# Complexity Issues in Computing Spectra, Pseudospectra and Resolvents

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#### Abstract

We display methods that allow for computations of spectra, pseudospectra and resolvents of linear operators on Hilbert spaces and also elements in unital Banach algebras. The paper considers two different approaches, namely, pseudospectral techniques and polynomial numerical hull theory. The former is used for Hilbert space operators whereas the latter can handle the general case of elements in a Banach algebra. This approach leads to multicentric holomorphic calculus. We also discuss some new types of pseudospectra and the recently defined Solvability Complexity Index.

Key words: spectrum, resolvent, pseudospectra, polynomial numerical hull, holomorphic functional calculus, multicentric calculus, solvability complexity index

#### 1 Introduction

The theme of this article is how to compute and approximate spectra of arbitrary closed operators on separable Hilbert spaces and arbitrary elements of a unital Banach algebra. This task is a fascinating mathematical problem, but it is strongly motivated by applications. The reason is as follows. After the triumph of quantum mechanics, operator and spectral theory became indispensable mathematical disciplines in order to support quantum theory and also to secure its mathematical foundations. The fundamental paper of Murray and von Neumann [33] (which was also very much motivated by quantum mechanics) on operator algebras showed how important abstractions of these issues were. In particular, one could then ask spectral questions not only about operators but also about elements in a unital  $C^*$ -algebra (or a von Neumann algebra), or more generally, a unital Banach algebra. There is a vast literature on how to analyze spectra of linear operators and the field is still very much active.

So far, so good, the only problem is that the theoretical physicist may not only want theorems about structural properties of spectra, one may actually want to determine the spectra completely. When faced with this problem the mathematician may first recall that even if the dimension of the Hilbert space is finite, this is not trivial. One quickly realizes that, due to Abel's contribution on the unsolvability of the quintic using radicals, one is doomed to fail if one tries to construct the spectrum in terms of finitely many arithmetic operations and radicals of the matrix elements of the operator. However, in finite dimensions, there is a vast theory on

how to obtain sequences of sets, whose construction only require finitely many arithmetic operations and radicals of the matrix elements, such that the sequence converges to the spectrum of the desired operator. Thus, at least in finite dimensions, one can construct the spectrum, and this construction automatically yields a method for approximating the spectrum. Even though this may be difficult in practice, one has a mathematical theory that guarantees that up to an arbitrarily small error, one can determine the spectra of operators on finite dimensional Hilbert spaces.

There is no automatic extension from the finite dimensional case, and the problem is therefore: what can be done in infinite dimensions? Moreover, how does one handle the case of an unbounded operator? Keeping the Schrödinger and Dirac operators in mind, one realizes that the unbounded cases may be the most important ones. We must emphasize that quite a lot is known about how to approximate spectra of Schrödinger and Dirac operators, but, as far as we know, even in the self-adjoint case, one still only knows how to deal with special cases, and current methods lack generality.

Bill Arveson commented in 1994 [3] on the situation of the computational spectral problem: "Unfortunately, there is a dearth of literature on this basic problem, and so far as we have been able to tell, there are no proven techniques." We will emphasize that this quote is concerned with the general problem, and if one has more structure available e.g. self-adjointness, then much more can be said. However, during the last two decades the importance of non-normal operators and their spectra has become increasingly evident. In particular, the growing interest in non-Hermitian quantum mechanics [9, 28], non-self-adjoint differential operators [19, 21] and in general non-normal phenomena [46, 47] has made non-self-adjoint operators and pseudospectral theory indispensable. This emphasizes the importance of the general problem and poses a slightly philosophical problem, namely, could there be operators whose spectra we can never determine? If such operators are indispensable in areas of mathematical physics it may lead to serious restrictions to our possible understanding of some physical systems. Fortunately, there have been some recent developments on the topic and due to the results in [27] the future may not be so pessimistic. For other papers related to the ideas presented in this papers we refer to [3, 4, 6, 10, 11, 12, 13, 14, 15, 16, 17, 24, 26, 30].

#### 1.1 Background and Notation

We will in this section review some basic definition and introduce the notation used in the article. Throughout the paper  $\mathcal{H}$  will always denote a separable Hilbert space,  $\mathcal{X}$  and  $\mathcal{Y}$  are Banach spaces,  $\mathcal{B}(\mathcal{H})$  and  $\mathcal{B}(\mathcal{X})$  the sets of bounded linear operators on  $\mathcal{H}$  and  $\mathcal{X}$ ,  $\mathcal{C}(\mathcal{H})$  and  $\mathcal{C}(\mathcal{X})$  the sets of densely defined closed linear operators on  $\mathcal{H}$  and  $\mathcal{X}$ , and  $\mathcal{SA}(\mathcal{H})$  the set of self-adjoint operators on  $\mathcal{H}$ . For  $T \in \mathcal{C}(\mathcal{H})$  or  $\mathcal{C}(\mathcal{X})$  the domain of T will be denoted by  $\mathcal{D}(T)$ . Furthermore,  $\mathcal{A}$  denotes a complex unital Banach algebra. We denote by  $a,b,\ldots$  generic elements in the algebra and the unit  $e \in \mathcal{A}$  satisfies  $\|e\| = 1$ . Thus for example, the spectrum of  $a \in \mathcal{A}$  is given by

$$\sigma(a) = \{ z \in \mathbb{C} : z - a \text{ does not have an inverse} \}.$$

If  $\mathcal{X}$  is a Banach space (or Hilbert space as before) then bounded operators  $B(\mathcal{X})$  is an important example of unital Banach algebras. The spectrum of an operator  $T \in \mathcal{C}(\mathcal{X})$  is defined slightly differently from the Banach algebra case:

$$\sigma(T) = \{ z \in \mathbb{C} : z - T \text{ does not have an inverse in } B(\mathcal{X}) \}.$$

