Spectral Approximation of Bounded Self-Adjoint Operators—A Short Survey

K. Kumar

Abstract Normal categories are essentially those arising as the category of principal left [right] ideals of a regular semigroup. These categories have been used in describing the structure of regular semigroups. The structure theory in this context is known as cross connection theory. Several associated categories can be derived from a normal category which are also of interest in the structure theory of regular semigroups. The subcategory of inclusions, the subcategory of retractons, the groupoid of isomorphisms etc. are some of the associated categories.

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1 Introduction

The fundamental question "How to approximate spectra of linear operators on separable Hilbert spaces?" was considered by many mathematicians, starting from Szegö in [21]. Several attempts have been made to make use of the finite dimensional theory

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K. Kumar (✉)
Department of Mathematics, PSMO College, Tirurangadi 676306, Kerala, India
e-mail: kiranbalu36@gmail.com

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in the computation of the spectrum of bounded operators in an infinite dimensional space through an asymptotic way. This approach found success in getting good estimates in the case of some self-adjoint operators. Significant efforts have been done by many mathematicians to build up a general theory for the approximation of the spectrum of bounded self-adjoint operators on an infinite dimensional Hilbert space. To quote some of the recent contributions in this direction are due to W.B. Arveson [1], Albrecht Böttcher et al. [4], E.B. Davies et al. [6, 7], I. Gohberg et al. [9], A. Hansen [11], etc. The list is nevertheless incomplete.

A short survey is presented here on various techniques used to approximate the spectrum of a bounded self-adjoint operator A on a separable complex Hilbert space $\mathbb{H}$. The finite dimensional compressions A_n of A are considered here. The asymptotic values of spectrum of A_n are used to study the nature of spectrum of A.

1.1 The Problem

Let $\{e_1, e_2, \ldots\}$ be an orthonormal basis for $\mathbb{H}$ and P_n be the projection of $\mathbb{H}$ onto the finite dimensional subspace $L_n = \text{span}\{e_1, e_2, \ldots, e_n\}$. The finite dimensional truncations $A_n = P_n A P_n$ of A can be treated as finite matrices by restricting their domains to the image of P_n. If we denote the infinite matrix $(a_{i,j}) = (\langle Ae_j, e_i\rangle)$ to be the matrix representation of A associated to the orthonormal basis $\{e_1, e_2, \ldots\}$, then the $n \times n$ matrix $(a_{i,j})_{1\le i,j\le n}$ coincides with the matrix representation of A_n restricted to the image of P_n.

Here we consider the following fundamental question. Can we approximate the spectrum of A using the eigenvalue sequences of the matrices $(a_{i,j})_{1\le i,j\le n}$. There are some disappointing examples in which the eigenvalues of truncations give little information about the spectrum. For instance, in the case of the right shift operator on the sequence space $l^2(\mathbb{Z})$, the eigenvalue sequence of the truncations is the constant sequence 0, while the spectrum is the whole closed unit circle. For a self-adjoint example, one can consider the operator A on $l^2(\mathbb{N})$, defined as follows:

$$A(x_n) = (x_{\pi(n)}), \tag{1.1}$$

where π is a suitably chosen permutation on $\mathbb{N}$. The essential properties required for the permutation π, are discussed in [1], due to which the truncation method fails to approximate the spectrum.

This article is a survey of some recent developments in this area. In the next section, we discuss the class of operators introduced by W.B. Arveson in [1] for which the spectrum is fully determined by the eigenvalues of their truncations except for some discrete eigenvalues that may lie between the bounds of essential spectrum. Also, the use of the truncation method to approximate the bounds and the discrete eigenvalues lying outside the bounds of the essential spectrum of a bounded self-adjoint operator is explained in this section. The recent advances in the spectral gap prediction problems are also discussed there. The use of preconditioners to modify the truncation method is explained with a couple of more recent results. In the third section, we briefly explain the quadratic projection method and second-order relative spectra with some recent modifications. A concluding section on the further possibilities ends the article.

2 Algebraic and Linear Algebraic Approach

First we report some of the algebraic developments in this area. The major contributions are due to W.B. Arveson, who generalized the notion of band-limited matrices in [1], and achieved some success in the case of a special class of operators. We start with some definitions and results below which will play a very important role in the approximation of the spectrum of bounded self-adjoint operators. The notation A_n is used to denote the matrix $(a_{i,j})_{1\le i,j\le n}$.

Definition 2.1 A **filtration** of a Hilbert space $\mathbb{H}$ is a sequence of finite dimensional subspaces of $\mathbb{H}$, $\{L_n; n \in \mathbb{N}\}$ such that $L_n \subset L_{n+1}$ and closure of the union $\bigcup_n L_n$ is $\mathbb{H}$.

Example 2.2 A typical example for filtration in a Hilbert space with an orthonormal basis is the following. Let $\{e_n : n \in \mathbb{Z}\}$ be the bilateral orthonormal basis for $\mathbb{H}$ and let $\{L_n\}$ be defined by $L_n = \text{span}\{e_{-n}, e_{-n+1}, \dots e_n\}$. Then $\{L_n; n \in \mathbb{Z}\}$ is a filtration.

Definition 2.3 Let $\{L_n : n \in \mathbb{N}\}$ be a filtration. And P_n be the projection onto L_n. The **degree** of a bounded operator A on $\mathbb{H}$ is defined by

$$\deg(A) = \sup_{n\ge 1} \text{rank}(P_n A - A P_n).$$

Corresponding to each filtration, a Banach $*-$algebra of operators called Arveson's class can be defined as follows.

Definition 2.4 A is an operator in the **Arveson's class** if $A = \sum_{n=1}^{\infty} A_n$, where $\deg(A_n) < \infty$ for every n and convergence is in the operator norm, in such a way that $\sum_{n=1}^{\infty}(1 + \deg(A_n)^{\frac{1}{2}})\|A_n\| < \infty$.

