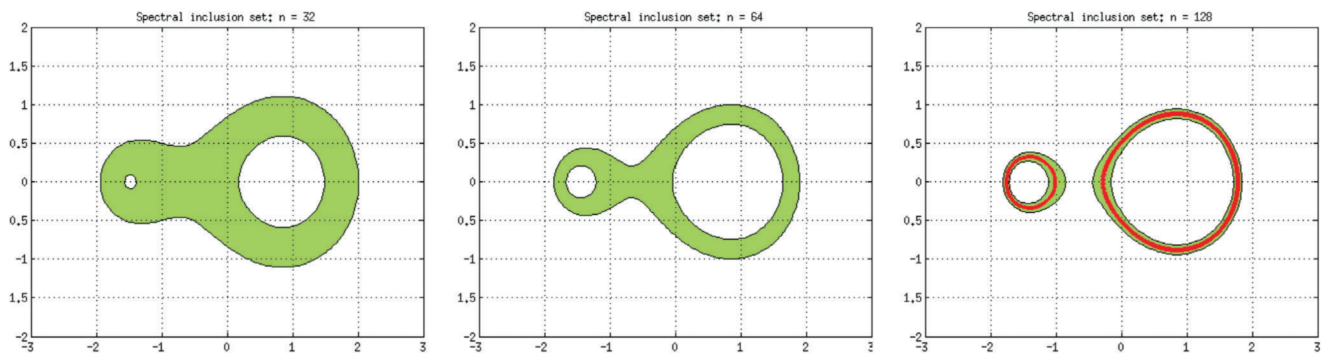
8 | EXAMPLES

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.

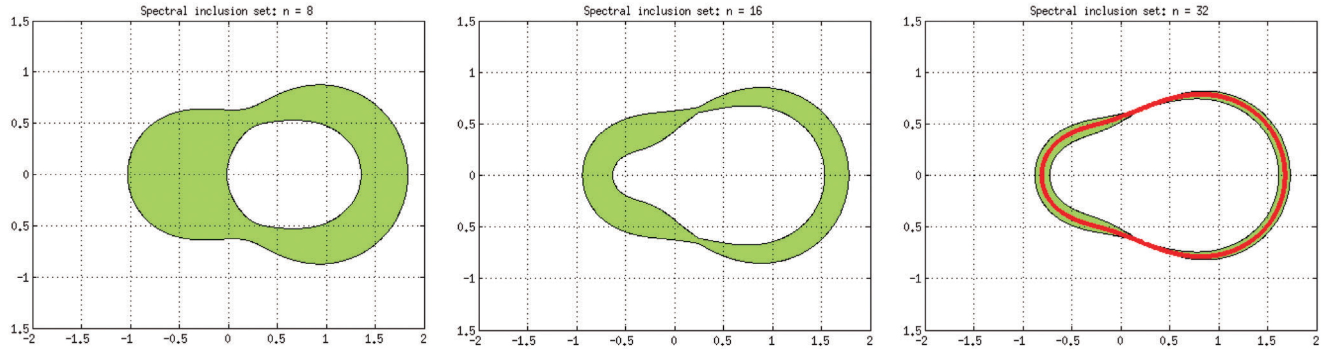
a) We start with the right shift, where the subdiagonal is $\alpha = (\dots, 1, 1, 1, \dots)$ and the main and superdigonal are $\beta = \gamma = (\dots, 0, 0, 0, \dots)$. The spectrum is the unit circle, and here are our supersets for $n \in \{4, 8, 16\}$:



b) Our next example is 3-periodic with subdiagonal $\alpha = (\dots, \mathbf{0}, 0, 0, \dots)$, main diagonal $\beta = (\dots, -\frac{3}{2}, 1, 1, \dots)$ and superdiagonal $\gamma = (\dots, \mathbf{1}, 2, 1, \dots)$, 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 $\alpha = (\dots, \mathbf{0}, 0, 0, \dots)$, main diagonal $\beta = (\dots, -\frac{1}{2}, 1, 1, \dots)$ and superdiagonal $\gamma = (\dots, \mathbf{1}, 2, 1, \dots)$, 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*, $\mathrm{spec}_{\mathrm{ess}}\, A$, 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,

$$A \;\cong\; \left(\begin{array}{ccc|c|ccc} \ddots & \ddots & & & & & \\ \ddots & A_{-2,-2} & A_{-2,-1} & & & & \\ & A_{-1,-2} & A_{-1,-1} & & & & \\ \hline & & & 0 & & & \\ \hline & & & & A_{1,1} & A_{1,2} & \\ & & & A_{2,1} & A_{2,2} & \ddots & \\ & & & & \ddots & \ddots & \end{array}\right) =: \left(\begin{array}{c|c|c} A_- & & \\ \hline & 0 & \\ \hline & & A_+ \end{array}\right),$$

so that

$$\mathrm{spec}_{\mathrm{ess}}\, A \;=\; \mathrm{spec}_{\mathrm{ess}}\, A_- \;\cup\; \mathrm{spec}_{\mathrm{ess}}\, A_+.$$

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

$$A \;=\; \begin{pmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & \ddots \\ & \ddots & \ddots \end{pmatrix} \;\cong\; \left(\begin{array}{ccc|ccc} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ \hline & & & A_{m+1,m+1} & A_{m+1,m+2} & \\ & & & A_{m+2,m+1} & A_{m+2,m+2} & \ddots \\ & & & & \ddots & \ddots \end{array}\right),$$

so that, with

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

we have

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

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

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

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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