We will denote orthonormal basis elements of  $\mathcal{H}$  by  $e_j$ , and if  $\{e_j\}_{j\in\mathbb{N}}$  is a basis and  $\xi\in\mathcal{H}$  then  $\xi_j=\langle \xi,e_j\rangle$ . The word basis will always refer to an orthonormal basis. If  $\mathcal{H}$  is a finite dimensional Hilbert space with a basis  $\{e_j\}$  then  $LT_{\text{pos}}(\mathcal{H})$  will denote the set of lower triangular matrices (with respect to  $\{e_j\}$ ) with positive elements on the diagonal. The closure of a set  $\Omega\in\mathbb{C}$  will be denoted by  $\overline{\Omega}$  or  $\text{cl}(\Omega)$ , and the interior of  $\Omega$  will be denoted by  $\Omega^o$ .

Convergence of sets in the complex plane will be quite crucial in our analysis and hence we need the Hausdorff metric as defined by the following.

**Definition 1.1.** For a set  $\Sigma \subset \mathbb{C}$  and  $\delta > 0$  we will let  $\omega_{\delta}(\Sigma)$  denote the  $\delta$ -neighborhood of  $\Sigma$  (i.e. the union of all  $\delta$ -balls centered at points of  $\Sigma$ ). Given two compact sets  $\Sigma, \Lambda \subset \mathbb{C}$  their Hausdorff distance is

$$d_H(\Sigma, \Lambda) = \max \left\{ \sup_{\lambda \in \Sigma} d(\lambda, \Lambda), \sup_{\lambda \in \Lambda} d(\lambda, \Sigma) \right\}$$

where  $d(\lambda, \Lambda) = \inf_{\rho \in \Lambda} |\rho - \lambda|$ . If  $\{\Lambda_n\}_{n \in \mathbb{N}}$  is a sequence of compact subsets of  $\mathbb{C}$  and  $\Lambda \subset \mathbb{C}$  is compact such that  $d_H(\Lambda_n, \Lambda) \to 0$  as  $n \to \infty$  we may use the notation  $\Lambda_n \longrightarrow \Lambda$ .

When it comes to unbounded subsets of  $\mathbb{C}$  one has to be a little careful, as the Hausdorff metric is no longer applicable. Instead one may use the *Attouch-Wets* metric defined by

$$d_{\mathrm{AW}}(\Sigma, \Lambda) = \sum_{i=1}^{\infty} 2^{-i} \min \left\{ 1, \sup_{|x| < i} |d(x, \Sigma) - d(x, \Lambda)| \right\},$$

where  $\Sigma$  and  $\Lambda$  are closed subsets of  $\mathbb{C}$ , and where  $d(x, \Sigma)$  is as above, which is well-defined even when  $\Sigma$  is unbounded. Note that the Attouch-Wets metric becomes, in some sense, a metric that represents *locally uniform* convergence of sets. This can easily be seen as follows. Let  $\Sigma \subset \mathbb{C}$  and  $\Sigma_n \subset \mathbb{C}$ ,  $n = 1, 2, \ldots$  be closed and non-empty. Then

$$d_{\mathrm{AW}}(\Sigma_n, \Sigma) \to 0$$
 if and only if  $d_{\mathcal{K}}(\Sigma_n, \Sigma) \to 0$  for any compact  $\mathcal{K} \subset \mathbb{C}$ ,

where

$$d_{\mathcal{K}}(\Sigma,\Lambda) = \max \left\{ \sup_{s \in \Sigma \cap \mathcal{K}} d(s,\Lambda), \sup_{t \in \Lambda \cap \mathcal{K}} d(t,\Sigma) \right\},$$

where we use the convention that  $\sup_{s\in\Sigma\cap\mathcal{K}}d(s,\Lambda)=0$  if  $\Sigma\cap\mathcal{K}=\emptyset$ . This also makes it clear that if we deal with bounded sets, the two metrics are equivalent.

#### 1.2 Overview of the paper

The discussion in this paper touches two different approaches for computing the spectrum. In  $pseudospectral\ techniques$  one studies the sets in which the resolvent of the operator T,

$$z \mapsto (z - T)^{-1}$$
,

becomes large (or does not exist). Polynomial numerical hulls on the other hand are based on sets

$$V_p(T) = \{ z \in \mathbb{C} : |p(z)| \le ||p(T)|| \}$$

where p is a monic polynomial, and thus they do not have recourse to any inversion of operators. We start with the pseudospectral theory and present some important variants to deal with operators. Then we define the  $Solvability\ Complexity\ Index$  which keeps track on how many levels an algorithm has limiting processes. We then discuss compact operators and show that the spectrum can be computed using algorithms with index 1. The next sections concern the indices of bounded and unbounded operators respectively.

Then we turn to polynomial numerical hull techniques. What is crucial is that all sets considered are *inclusion sets* for the spectrum. For example, intersecting the  $V_p(T)$  over all first degree polynomials gives the closure of the numerical range while intersecting over all polynomials equals the polynomially convex hull of the spectrum. The algorithms have a natural set up within Banach algebras and for example, the spectrum of an algebra element (within the subalgebra it generates) can be computed with just one limiting process *provided* that one assumes that the norm of an element is available as a single operation.

It turns out that, as a byproduct, one obtains an explicit representation for the resolvent which then leads to an approach for algorithmic holomorphic calculus with low complexity.

### 2 Pseudospectra and their Close Cousins

Pseudospectral theory is now a mainstay in spectral analysis and we refer the reader to [47] for a thorough introduction to the topic. Before we introduce other types of pseudospectra we will recall the definition of the pseudospectrum and discuss some of its quite pleasant properties.