In case each L_n is the span of finite number of elements in the basis as defined in Example 2.2, the following gives a concrete description of operators in the Arveson's class.

Theorem 2.5 ([1]) *Let $\{L_n; n \in \mathbb{Z}\}$ be the filtration defined in Example 2.2. Also let $(a_{i,j})$ be the matrix representation of a bounded operator A, with respect to $\{e_n\}$, and for every $k \in \mathbb{Z}$ let*

$$d_k = \sup_{i\in\mathbb{Z}} |a_{i+k,i}|$$

be the sup norm of the kth diagonal of $(a_{i,j})$. *Then A will be in the Arveson's class whenever the series* $\sum_k |k|^{1/2} d_k$ *converges.*

In particular, any operator whose matrix representation $(a_{i,j})$ is band-limited, in the sense that $a_{i,j} = 0$ whenever $|i - j|$ is sufficiently large, must be in the Arveson's class. Before stating the spectral inclusion theorems for arbitrary self-adjoint operators and for operators in the Arveson's class, recall the notion of essential points and transient points.

Definition 2.6 Essential point: A real number λ is an essential point of A, if for every open set U containing λ, $\lim_{n\to\infty} N_n(U) = \infty$, where $N_n(U)$ is the number of eigenvalues of A_n in U.

Definition 2.7 Transient point: A real number λ is a transient point of A if there is an open set U containing λ, such that sup $N_n(U)$ with n varying on the set of all natural number, is finite.

Remark 2.8 It should be noted that a number can be neither transient nor essential.

Denote $\Lambda = \{\lambda \in R; \lambda = \lim \lambda_n, \lambda_n \in \sigma(A_n)\}$ and Λ_e as the set of all essential points. The following spectral inclusion results for a bounded self-adjoint operator A is of high importance.

Theorem 2.9 ([1]) *The spectrum of a bounded self-adjoint operator is contained in the set of all limit points of the eigenvalue sequences of its truncations. Also, the essential spectrum is contained in the set of all essential points, i.e.,*

$$\sigma(A) \subseteq \Lambda \subseteq [m, M] \text{ and } \sigma_e(A) \subseteq \Lambda_e.$$

Equality in one of the above inclusion for bounded self-adjoint operators in the Arveson's class, was also proved in [1]. The precise result is the following.

Theorem 2.10 ([1]) *If A is a bounded self-adjoint operator in the Arveson's class, then* $\sigma_e(A) = \Lambda_e$ *and every point in* Λ *is either transient or essential.*

Remark 2.11 The above two theorems enable us to confine our attention to the limiting set Λ and the essential points Λ_e, in the task of computation of spectrum and essential spectrum of a bounded self-adjoint operator, respectively. Now the following issues may arise. The limiting set Λ may contain points which does not belong to the spectrum. Such points are called spurious eigenvalues. In the case of an operator in the Arveson's class, the essential points will give all information about essential spectrum, while the transient points may be misleading. Here we loose only information about eigenvalues of finite multiplicity. But this is very important if such points exist between the lower and upper bounds of essential spectrum, since they lead to the existence of spectral gaps between these bounds.

2.1 Operators with Connected Essential Spectrum

Things can be more difficult in the case of an arbitrary bounded self-adjoint operator. There may exist essential points, which are not spectral values. The operator given by the Eq. (1.1) is of that kind. However, the inclusion in Theorem 2.9 helps us to determine the spectrum, with an additional assumption of connectedness of the essential spectrum. The details of this claim are given below, which is a brief review of the article [4] with some slight modifications. This will play a key role in the forthcoming sections.

Recall that, for a bounded self-adjoint operator A, the spectrum $\sigma(A)$ is contained in the interval $[m, M]$ and the essential spectrum $\sigma_e(A)$ in $[\nu, \mu]$, where m, M, ν, μ, are bounds of $\sigma(A)$ and $\sigma_e(A)$, respectively. The following definitions and preliminary results are needed further.

Definition 2.12 Consider the singular number s_k, k natural number,

$$s_k\,(A) = \inf\,\{\|A - F\|\,;\, F \in \mathbb{B}(\mathbb{H}), \text{rank } F \leq k-1\}$$

is the kth **approximation number** of A.

Clearly, we have $\|A\| = s_1\,(A) \geq s_2\,(A) \geq \cdots \geq 0$

Theorem 2.13

- [9] $\lim_{k\to\infty} s_k\,(A) = \|A\|_{ess}$ *where* $\|A\|_{ess}$ *is the essential norm.*
- [4] $\lim_{n\to\infty} s_k\,(A_n) = s_k\,(A)$.

Remark 2.14 For $|A| = (A^*A)^{1/2}$, in case A is a finite matrix, the approximation numbers are the eigenvalues of $|A|$. That is $s_k\,(A) = \lambda_k(|A|)$, where $\lambda_k\,(|A|)$ is the kth eigenvalue of $|A|$.

Theorem 2.15 ([9]) *The set* $\sigma(|A|) - \left[0, \|A\|_{ess}\right]$ *is at most countable,* $\|A\|_{ess}$ *is the only possible accumulation point, and all the points of the set are eigenvalues with finite multiplicity of* $|A|$. *Furthermore if*

$$\lambda_1(|A|) \geq \lambda_2(|A|) \geq \cdots \geq \lambda_N(|A|)$$

are those N eigenvalues (N can be infinity), then

$$s_k\,(A) = \begin{cases} \lambda_k(|A|), \; \textit{if}\, N = \infty \; \textit{or}\, 1 \leq k \leq N \\ \|A\|_{ess,} \; \textit{if}\, N < \infty \, \textit{and}\, k \geq N+1 \end{cases} \tag{2.1}$$

Corollary 2.16

$$\lim_{n\to\infty} \lambda_k\,(|A_n|) = \lim_{n\to\infty} s_k\,(A_n) = s_k\,(A) = \begin{cases} \lambda_k\,(|A|) \; if\, N = \infty\, or\; 1 \leq k \leq N \\ \|A\|_{ess} \; if \; N < \infty \, and\, k \geq N+1 \end{cases}$$

Remark 2.17 The above result will play a key role in the approximation of spectrum. Considering the positive operator $A - mI$, it can be deduced that the set $\sigma(A) \cap (\mu, M]$ is at most countable and that consists of eigenvalues of finite multiplicity by Theorem 2.15. Also μ is the only possible accumulation point. Let these eigenvalues be

$$\lambda_R^+(A) \leq \cdots \leq \lambda_2^+(A) \leq \lambda_1^+(A).$$

Similarly by considering the operator $MI - A$, it can be observed that $\sigma(A) \cap [m, \nu)$ consists of at most countably many eigenvalues of finite multiplicity with only possible accumulation point ν. Let

$$\lambda_1^-(A) \leq \lambda_2^-(A) \leq \cdots \leq \lambda_S^-(A)$$

be those eigenvalues. Also the numbers R and S can be infinity. Arrange the eigenvalues of A_n as

$$\lambda_1(A_n) \geq \lambda_2(A_n) \geq \cdots \geq \lambda_n(A_n).$$

From here onwards, the above notations will be used.

Now we prove the following result from [4] which is the major tool that is used frequently in this note.

Theorem 2.18 *For every fixed integer k we have*

$$\lim_{n\to\infty} \lambda_k(A_n) = \begin{cases} \lambda_k^+(A), & \text{if } R = \infty \text{ or } 1 \leq k \leq R \\ \mu, & \text{if } R < \infty \text{ and } k \geq R+1 \end{cases}$$

$$\lim_{n\to\infty} \lambda_{n+1-k}(A_n) = \begin{cases} \lambda_k^-(A), & \text{if } S = \infty \text{ or } 1 \leq k \leq S \\ \nu, & \text{if } S < \infty \text{ and } k \geq S+1 \end{cases}$$

In particular,

$$\lim_{k\to\infty} \lim_{n\to\infty} \lambda_k(A_n) = \mu \text{ and } \lim_{k\to\infty} \lim_{n\to\infty} \lambda_{n+1-k}(A_n) = \nu.$$

Proof The following observations are made first.

$$|A - mI| = A - mI, \; P_n(A - mI)P_n = A_n - mI_n, \text{ and } |A_n - mI_n| = A_n - mI_n.$$

Hence from the above corollary, we have

$$\lim_{n\to\infty} \lambda_k(A_n - mI_n) = \begin{cases} \lambda_k(A - mI), & \text{if } R = \infty \text{ or } 1 \leq k \leq R \\ \|A - mI\|_{ess}, & \text{if } R < \infty \text{ and } k \geq R+1 \end{cases} \tag{2.2}$$

Similarly, by considering the operator $MI - A$, we get

$$\lim_{n\to\infty} \lambda_k(MI_n - A_n) = \begin{cases} \lambda_k(MI - A), & \text{if } S = \infty \text{ or } 1 \le k \le S \\ \|MI - A\|_{ess}, & \text{if } S < \infty \text{ and } k \ge S+1 \end{cases} \tag{2.3}$$

Also we have the following identities

$$\|A - mI\|_{ess} = \mu - m, \quad \|MI - A\|_{ess} = M - \nu. \tag{2.4}$$

$$\lambda_k(A_n - mI_n) = \lambda_k(A_n) - m, \quad \lambda_k(MI_n - A_n) = M - \lambda_{n+1-k}(A_n). \tag{2.5}$$

$$\lambda_k(A - mI) = \lambda_k^+(A) - m, \quad \lambda_k(MI - A) = M - \lambda_k^-(A). \tag{2.6}$$

Substituting them in Eqs. (2.2) and (2.3), we get

$$\lim_{n\to\infty} \lambda_k(A_n) = \begin{cases} \lambda_k^+(A), & \text{if } R = \infty \text{ or } 1 \le k \le R \\ \mu, & \text{if } R < \infty \text{ and } k \ge R+1 \end{cases}$$

$$\lim_{n\to\infty} \lambda_{n+1-k}(A_n) = \begin{cases} \lambda_k^-(A), & \text{if } S = \infty \text{ or } 1 \le k \le S \\ \nu, & \text{if } S < \infty \text{ and } k \ge S+1 \end{cases}$$

Hence the proof. □

Remark 2.19 The above results are also true if we replace A_n by some other sequence A_{1n} of self-adjoint operators with the property that

$$\|A_n - A_{1n}\| \to 0 \text{ as } n \to \infty$$

In order to justify this, we need only to recall an important inequality concerning the eigenvalues of self-adjoint matrices A, B (refer e.g. to [2])

$$|\lambda_k(A) - \lambda_k(B)| \le \|A - B\|.$$

Remark 2.20 By Theorem 2.18, all the discrete spectral values lying outside the bounds of essential spectrum and the upper and lower bounds of the essential spectrum can be approximated. Note that, the theorem points out exactly the particular sequence that converges to a discrete spectral value. But how fast does the convergence take place, is still not known. Looking at some concrete situations, one may hope for a better rate of convergence.

Even the rate of convergence is not estimated, it can be proved that the order of convergence is the same as the order of convergence of approximation numbers. The following theorem gives a vague idea about the rate of convergence.