**Definition 2.1.** Let T be a closed operator on a Hilbert space  $\mathcal{H}$  such that  $\sigma(T) \neq \mathbb{C}$ , and  $\epsilon > 0$ . The  $\epsilon$ -pseudospectrum of T is defined as the set

$$\sigma_{\epsilon}(T) = \sigma(T) \cup \{z \notin \sigma(T) : \|(z - T)^{-1}\| > \epsilon^{-1}\}.$$

Note that, for  $\epsilon > 0$ , the mapping  $\mathcal{B}(\mathcal{H}) \ni T \mapsto \overline{\sigma_{\epsilon}(T)} \in \mathcal{F}$ , where  $\mathcal{F}$  denotes the collection of compact subsets of  $\mathbb{C}$  equipped with the Hausdorff metric, is a continuous mapping. This is a nice property that is not shared by the spectrum. In particular, it is well known that the mapping  $\mathcal{B}(\mathcal{H}) \ni T \mapsto \sigma(T) \in \mathcal{F}$  is discontinuous (see [27] for examples). The nice property of continuity is one reason why the pseudospectrum has become popular and very important in applications [26], although there are many other justifications for the enthusiasm for the pseudospectum [47, 45]. Note, however, that the continuity property ends with  $\mathcal{B}(\mathcal{H})$ . In particular, as a result of the fundamental paper by Shargorodsky [41], the mapping  $\mathcal{C}(\mathcal{H}) \ni T \mapsto \overline{\sigma_{\epsilon}(T)}$ , where  $\mathcal{C}(\mathcal{H})$  is equipped with the graph metric (see [27]), may not be continuous. This is also the case in the bounded example if the Hilbert space is replaced by a Banach space.

In [25] and [27] some new variants of the pseudospectrum were introduced. We will recall these sets here and discuss some of their nice properties. Before we introduce the different pseudospectra we need to define a convenient function.

**Definition 2.2.** Define, for  $n \in \mathbb{Z}_+$  the function  $\Phi_n : \mathcal{B}(\mathcal{H}) \times \mathbb{C} \to \mathbb{R}$  by

$$\Phi_n(S,z) = \min\left\{\lambda^{1/2^{n+1}}: \lambda \in \sigma\left(\left((S-z)^*\right)^{2^n}(S-z)^{2^n}\right)\right\}.$$

Define also for  $T \in \mathcal{B}(\mathcal{H})$ 

$$\gamma_n(z) = \min[\Phi_n(T, z), \Phi_n(T^*, \bar{z})]. \tag{2.1}$$

#### 2.1 The $(n, \epsilon)$ -pseudospectrum

We will now introduce the  $(n, \epsilon)$ -pseudospectrum, which is an extension of the usual pseudospectrum. (This set was actually first introduced in [25].)

**Definition 2.3.** Let T be a closed operator on a Hilbert space  $\mathcal{H}$  such that  $\sigma(T) \neq \mathbb{C}$ , and let  $n \in \mathbb{Z}_+$  and  $\epsilon > 0$ . The  $(n, \epsilon)$ -pseudospectrum of T is defined as the set

$$\sigma_{n,\epsilon}(T) = \sigma(T) \cup \{z \notin \sigma(T) : \|(z-T)^{-2^n}\|^{1/2^n} > \epsilon^{-1}\}.$$

As we will see in the next theorem, the  $(n, \epsilon)$ -pseudospectrum has all the nice continuity properties that the pseudospectrum has, but it also approximates the spectrum arbitrarily well for large n.

**Theorem 2.4.** [27] Let  $T \in \mathcal{B}(\mathcal{H})$ ,  $\gamma_n$  be defined as in (2.1) and  $\epsilon > 0$ . Then the following is true:

- (i)  $\sigma_{n+1,\epsilon}(T) \subset \sigma_{n,\epsilon}(T)$ .
- (ii)  $\sigma_{n,\epsilon}(T) = \{ z \in \mathbb{C} : \gamma_n(z) < \epsilon \}.$
- (iii)  $\operatorname{cl}(\{z : \gamma_n(z) < \epsilon\}) = \{z : \gamma_n(z) \le \epsilon\}.$
- (iv) Let  $\omega_{\epsilon}(\sigma(T))$  denote the  $\epsilon$ -neighborhood around  $\sigma(T)$ . Then

$$d_H\left(\overline{\sigma_{n,\epsilon}(T)}, \overline{\omega_{\epsilon}(\sigma(T))}\right) \longrightarrow 0, \quad n \to \infty.$$

(v) If  $\{T_k\} \subset \mathcal{B}(\mathcal{H})$  and  $T_k \to T$  in norm, it follows that

$$d_H\left(\overline{\sigma_{n,\epsilon}(T_k)},\overline{\sigma_{n,\epsilon}(T)}\right) \longrightarrow 0, \qquad k \to \infty.$$

Note that the definition of the  $(n, \epsilon)$ -pseudospectrum carries over to the abstract case of a unital Banach algebra. In particular, we will have the following definition.

**Definition 2.5.** Let  $a \in \mathcal{A}$  where  $\mathcal{A}$  is a unital Banach algebra,  $n \in \mathbb{Z}_+$  and  $\epsilon > 0$ . The  $(n, \epsilon)$ -pseudospectrum of a is defined as the set

$$\sigma_{n,\epsilon}(a) = \sigma(a) \cup \{z \notin \sigma(a) : \|(z-a)^{-2^n}\|^{1/2^n} > \epsilon^{-1}\}.$$

However, all of the properties (i)-(v) may not carry over in the abstract case. For example, (ii) and (iii) does not even make sense, since an involution mapping  $a \mapsto a^*$  is needed to define the function  $\gamma$ . Also, property (v) may not carry over. In fact, by the fundamental result of Shargorodsky [41], it is known that pseudospectra of Banach space operators can "jump". More precisely one can have that

$$\overline{\sigma_{\epsilon}(a)} \neq \sigma(a) \cup \{ z \notin \sigma(a) : \|(z-a)^{-1}\| \ge \epsilon^{-1} \}$$

for a being a bounded operator on a certain Banach space. However, properties (i) and (iv) carry over and this can be seen as follows. First, we need the following proposition from [27]:

**Proposition 2.6.** [27] Let  $f: \mathbb{C} \to [0,\infty)$  be continuous and let  $\{f_k\}_{k\in\mathbb{N}}$  be a sequence of functions such that  $f_k: \mathbb{C} \to [0,\infty)$  and  $f_k \to f$  locally uniformly. Suppose that one of the two following properties are satisfied.