Theorem 2.21 ([14]) *If* $s_k(A_n) - s_k(A) = O(\theta_n)$, *where* θ_n *goes to* 0 *as n tends to* ∞, *then*

$$\lambda_k(A_n) = \begin{cases} \lambda_k^+(A) + O(\theta_n), & \textit{if } R = \infty \textit{ or } 1 \le k \le R \\ \mu + O(\theta_n), & \textit{if } R < \infty \textit{ and } k \ge R+1 \end{cases}$$

$$\lambda_{n+1-k}(A_n) = \begin{cases} \lambda_k^-(A) + O(\theta_n), & \textit{if } S = \infty \textit{ or } 1 \le k \le S \\ \nu + O(\theta_n), & \textit{if } S < \infty \textit{ and } k \ge S+1 \end{cases}$$

where R and S are the same notations used in Theorem 2.18.

Proof Let N be the number of eigenvalues lying in $\sigma(|A|) - \left[0, \|A\|_{ess}\right]$. From identity (2.1), and the the fact that $s_k(A_n) = \lambda_k(|A_n|)$, we have the following identity.

$$s_k(A_n) - s_k(A) = \begin{cases} \lambda_k(|A_n|) - \lambda_k(|A|), & \text{if } N = \infty \text{ or } 1 \le k \le N \\ \lambda_k(|A_n|) - \|A\|_{ess}, & \text{if } N < \infty \text{ and } k \ge N+1 \end{cases}$$

Since by hypothesis, $s_k(A_n) - s_k(A) = O(\theta_n)$,

$$\lambda_k(|A_n|) - \lambda_k(|A|) = O(\theta_n), \quad \text{if } N = \infty \text{ or } 1 \le k \le N,$$

$$\lambda_k(|A_n|) - \|A\|_{ess} = O(\theta_n), \quad \text{if } N < \infty \text{ and } k \ge N+1.$$

Applying this to the positive operators $A - mI$, and $MI - A$, with the notations used in Theorem 2.18, we get the following conclusions.

$$\lambda_k(A_n - mI_n) = \begin{cases} \lambda_k(A - mI) + O(\theta_n), & \text{if } R = \infty \text{ or } 1 \le k \le R \\ \|A - mI\|_{ess} + O(\theta_n), & \text{if } R < \infty \text{ and } k \ge R+1 \end{cases}$$

and

$$\lambda_k(MI_n - A_n) = \begin{cases} \lambda_k(MI - A) + O(\theta_n), & \text{if } S = \infty \text{ or } 1 \le k \le S \\ \|MI - A\|_{ess} + O(\theta_n), & \text{if } S < \infty \text{ and } k \ge S+1 \end{cases}$$

Also from the identities (2.4)–(2.6), we get the desired conclusions

$$\lambda_k(A_n) = \begin{cases} \lambda_k^+(A) + O(\theta_n), & \text{if } R = \infty \text{ or } 1 \le k \le R \\ \mu + O(\theta_n), & \text{if } R < \infty \text{ and } k \ge R+1 \end{cases}$$

$$\lambda_{n+1-k}(A_n) = \begin{cases} \lambda_k^-(A) + O(\theta_n), & \text{if } S = \infty \text{ or } 1 \le k \le S \\ \nu + O(\theta_n), & \text{if } S < \infty \text{ and } k \ge S+1 \end{cases}$$

Hence the proof. □

The above theorem is the first result regarding the rate of convergence in the approximations done in Theorem 2.18. So far there is no evidence of remainder estimation and the error estimation in these approximations in the case of an arbitrary self-adjoint operator to the best of our knowledge. The subsequent theorem taken from [4] denies the existence of spurious eigenvalues (points in Λ those are not part of the spectrum) under the assumption of connectedness of essential spectrum.

Theorem 2.22 ([4]) *If A is a self-adjoint operator and if $\sigma_e(A)$ is connected, then* $\sigma(A) = \Lambda$.

Remark 2.23 It is worthwhile to notice that the connectedness of essential spectrum enables us to compute the spectrum using finite dimensional truncations. Thus, if we cannot determine the spectrum fully by the truncations, then the essential spectrum is not connected. In short, if there is a spurious eigenvalue, then there exists a gap in the essential spectrum.

Remark 2.24 The converse of the above observation need not be true. That is the existence of a spectral gap does not lead to the existence of a spurious eigenvalue. For example, if we take A to be be the projection operator on to some closed subspace of $\mathbb{H}$, then the eigenvalues of truncations are 0 and 1 only. There we have $\Lambda = \sigma(A) = \{0, 1\}$. Hence no spurious eigenvalues, but still there is a gap.

In summary, the upper and lower bounds of the essential spectrum can be computed using the sequence of eigenvalues of finite dimensional truncations. Also the discrete eigenvalues lying below and above these bounds can be computed. The above results pinpointing the particular sequence of eigenvalues that converges to a particular eigenvalue of the operator. Now the remaining part is the computation of essential spectrum. The problem is whether it is possible to locate the gaps in the essential spectrum using these truncations. If it is possible, then the spectrum is fully determined up to some discrete eigenvalues that may have trapped between these gaps.

2.2 Gaps in the Essential Spectrum

The following theorem is an attempt to predict the existence of spectral gaps, using the finite dimensional truncations. The notation $\#S$ is used to denote the number of elements in the set S and w_{nk} is used to denote an averaging sequence. That is $0 \leq w_{nk} \leq 1$, and $\sum_{k=1}^{n} w_{nk} = 1$.

Theorem 2.25 ([13]) *Let A be a bounded self-adjoint operator, and $\lambda_{n1}(A_n) \geq \lambda_{n2}(A_n) \geq \cdots \geq \lambda_{nn}(A_n)$ be the eigenvalues of A_n arranged in decreasing order. For each positive integer n, let $a_n = \sum_{k=1}^{n} w_{nk}\lambda_{nk}$ be the convex combination of eigenvalues of A_n. If there exists a $\delta > 0$ and $K > 0$ such that*

$$\#\left\{\lambda_{nj};\ \left|a_n - \lambda_{nj}\right| < \delta\right\} < K \tag{2.7}$$

and in addition if $\sigma_e(A)$ and $\sigma(A)$ have the same upper and lower bounds, then $\sigma_e(A)$ has a gap.