- (i)  $f_k \to f$  monotonically from above.
- (ii) For  $\epsilon > 0$ , then  $\operatorname{cl}(\{z : f(z) < \epsilon\}) = \{z : f(z) < \epsilon\}$ .

Then, it follows that

$$d_{AW}(\operatorname{cl}(\{z: f_k(z) < \epsilon\}), \operatorname{cl}(\{z: f(z) < \epsilon\})) \longrightarrow 0, \quad k \to \infty$$

Note that (i) follows by the definition of  $\sigma_{n,\epsilon}(a)$  and the fact that

$$\|(z-a)^{-2^{n+1}}\|^{-1/2^{n+1}} \ge \|(z-a)^{-2^n}\|^{-1/2^{n+1}} \|(z-a)^{-2^n}\|^{-1/2^{n+1}}$$
$$= \|(z-a)^{-2^n}\|^{-1/2^n}.$$

To see that (iv) is also true in the general case define

$$f(z) = \operatorname{dist}(z, \sigma(a)),$$

and define

$$f_n(z) = \begin{cases} \|(z-a)^{-2^n}\|^{-1/2^n} & z \notin \sigma(a) \\ 0 & z \in \sigma(a). \end{cases}$$

After observing that

$$f(z) = 1/\rho((z-a)^{-1}),$$

where  $\rho((z-a)^{-1})$  denotes the spectral radius of  $((z-a)^{-1})$ , we can apply the spectral radius formula, a straightforward argument via Dini's Theorem and deduce that  $f_n \to f$  locally uniformly and monotonically from above. By invoking Proposition 2.6 we are done.

#### 2.2 The Residual Pseudospectrum

The disadvantage of the  $(n, \epsilon)$ -pseudospectrum is that even though one can estimate the spectrum by taking n very large or  $\epsilon$  very small, n may have to be too large or  $\epsilon$  too small for practical purposes (this would depend on the computer used). Thus, since we only have the estimate  $\sigma(T) \subset \sigma_{n,\epsilon}(T)$  for  $T \in \mathcal{B}(\mathcal{H}), \epsilon > 0$ , it is important to get a "lower" bound on  $\sigma(T)$  i.e. we want to find a set  $\theta \subset \mathbb{C}$  such that  $\theta \subset \sigma(T)$ . A candidate for this is described in the following.

**Definition 2.7.** Let  $T \in \mathcal{B}(\mathcal{H})$  and  $\Phi_0$  be defined as in Definition 2.2. Let  $\zeta_1(z) = \Phi_0(T, z)$   $\zeta_2(z) = \Phi_0(T^*, \bar{z})$ . Now let  $\epsilon > 0$  and define the  $\epsilon$ -residual pseudospectrum to be the set

$$\sigma_{\text{res},\epsilon}(T) = \{z : \zeta_1(z) > \epsilon, \zeta_2(z) = 0\}$$

and the adjoint  $\epsilon$ -residual pseudospectrum to be the set

$$\sigma_{\mathrm{res}^*,\epsilon}(T) = \{z : \zeta_1(z) = 0, \zeta_2(z) > \epsilon\}.$$

**Theorem 2.8.** [27] Let  $T \in \mathcal{B}(\mathcal{H})$  and let  $\{T_k\} \subset \mathcal{B}(\mathcal{H})$  such that  $T_k \to T$  in norm, as  $k \to \infty$ . Then for  $\epsilon > 0$  we have the following:

(i) 
$$\sigma(T) \supset \bigcup_{\epsilon > 0} \sigma_{\text{res},\epsilon}(T) \cup \sigma_{\text{res}^*,\epsilon}(T)$$
.

(ii) 
$$\operatorname{cl}(\{z \in \mathbb{C} : \zeta_1(z) < \epsilon\}) = \{z \in \mathbb{C} : \zeta_1(z) \le \epsilon\}.$$

(iii) 
$$\operatorname{cl}(\{z \in \mathbb{C} : \zeta_2(z) < \epsilon\}) = \{z \in \mathbb{C} : \zeta_2(z) \le \epsilon\}.$$

(iv)

$$d_H(\operatorname{cl}(\sigma_{\operatorname{res},\epsilon}(T_k)),\operatorname{cl}(\sigma_{\operatorname{res},\epsilon}(T))) \longrightarrow 0, \qquad k \to \infty.$$

(v) 
$$d_H(\operatorname{cl}(\sigma_{\operatorname{res}^*,\epsilon}(T_k)),\operatorname{cl}(\sigma_{\operatorname{res}^*,\epsilon}(T))) \longrightarrow 0, \qquad k \to \infty$$

Note that the definition of the residual pseudospectrum and the adjoint residual pseudospectrum does not extend to an arbitrary unital Banach algebra because of the lack of an involution. However, if we have a unital Banach algebra  $\mathcal{A}$  with an involution we can define the following functions: Let  $a \in \mathcal{A}$  and define

$$\zeta_{a,1}(z) = \min \left\{ \sqrt{\lambda} : \lambda \in \sigma \left( (a-z)^* (a-z) \right) \right\}$$

$$\zeta_{a,2}(z) = \min \left\{ \sqrt{\lambda} : \lambda \in \sigma \left( (a-z)(a-z)^* \right) \right\},$$

then, clearly, Definition 2.7 extends to elements in  $\mathcal{A}$ . The question on whether properties (i)-(v) in Theorem 2.8 extends to  $\mathcal{A}$  is delicate. We will not make any predictions, however, we would like to point out that the proof of Theorem 2.8 [27] makes use of a crucial result, namely

**Theorem 2.9.** (Shargorodsky)[41] Let  $\Omega$  be an open subset of  $\mathbb{C}$ , X be a Banach space and Y be a uniformly convex Banach space. Suppose  $A: \Omega \to \mathcal{B}(X,Y)$  is an analytic operator valued function such that A'(z) is invertible for all  $z \in \Omega$ . If  $||A(z)|| \leq M$  for all  $z \in \Omega$  then ||A(z)|| < M for all  $z \in \Omega$ .

# 3 The Solvability Complexity Index

Let  $T \in \mathcal{B}(\mathcal{H})$  and suppose that we would like to compute  $\sigma(T)$ . This is a non-trivial computational problem even if the dimension of the Hilbert space is finite, say N. In that case the QR-algorithm may be the method of choice and with suitable assumptions on T one can guarantee that if  $\theta_n = \{\omega_{1,n}, \ldots, \omega_{N,n}\}$  are the elements on the diagonal of  $T_n$ , where  $T_n$  is the n-th term in the QR-iteration, then

$$d_H(\theta_n, \sigma(T)) \longrightarrow 0, \qquad n \to \infty.$$

What is crucial is that there is only one numerical parameter tending to infinity. Now, suppose that  $T \in \mathcal{B}(\mathcal{H})$  is compact. Let  $\{e_j\}$  be a basis for  $\mathcal{H}$  and let  $P_m$  be the projection onto  $\operatorname{span}\{e_1,\ldots,e_m\}$ . In that case it follows that

$$d_H(\sigma(P_mT\lceil_{P_m\mathcal{H}}),\sigma(T))\longrightarrow 0, \qquad m\to\infty.$$

Thus, a way of computing  $\sigma(T)$  is to use the QR-algorithm (or any other appropriate convergent method, also, for the sake of the argument we assume that the QR-algorithm converges) on  $P_mT\lceil_{P_m\mathcal{H}}$  for sufficiently large m. Let  $\{\omega_{1,n}^{(m)},\ldots\omega_{m,n}^{(m)}\}$  denote the elements of the diagonal of  $\widetilde{T}_{n,m}$  where  $\widetilde{T}_{n,m}$  is the n-th term in the QR-iteration of the matrix  $P_mT\lceil_{P_m\mathcal{H}}$  with respect to the basis  $\{e_i\}$ . In this case we may express  $\sigma(T)$  as

$$\sigma(T) = \lim_{m \to \infty} \lim_{n \to \infty} \{\omega_{1,n}^{(m)}, \dots \omega_{m,n}^{(m)}\}.$$

Hence, we have a way of computing  $\sigma(T)$  but it requires two limits with indices n and m. The question is then: what about the general problem? Suppose that we have no more information about the operator except that it is bounded. How many limits will we need to compute the spectrum? This is the motivation for the Solvability Complexity Index, namely, we want the Solvability Complexity Index to indicate how many limiting processes do we need to compute the spectrum (or any other set e.g. the pseudospectrum).

We will now define the Solvability Complexity Index, but before that we need the definition of a set of estimating functions of order k. The motivation behind the definition is that the estimating functions should be a method used in actual computations and the integer k determines how many limiting processes (a la the example above) there are in order to assure convergence. Note that we also want to include unbounded operators and thus more formally we have the following.

**Definition 3.1.** Let  $\mathcal{H}$  be a Hilbert space spanned by  $\{e_j\}_{j\in\mathbb{N}}$  and let

$$\Upsilon = \{ T \in \mathcal{C}(\mathcal{H}) : \operatorname{span}\{e_i\}_{n \in \mathbb{N}} \subset \mathcal{D}(T) \}. \tag{3.1}$$

Let  $\mathcal{E} \subset \Upsilon$  and  $\Xi : \mathcal{E} \to \mathcal{F}$ , where  $\mathcal{F}$  denotes the family of closed subsets of  $\mathbb{C}$ . Let

$$\Pi_{\mathcal{E}} = \{ \{x_{ii}\}_{i i \in \mathbb{N}} : \exists T \in \mathcal{E}, x_{ii} = \langle Te_i, e_i \rangle \}.$$

A set of estimating functions of order k for  $\Xi$  is a family of functions

$$\begin{split} \Gamma_{n_1}: \Pi_{\mathcal{E}} \to \mathcal{F}, \\ \Gamma_{n_1,n_2}: \Pi_{\mathcal{E}} \to \mathcal{F}, \\ & \vdots \\ \Gamma_{n_1,\dots,n_{k-1}}: \Pi_{\mathcal{E}} \to \mathcal{F}, \\ \Gamma_{n_1,\dots,n_k}: \left\{ \{x_{ij}\}_{i,j \leq N(n_1,\dots,n_k)}: \{x_{ij}\}_{i,j \in \mathbb{N}} \in \Pi_{\mathcal{E}} \right\} \to \mathcal{F}, \end{split}$$

where  $N(n_1, \ldots, n_k) < \infty$  depends on  $n_1, \ldots, n_k$ , with the following properties:

- (i) The evaluation of  $\Gamma_{n_1,...,n_k}(\{x_{ij}\})$  requires only finitely many arithmetic operations and radicals of the elements  $\{x_{ij}\}_{i,j \leq N(n_1,...,n_k)}$ .
- (ii) Also, we have the following relations between the limits:

$$\Xi(T) = \lim_{n_1 \to \infty} \Gamma_{n_1}(\{x_{ij}\}),$$

$$\Gamma_{n_1}(\{x_{ij}\}) = \lim_{n_2 \to \infty} \Gamma_{n_1, n_2}(\{x_{ij}\}),$$

$$\vdots$$

$$\Gamma_{n_1, \dots, n_{k-1}}(\{x_{ij}\}) = \lim_{n_k \to \infty} \Gamma_{n_1, \dots, n_k}(\{x_{ij}\}).$$

The limit is understood to be in the Attouch-Wets metric.