Remark 2.26 There is possibility for the presence of discrete eigenvalues inside the gaps in the above case.

Remark 2.27 The special case which is more interesting is when $w_{nk} = \frac{1}{n}$, for all n. In that case, we are actually looking at the averages of eigenvalues of truncations and these averages can be computed using the trace at each level.

Remark 2.28 It is to be noted that all the points of the form $a_n = \sum_{k=1}^{n} w_{nk}\lambda_{nk}$ are in the numerical range of A_n. Therefore, the result can be made simpler in the language of numerical range. However it is not easy to compute the numbers in the expression (2.7). Here we treated it as a deviation from the mean value. Hence the condition (2.7) may be interpreted as a restriction to the deviation of the eigenvalues of truncations from their central tendency. Nevertheless the computations still remain difficult.

In Theorem 2.25, the weighted mean of the eigenvalues at each level and its deviation is analyzed. The following special choice of the weights are interesting.

Special Choice

Let us consider an instance where these weights w_{nk} arise naturally associated to a self-adjoint operator on a Hilbert space. Let $A_n = \sum_{k=1}^{n} \lambda_{n,k} Q_{n,k}$ be the spectral resolution of A_n. Define $w_{nk} = \langle Q_{n,k}e_1, e_1 \rangle$. Then $0 \leq w_{nk} \leq 1$ and $\sum_{k=1}^{n} w_{nk} = 1$. Now

$$\sum_{k=1}^{n} w_{nk}\lambda_{nk} = \sum_{k=1}^{n} \lambda_{nk}\langle Q_{n,k}e_1, e_1 \rangle = \langle A_n e_1, e_1 \rangle = \langle A e_1, e_1 \rangle = a_{11}.$$

Therefore by Theorem 2.25, if there exists a $\delta > 0$ and a $K > 0$, such that

$$\# \left\{ \lambda_{nj};\, \left| a_{11} - \lambda_{nj} \right| < \delta \right\} < K$$

then there exists a gap in the essential spectrum of A. Hence if the first entry in the matrix representation of A, is not an essential point, then there exists a gap in the essential spectrum.

Remark 2.29 All points of the form $\langle Ae_i, e_i \rangle = a_{ii}$ are in the numerical range which lies between the bounds of the essential spectrum, in the case that the bounds coincide with the bounds of the spectrum. Hence in that case, if a_{ii} is not an essential point for some i, then that will lead to the existence of a spectral gap. That means if any one of the diagonal entries in the matrix representation of A is not an essential point, then there exists a gap in the essential spectrum as indicated in the above special choice of w_{nk}.

The following is an example where the first entry a_{11} is a transient point and the spectral gap prediction is valid.

Example 2.30 Define a bounded self-adjoint operator A on $l^2(\mathbb{N})$, as follows.

$$A(x_n) = (x_{n-1} + x_{n+1}) + (v_n x_n), x_0 = 0;$$

where the periodic sequence $(v_n) = (1, 2, 3, 1, 2, 3, \ldots)$. The matrix representation of A, associated to the standard orthonormal basis, is tridiagonal. The diagonal entries are the entries in the periodic sequence (v_n) and upper and lower diagonal will be 1. Such matrices can be identified as the block Toeplitz operator with corresponding matrix valued symbol given by

$$\tilde{f}(\theta) = \begin{bmatrix} 1 & 1 & e^{i\theta} \\ 1 & 2 & 1 \\ e^{-i\theta} & 1 & 3 \end{bmatrix}.$$

By our special choice above, Theorem 2.25 guarantees that if $\langle A(e_1), e_1 \rangle = 1$ is a transient point, then $\sigma_e(A)$ has a gap. The fact that 1 is a transient point, is a consequence of discrete Borg theorem [8, 10] and some numerical computations. The interval $\left(\frac{3-\sqrt{5}}{2}, \frac{5-\sqrt{5}}{2}\right)$ is a spectral gap an 1 lies in that gap.

2.3 Preconditioners in Spectral Approximation

Here we try to modify the truncation method with the help of the notions of preconditioners and the convergence of matrix sequences in the sense of eigenvalue clustering. Recall that in the numerical analysis literature, the preconditioner associated with a matrix is used to make the iteration process more efficient. Here we use different notions of matrix convergence in the sense of eigenvalue clustering to study the spectral approximation by preconditioners. That is, the A_n's will be replaced by its preconditioner to perform approximation of spectrum.

We start with defining different notions of convergence of matrix sequences in the sense of eigenvalue clustering. Such notions were used in the special case of Toeplitz matrices in [20], and generalized into the arbitrary case in [12].

Definition 2.31 Let $\{A_n\}$ and $\{B_n\}$ be two sequences of $n \times n$ Hermitian matrices. We say that $A_n - B_n$ converges to 0 in the ***strong cluster sense*** if for any $\epsilon > 0$, there exist integers $N_{1,\epsilon}, N_{2,\epsilon}$ such that all the singular values $\sigma_j(A_n - B_n)$ lie in the interval $[0, \epsilon)$ except for at most $N_{1,\epsilon}$ (independent of the size n) singular values for all $n > N_{2,\epsilon}$.

If the number $N_{1,\epsilon}$ does not depend on ϵ, we say that $A_n - B_n$ converges to 0 in the ***uniform cluster sense***. And if $N_{1,\epsilon}$ depends on ϵ, n and is of $o(n)$, we say that $A_n - B_n$ converges to 0 in ***weak cluster sense***.