**Definition 3.2.** Let  $\mathcal{H}$  be a Hilbert space spanned by  $\{e_j\}_{j\in\mathbb{N}}$ , define  $\Upsilon$  as in (3.1), and let  $\mathcal{E}\subset\Upsilon$ . A set valued function

$$\Xi:\mathcal{E}\subset\mathcal{C}(\mathcal{H}) o\mathcal{F}$$

is said to have Solvability Complexity Index k if k is the smallest integer for which there exists a set of estimating functions of order k for  $\Xi$ . Also,  $\Xi$  is said to have infinite Solvability Complexity Index if no set of estimating functions exists. If there is a function

$$\Gamma: \{\{x_{ij}\}: \exists T \in \mathcal{E}, x_{ij} = \langle Te_i, e_i \rangle\} \to \mathcal{F}$$

such that  $\Gamma(\lbrace x_{ij} \rbrace) = \Xi(T)$ , and the evaluation of  $\Gamma(\lbrace x_{ij} \rbrace)$  requires only finitely many arithmetic operations and radicals of a finite subset of  $\lbrace x_{ij} \rbrace$ , then  $\Xi$  is said to have Solvability Complexity Index zero. The Solvability Complexity Index of a function  $\Xi$  will be denoted by  $SCI(\Xi)$ .

- **Example 3.3** (i) Let  $\mathcal{H}$  be a Hilbert space with basis  $\{e_j\}$ ,  $\mathcal{E} = \mathcal{B}(\mathcal{H})$  and  $\Xi(T) = \sigma(T)$  for  $T \in \mathcal{B}(\mathcal{H})$ . Suppose that  $\dim(\mathcal{H}) \leq 4$ . Then  $\Xi$  must have complexity index zero, since one can obviously express the eigenvalues of T using finitely many arithmetic operations and radicals of the matrix elements  $x_{ij} = \langle Te_j, e_i \rangle$ .
  - (ii) If  $\dim(\mathcal{H}) \geq 5$  then obviously  $SCI(\Xi) > 0$ , by the much celebrated theory of Abel on the insolubility of the quintic using radicals.
- (iii) Now, what about compact operators? Suppose for a moment that we can show that  $SCI(\Xi) = 1$  if  $\dim(\mathcal{H}) < \infty$ . A standard way of determining the spectrum of a compact operator T is to let  $P_n$  be the projection onto  $\operatorname{span}\{e_j\}_{j\leq n}$  and compute the spectrum of  $P_nA\lceil_{P_n\mathcal{H}}$ . This approach is justified since  $\sigma(P_nA\lceil_{P_n\mathcal{H}}) \to \sigma(T)$  as  $n \to \infty$ . By the assumption on the complexity index in finite dimensions it follows that if  $\mathcal{E}$  denotes the set of compact operators then  $SCI(\Xi) \leq 2$ .

## 4 The Compact Case

The reasoning in the example does not say anything about what the Solvability Complexity Index of spectra of compact operators is, it only suggest that the standard way of approximating spectra of such operators will normally make use of a construction requiring two limits, and hence it gives us an upper bound. However, we may very well ask the question: if  $\mathcal{E}$  is the set of compact operators on  $\mathcal{H}$  and  $\Xi(T) = \sigma(T)$  for  $T \in \mathcal{E}$ , what is  $SCI(\Xi)$ ? This is the topic of the next theorem.

**Theorem 4.1.** Let  $\{e_j\}_{j\in\mathbb{N}}$  be a basis for the Hilbert space  $\mathcal{H}$ . Let

$$\mathcal{E} = \{T \in \mathcal{B}(\mathcal{H}) : T \text{ is compact}\}\$$

and  $\Xi: \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi(T) = \sigma(T)$ . Then  $SCI(\Xi) = 1$ .

*Proof.* Let, for  $n \in \mathbb{N}$ ,  $P_n$  denote the projection onto span $\{e_1, \ldots, e_n\}$ . Define also

$$\Theta_n = \{ z \in \mathbb{C} : \operatorname{Re} z, \operatorname{Im} z = r\delta, r \in \mathbb{Z}, |r| \le n \}, \qquad \delta = \sqrt{\frac{1}{n}}, \tag{4.1}$$

and let

$$\Gamma_n(\lbrace x_{ij}\rbrace) = \lbrace z \in \Theta_n : \nexists L \in LT_{pos}(P_n\mathcal{H}), T_{1/n}(z) = LL^* \rbrace,$$

where  $LT_{pos}(P_n\mathcal{H})$  denotes the lower triangular matrices in  $P_n\mathcal{H}$  (with respect to  $\{e_1,\ldots,e_n\}$ ) with positive elements on the diagonal and

$$T_{1/n}(z) = (P_n(T-z)P_n)^* P_n(T-z)P_n - \frac{1}{n^2} P_n.$$

We claim that  $\Gamma_n$  can be evaluated using only finitely many arithmetic operations and radicals of the matrix elements  $\{x_{ij}\}$ . Indeed, to determine if  $z \in \Theta_k$  is in  $\Gamma_k(\{x_{ij}\})$  one has to determine

if  $T_{1/n}(z)$  has a Cholesky decomposition or not. This can indeed be done by using finitely many arithmetic operations and radicals of  $\{x_{ij}\}$ . The fact that  $\Theta_n$  contains only finitely many elements yields the assertion. To see that

$$d_H(\Gamma_n(\lbrace x_{ij} \rbrace), \sigma(T)) \longrightarrow 0, \quad n \to \infty,$$

one uses that fact that  $\sigma(P_nKP_n) \to \operatorname{sp}(T)$  and the definition of the pseudospectrum. We omit the details.

This gives us the obvious corollary for operators on finite dimensional Hilbert spaces.

**Corollary 4.2.** Let  $\{e_j\}_{j=1}^N$  be a basis for the Hilbert space  $\mathcal{H}$ , and suppose that  $5 \leq N < \infty$ . Let  $\mathcal{E} = \mathcal{B}(\mathcal{H})$  and  $\Xi : \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi(T) = \sigma(T)$ . Then  $SCI(\Xi) = 1$ .

#### 5 The Bounded Case

As we saw in the previous section, handling the compact case essentially relies on the fact that the spectral properties of a section  $P_nTP_n$  of a compact operator T resemble the spectral properties of T for large n (here  $P_n$  is as in the proof of Theorem 4.1). This may not be the case for an arbitrary bounded operator. In this case completely different techniques must be used.

**Theorem 5.1.** [27] Let  $\{e_j\}_{j\in\mathbb{N}}$  be a basis for the Hilbert space  $\mathcal{H}$  and let  $\mathcal{E} = \mathcal{B}(\mathcal{H})$ . Define, for  $n \in \mathbb{Z}_+, \epsilon > 0$ , the set valued functions

$$\Xi_1, \Xi_2, \Xi_3, \Xi_4, \Xi_5: \mathcal{E} \to \mathcal{F}$$

by

$$\Xi_1(T) = \overline{\sigma_{n,\epsilon}(T)}, \quad \Xi_2(T) = \overline{\omega_{\epsilon}(\sigma(T))}, \quad \Xi_3(T) = \sigma(T),$$
$$\Xi_4(T) = \overline{\sigma_{\mathrm{res},\epsilon}(T)}, \quad \Xi_5(T) = \overline{\sigma_{\mathrm{res}*,\epsilon}(T)}.$$

Then

$$\begin{split} SCI(\Xi_1) \leq 2, & SCI(\Xi_2) \leq 3, & SCI(\Xi_3) \leq 3, \\ SCI(\Xi_4) \leq 2, & SCI(\Xi_5) \leq 2. \end{split}$$

We will not prove the theorem here, but refer to [27] for details. However, we will sketch the ideas on how to construct the set of estimating functions. We start by constructing a set of estimating functions for  $\Xi_1$ . In particular, given the matrix elements  $x_{ij} = \langle Te_j, e_i \rangle$  of  $T \in \mathcal{B}(\mathcal{H})$  we define the following:

$$\Gamma_{n_{1},n_{2}}(\lbrace x_{ij}\rbrace) = \lbrace z \in \Theta_{n_{1}} : \nexists L \in LT_{pos}(P_{n_{1}}\mathcal{H}), T_{\epsilon,n_{1},n_{2}}(z) = LL^{*}\rbrace 
\cup \lbrace z \in \Theta_{n_{1}} : \nexists L \in LT_{pos}(P_{n_{1}}\mathcal{H}), \widetilde{T}_{\epsilon,n_{1},n_{2}}(z) = LL^{*}\rbrace, 
\Gamma_{n_{1}}(\lbrace x_{ij}\rbrace) = \lbrace z \in \Theta_{n_{1}} : (-\infty,0] \cap \sigma(T_{\epsilon,n_{1}}(z)) \neq \emptyset \rbrace 
\cup \lbrace z \in \Theta_{n_{1}} : (-\infty,0] \cap \sigma(\widetilde{T}_{\epsilon,n_{1}}(z)) \neq \emptyset \rbrace, \qquad n_{1}, n_{2} \in \mathbb{N},$$
(5.1)

where  $LT_{pos}(P_m\mathcal{H})$  denotes the set of lower triangular matrices in  $\mathcal{B}(P_m\mathcal{H})$  (with respect to  $\{e_i\}$ ) with strictly positive diagonal elements and

$$T_{\epsilon,n_{1},n_{2}}(z) = T_{n_{1},n_{2}}(z) - \epsilon^{2^{n+1}} I,$$

$$\widetilde{T}_{\epsilon,n_{1},n_{2}}(z) = \widetilde{T}_{n_{1},n_{2}}(z) - \epsilon^{2^{n+1}} I,$$

$$T_{\epsilon,n_{1}}(z) = T_{n_{1}}(z) - \epsilon^{2^{n+1}} I,$$

$$\widetilde{T}_{\epsilon,n_{1}}(z) = \widetilde{T}_{n_{1}}(z) - \epsilon^{2^{n+1}} I,$$
(5.2)

where  $T_{n_1,n_2}$ ,  $\widetilde{T}_{n_1,n_2}$ ,  $T_{n_1}$  and  $\widetilde{T}_{n_1}$  are defined by

$$T_{m}(z) = P_{m}((T-z)^{*})^{2^{n}}(T-z)^{2^{n}}|_{P_{m}\mathcal{H}},$$

$$T_{m,k}(z) = P_{m}((P_{k}(T-z)P_{k})^{*})^{2^{n}}(P_{k}(T-z)P_{k})^{2^{n}}|_{P_{m}\mathcal{H}},$$

$$\tilde{T}_{m}(z) = P_{m}(T-z)^{2^{n}}((T-z)^{*})^{2^{n}}|_{P_{m}\mathcal{H}},$$

$$\tilde{T}_{m,k}(z) = P_{m}(P_{k}(T-z)P_{k})^{2^{n}}((P_{k}(T-z)P_{k})^{*})^{2^{n}}|_{P_{m}\mathcal{H}}.$$