Here the aim is to modify the truncation method by replacing A_n by some other *simpler* sequence of matrices B_n, where $\{A_n\} - \{B_n\}$ converges to 0 in the strong cluster sense (weak or uniform cluster sense, respectively). We study the effect of this replacement in the well-known results obtained by truncation method. We prove a couple of results which show that the convergence in the strong or uniform cluster sense is equivalent to the compact perturbation of operators. These are the modified versions of the results proved in [15].

Theorem 2.32 *Let $A, B \in B(\mathcal{H})$ be self-adjoint operators. Then the operator $R = A - B$ is compact if and only if the sequence of truncations $A_n - B_n$ converges to the zero matrix in the strong cluster.*

Proof First assume that $R = A - B$ is compact and its spectrum $\sigma(R) = \{\lambda_k(R) : k = 1, 2, 3, \ldots\} \bigcup \{0\}$. Here 0 is the only accumulation point of the spectrum. Hence $\lambda_k(R) \to 0$ as $k \to \infty$. Hence for any given $\epsilon > 0$, there exists a positive integer $N_{1,\epsilon}$ such that

$$\lambda_k(R) \in \left(\frac{-\epsilon}{2}, \frac{\epsilon}{2}\right), \text{ for every } k > N_{1,\epsilon}.$$

Also since R is compact, the truncation $R_n = A_n - B_n$ converges to R in the operator norm topology. Therefore, the eigenvalues of truncations converges to the eigenvalues of R. That is

$$\lambda_k(R_n) \to \lambda_k(R) \text{ as } n \to \infty, \text{ for each } k.$$

In particular, for every $k > N_{1,\epsilon}$, there exists a positive integer $N_{2,\epsilon}$ such that

$$\lambda_k(R_n) - \lambda_k(R) \in \left(\frac{-\epsilon}{2}, \frac{\epsilon}{2}\right), \text{ for every } n > N_{2,\epsilon}.$$

Therefore, when $n > N_{2,\epsilon}$, all the eigenvalues $\lambda_k(R_n)$ of $R_n = A_n - B_n$, except for at most $N_{1,\epsilon}$ eigenvalues, are in the interval $(-\epsilon, \epsilon)$. That is $R_n = A_n - B_n$ converges to 0 in the strong cluster.

For the converse part, assume that $A_n - B_n$ converges to the zero matrix in the strong cluster. Then for any $\lambda \neq 0$, choose an $\epsilon > 0$ such that λ is outside the interval $(-\epsilon, \epsilon)$. Corresponding to this ϵ, there exist positive integers $N_{1,\epsilon}, N_{2,\epsilon}$ such that $\sigma(A_n - B_n)$ is contained in $(-\epsilon, \epsilon)$, for every $n > N_{2,\epsilon}$, except for possibly $N_{1,\epsilon}$ eigenvalues. Now consider the counting function $N_n(U)$ of eigenvalues of $A_n - B_n$ in U. For any neighborhood U of λ that does not intersect with $(-\epsilon, \epsilon)$, $N_n(U)$ is bounded by the number $N_{1,\epsilon}$. Hence λ is not an essential point of $A - B$. Therefore, it is not in the essential spectrum (see Theorem 2.3 of [1]). Since $\lambda \neq 0$ was arbitrary, this shows that the essential spectrum of $A - B$ is the singleton set $\{0\}$. Hence it is a compact operator and the proof is completed. □

Theorem 2.33 *Let $A, B \in B(\mathcal{H})$ be self-adjoint operators. Then the operator $R = A - B$ is of finite rank if and only if the truncations $A_n - B_n$ converges to the zero matrix in the uniform cluster.*

Proof The proof is an imitation of the proof of Theorem 2.32, differs only in the choice of $N_{1,\epsilon}$ to be independent of ϵ. However the details are given below. First assume that R = A − B is a finite rank operator with rank N_1, and its spectrum $\sigma(R) = \{\lambda_k(R) : k = 1, 2, 3, \dots N_1\} \bigcup \{0\}$. Since the truncation $R_n = A_n - B_n$ converges to R in the operator norm topology, the eigenvalues of truncations converges to the eigenvalues of R. That is

$$\lambda_k(R_n) \to \lambda_k(R) \text{ as } n \to \infty, \text{ for each } k = 1, 2, 3, \dots N_1.$$

For every $k > N_1$, $\lambda_k(R_n)$ converges to 0 by [4]. Hence for a given $\epsilon > 0$, there exists a positive integer $N_{2,\epsilon}$ such that

$$\lambda_k(R_n) \in (-\epsilon, \epsilon)\,, \text{ for every } n > N_{2,\epsilon} \text{ and for each } k > N_1.$$

Therefore, when $n > N_{2,\epsilon}$, all the eigenvalues $\lambda_k(R_n)$ of $R_n = A_n - B_n$, except for the first N_1 eigenvalues, are in the interval $(-\epsilon, \epsilon)$. That is $A_n - B_n$ converges to 0 in the uniform cluster.

For the converse part, assume that $A_n - B_n$ converges to the zero matrix in the uniform cluster. Then for any $\epsilon > 0$, there exist positive integers $N_1, N_{2,\epsilon}$ such that $\sigma(A_n - B_n)$ is contained in $(-\epsilon, \epsilon)$, for every $n > N_{2,\epsilon}$, except for possibly N_1 eigenvalues. As in the proof of Theorem 2.32, we obtain 0 is the only element in the essential spectrum. Hence $R = A - B$ is a compact operator. In addition to this, R can have at most N_1 eigenvalues. To see this, notice that all the eigenvalues of a compact operator are obtained as the limits of sequence of eigenvalues of its truncations. In this case at most N_1 such sequence can go to a nonzero limit. Hence R is a finite rank operator and the proof is completed. □

Remark 2.34 The above results have the following implications. Since a compact perturbation may change the discrete eigenvalues, the above results show that the convergence of preconditioners in the sense of eigenvalue clustering, is not sufficient to use them in the spectral approximation problems. Nevertheless one can use it in the spectral gap prediction problems, since the compact perturbation preserves essential spectrum.

Remark 2.35 The analysis of weak convergence is yet to be carried out.

We end this section with the example of Frobenius optimal preconditioners, which are useful in the context of infinite linear systems with Toeplitz structure (see [20] for details).

Example 2.36 Let $\{U_n\}$ be a sequence of unitary matrices over $\mathbb{C}$, where U_n is of order n for each n. For each n, we define the commutative algebra M_{U_n} of matrices as follows.

$$M_{U_n} = \left\{A \in M_n\left(\mathbb{C}\right); {U_n}^* A U_n \text{ complex diagonal}\right\}$$

Recall that $M_n(\mathbb{C})$ is a Hilbert space with respect to the classical Frobenius scalar product,

$$\langle A, B\rangle = \text{trace } (B^* A).$$

Observe that M_{U_n} is a closed convex set in $M_n(\mathbb{C})$ and hence, corresponding to each $A \in M_n(\mathbb{C})$, there exists a unique matrix $P_{U_n}(A)$ in M_{U_n} such that

$$\|A - X\|_2^2 \geq \left\|A - P_{U_n}(A)\right\|_2^2 \text{ for every } X \in M_{U_n}.$$

For each $A \in \mathbb{B}(\mathbb{H})$, consider the sequence of matrices $P_{U_n}(A_n)$ as the Frobenius optimal preconditioners of A_n. In the case A is the Toeplitz operator with continuous symbol, there are many good examples of matrix algebras such that the associated Frobenius optimal preconditioners are of low complexity and have faster rate of convergence.

3 Analytical Approach

The concepts of second-order relative spectra and quadratic projection method, which are almost synonyms of the other, were used in the spectral pollution problems and in determining the eigenvalues in the gaps by E.B. Davies, Levitin, Shagorodsky, etc. (see [5–7, 17]). In all these articles, the idea is to reduce the spectral approximation problems into the estimation of a particular function, related to the distance from the spectrum. This particular function is usually approximated by a sequence of functions related to the eigenvalues of truncations of the operator under concern.

First, we shall briefly mention the work done by E.B. Davies [6] and E.B. Davies and M. Plum [7], which is of great interest, where he considered functions which are related to the distance from the spectrum.

3.1 Distance from the Spectrum

In the paper published in 1998 [6], E.B. Davies considered the function F defined by

$$F(t) = \inf\left\{\frac{\|A(x) - tx\|}{\|x\|} : 0 \neq x \in \mathbb{L}\right\} \tag{3.1}$$

where $\mathbb{L}$ is a subspace of $\mathbb{H}$. Then he observed the following.

- F is Lipschitz continuous and satisfies $|F(s) - F(t)| \leq |s - t|$, for all $s, t \in \mathbb{R}$.
- $F(t) \geq d(t, \sigma(A)) = dist(t, \sigma(A))$.
- If $0 \leq F(t) \leq \delta$, then $\sigma(A) \cap [t - \delta, t + \delta] \neq \emptyset$.

From these observations, he obtained some bounds for the eigenvalues in the spectral gap of A, and found it useful in some concrete situations. For the efficient computation of the function F, he considered family of operators $N(s)$ on the given finite dimensional subspace $\mathbb{L}$, defined by

$$N(s) = A_{\mathbb{L}}^* A_{\mathbb{L}} - 2sPA_{\mathbb{L}} + s^2 I_{\mathbb{L}} \tag{3.2}$$

where P is the projection onto $\mathbb{L}$ and the notation $A_{\mathbb{L}}$ means A restricted to $\mathbb{L}$. The eigenvalues of these family of finite dimensional operators form sequence of real analytic functions (functions which map s to the eigenvalues of $N(s)$). He used these sequence to approximate the function F and thereby obtain information about the spectral properties of A. The main result is stated below, under the assumption that A is bounded.

Theorem 3.1 *Suppose $\{\mathbb{L}_n\}_{n=1}^{\infty}$ is an increasing sequence of closed subspaces of $\mathbb{H}$. If F_n is the functions associated with $\mathbb{L}_n$ according to (3.1), then F_n decreases monotonically and converge locally uniformly to $d(., \sigma(A))$. In particular, $s \in \sigma(A)$ if and only if*

$$\lim_{n\to\infty} F_n(s) = 0.$$

In the article on spectral pollution [7] in 2004, the above method was linked with various techniques due to Lehmann [16], Behnke et al. [3], Zimmerman et al. [22]. The problem of spurious eigenvalues in a spectral gap was addressed by considering the following function.

$$F(t) = \inf\{\|A(x) - tx\| : \ x \in \mathbb{L}, \|x\| = 1\}$$

If we define $F_n(t) = \inf\{\|A(x) - tx\| : \ x \in \mathbb{L}_n, \|x\| = 1\}$, then the following results shall be obtained.

- Given $\epsilon > 0$, there exists an N_ϵ such that $n \geq N_\epsilon$ implies

$$F(t) \leq F_n(t) \leq F(t) + \epsilon \ \text{ for all } \ t \in \mathbb{R}$$

- $\sigma(A) \cap [t - F_n(t), t + F_n(t)] \neq \emptyset$ for every $t \in \mathbb{R}$.

These observations were useful in obtaining some bounds for the eigenvalues between the bounds of essential spectrum. This was established with some numerical evidence in [7] for bounding eigenvalues for some particular operators.

Levitin and Shargorodsky considered the problem of spectral pollution in [17]. They suggested the usage of second-order relative spectra, to deal the problem. For the sake of completion, the definition is given below.

Definition 3.2 ([17]) Let $\mathbb{L}$ be a finite dimensional subspace of $\mathbb{H}$. A complex number z is said to belong to the second-order spectrum $\sigma_2(A, \mathbb{L})$ of A relative to $\mathbb{L}$ if there exists a nonzero u in $\mathbb{L}$ such that

$$\langle (A - zI)u, (A - \bar{z}I)v \rangle = 0, \text{ for every } v \in \mathbb{L}$$

They proved that the second-order relative spectrum intersects with every disk in the complex plane with diameter is an interval which intersect with the spectrum of A (Lemma 5.2 of [17]). They also provided some numerical results in case of some Multiplication and Differential operators, which indicated the effectiveness of second-order relative spectra in avoiding the spectral pollution. In [5], Boulton and Levitin used the quadratic projection method to avoid spectral pollution in the case of some particular Schrodinger operators.

3.2 Distance from the Essential Spectrum

To predict the existence of a gap in the essential spectrum, we need to know whether a number λ in (ν, μ) belongs to the spectrum or not. If it is not a spectral value, then there exists an open interval between (ν, μ) as a part of the compliment of the spectrum, since the compliment is an open set. We observe that the spectral gap prediction is possible by computing values of the following function.

Definition 3.3 Define the nonnegative valued function f on the real line $\mathbb{R}$ as follows.

$$f(\lambda) = \nu_\lambda = \inf \sigma_e((A - \lambda I)^2).$$

The primary observation is that we can predict the existence of a gap inside the essential spectrum by evaluating the function and checking whether it attains a nonzero value. The nonzero values of this function give the indication of spectral gaps.

Theorem 3.4 *The number λ in the interval (ν, μ) is in the gap if and only if $f(\lambda) > 0$. Also one end point of the gap will be $\lambda \pm \sqrt{f(\lambda)}$.*

The advantage of considering $f(\lambda)$ is that, it is the lower bound of the essential spectrum of the operator $(A - \lambda I)^2$, which we can compute using the finite dimensional truncations with the help of Theorem 2.18. So the computation of $f(\lambda)$, for each λ, is possible. This enables us to predict the gap using truncations. Also here we are able to compute one end point of a gap. The other end point is possible to compute by Theorem 2.3 of [18], which is stated below.

Theorem 3.5 ([18]) *Let A be a bounded self-adjoint operator and $\sigma_e(A) = [a, b] \bigcup [c, d]$, where $a < b < c < d$. Assume that b is known and not an accumulation point of the discrete spectra of A. Then c can be computed by truncation method.*

Coming back to the Arveson's class, we observe that the essential points and hence the essential spectrum is fully determined by the zeros of the function in the Definition 3.3.

Corollary 3.6 *If A is a bounded self-adjoint operator in the Arveson's class, then λ is an essential point if and only if $f(\lambda) = 0$.*

When one wishes to apply the above results to determine the gaps in the essential spectrum of a particular operator, one has to face the following problems. To check for each λ in (ν, μ), is a difficult task from the computational point of view. Also taking truncations of the square of the operator may lead to difficulty. Note that $(P_n A P_n)^2$ and $P_n A^2 P_n$ are entirely different. So we may have to do more computations to handle the problem.

Another problem is the rate of convergence and estimation of the remainder term. For each λ in (ν, μ), the value of the function $f(\lambda)$ has to be computed. This computation involves truncation of the operator $(A - \lambda I)^2$ and the limiting process of sequence of eigenvalues of each truncation. The rate of convergence of these approximations and the remainder estimate are the questions of interest.

Below, the function $f(.)$ is approximated by a double sequence of functions, which arise from the eigenvalues of truncations of operators.

Theorem 3.7 ([14]) *Let $f_{n,k}$ be the sequence of functions defined by $f_{n,k}(\lambda) = \lambda_{n+1-k}\left(P_n (A - \lambda I)^2 P_n\right)$. Then $f(.)$ is the uniform limit of a subsequence of $\{f_{n,k}(.)\}$ on all compact subsets of the real line.*

The following result makes the computation of $f(\lambda)$ much easier for a particular class of operators. When the operator is truncated first and square the truncation rather than truncating the square of the operator, the difficulty of squaring a bounded operator is reduced. The computation needs only to square the finite matrices.

Theorem 3.8 ([14]) *If $\|P_n A - A P_n\| \to 0$ as $n \to \infty$, then*

$$\lim_{k\to\infty}\lim_{n\to\infty} \lambda_{n+1-k}\left(P_n (A - \lambda I)^2 P_n\right) = \lim_{k\to\infty}\lim_{n\to\infty} \lambda_{n+1-k}\left(P_n (A - \lambda I) P_n\right)^2.$$

Remark 3.9 The function $f(.)$ that is considered here is directly related to the distance from the essential spectrum, while Davies' function was related with the distance from the spectrum. Here the approximation results in [4], especially Theorem 2.18 are used to approximate the function. But it is still not known to us whether these results are useful from a computational point of view. The methods due to Davies et al. were applied in the case of some Schrodinger operators with a particular kind of potentials in [5, 17]. We hope that a combined use of both methods may give a better understanding of the spectrum.

4 Concluding Remarks and Further Problems

The goal of such developments is to use the finite dimensional techniques into the spectral analysis of bounded self-adjoint operators on infinite dimensional Hilbert spaces. This also leads to a large number of open problems of different flavors. We shall quote some of them here.

- The numerical algorithms have to be developed to approximate spectrum and essential spectrum using the eigenvalue sequence of truncations, with emphasis on the computational feasibility.
- The random versions of the spectral approximation problems are another area to be investigated. The related work is already under progress in [14].
- The use of preconditioners has its origin in the numerical linear algebra literature, especially in the case of Toeplitz operators. One can expect good estimates on such concrete examples.
- The unbounded operators shall be considered and the approximation techniques have to be developed.

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