One can then argue that the evaluation of  $\Gamma_{n_1,n_2}(\{x_{ij}\})$  indeed requires only finitely many arithmetic operations and radicals. This is pretty straightforward, however, showing that

$$\Xi_1(T) = \lim_{n_1 \to \infty} \Gamma_{n_1}(\{x_{ij}\}),$$
  
$$\Gamma_{n_1}(\{x_{ij}\}) = \lim_{n_2 \to \infty} \Gamma_{n_1, n_2}(\{x_{ij}\}),$$

requires some more work. As long as we can establish that our construction actually yields a set of estimating functions of order two for  $\Xi_1$  we can deduce that  $SCI(\Xi_1) \leq 2$  and then Theorem 2.4 yields that  $SCI(\Xi_2) \leq 3$ . The fact that  $SCI(\Xi_3) \leq 3$  is clear from the fact that  $SCI(\Xi_1) \leq 2$ .

Remark 5.2 It is tempting to try clever ways of subsequencing in order to reduce the bound on the Solvability Complexity Index. However, the trained eye of an operator theorist will immediately spot the difficulties with such a strategy. This is confirmed in the following proposition.

**Proposition 5.3.** Let  $\epsilon > 0$ , n = 0 and  $\Gamma_{n_1,n_2}$  be defined as in (5.1). There does NOT exists a subsequence  $\{k_m\}_{m \in \mathbb{N}}$  such that

$$\Gamma_{m,k_m}(\{x_{ij}\}) \longrightarrow \overline{\sigma_{\epsilon}(T)}, \qquad m \to \infty, \quad x_{ij} = \langle Te_j, e_i \rangle, \quad \forall T \in \mathcal{B}(\mathcal{H}).$$

*Proof.* We will argue by contradiction and suppose that such a subsequence exists. Then, obviously may assume that  $k_m > m$  for all  $m \in \mathbb{N}$ . Now define the operator S on span $\{e_j\}_{j \in \mathbb{N}}$  by

$$\langle Se_j, e_i \rangle = \begin{cases} 1 + \epsilon & i = m, j = k_m + 1, \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to see that S extends to a bounded operator on  $\mathcal{H}$  with  $||S|| \leq 1$ . Define  $T = S + S^*$ . Then a straightforward computation gives that for m > 1 (since  $k_m > m$ ) it follows that

$$P_m T^* T P_m = (1 + \epsilon)^2 P_m, \qquad P_m T^* P_{k_m} T P_m = (1 + \epsilon)^2 P_{m-1}.$$
 (5.3)

And it is this equation that will yield the contradiction. Letting  $x_{ij} = \langle Te_j, e_i \rangle$  we have (as argued above) that  $\Gamma_m(\{x_{ij}\}) \longrightarrow \overline{\sigma_{\epsilon}(T)}$ , as  $m \to \infty$ , and by hypothesis that

$$\Gamma_{m,k_m}(\{x_{ij}\}) \longrightarrow \overline{\sigma_{\epsilon}(T)}, \qquad m \to \infty,$$

hence

$$d_H(\Gamma_m(\lbrace x_{ij}\rbrace), \Gamma_{m,k_m}(\lbrace x_{ij}\rbrace)) \longrightarrow 0, \qquad m \to \infty.$$
 (5.4)

It is the latter statement that is not true, and therefore gives us the desired contradiction. We will now demonstrate why. Note that

$$\Gamma_m(\{x_{ij}\}) = \{z \in \mathbb{C} : (-\infty, 0] \cap \sigma(T_{\epsilon, m}(z)) \neq \emptyset\}$$
$$\cup \{z \in \mathbb{C} : (-\infty, 0] \cap \sigma(\widetilde{T}_{\epsilon, m}(z)) \neq \emptyset\},\$$

where

$$T_{\epsilon,m}(z) = P_m T^* T|_{P_m \mathcal{H}} - P_m \bar{z} T|_{P_m \mathcal{H}} - P_m z T^*|_{P_m \mathcal{H}} - (\epsilon - |z|)I,$$

$$\tilde{T}_{\epsilon,m}(z) = P_m T^* T|_{P_m \mathcal{H}} - P_m \bar{z} T|_{P_m \mathcal{H}} - P_m z T^*|_{P_m \mathcal{H}} - (\epsilon - |z|)I.$$

Hence, by the first part of (5.3) and the fact that  $||T|| \le 2$  it follows that

$$(-\infty, 0] \cap \sigma(T_{\epsilon,m}(z)) = \emptyset, \qquad (-\infty, 0] \cap \sigma(\widetilde{T}_{\epsilon,m}(z)) = \emptyset, \qquad |z| \le 1/8.$$

In particular,

$$\mathbb{D}(0,1/8) \cap \Gamma_m(\{x_{ij}\}) = \emptyset, \quad \forall m \in \mathbb{N} \setminus \{1\}, \tag{5.5}$$

where  $\mathbb{D}(0,1/8)$  denotes the closed disc centered at zero with radius 1/8. On the other hand we have that

$$\Gamma_{m,k_m}(\{x_{ij}\}) = \{z \in \mathbb{C} : (-\infty, 0] \cap \sigma(T_{\epsilon,m,k_m}(z)) \neq \emptyset\}$$
$$\cup \{z \in \mathbb{C} : (-\infty, 0] \cap \sigma(\widetilde{T}_{\epsilon,m,k_m}(z)) \neq \emptyset\},$$

where

$$T_{\epsilon,m,k_m}(z) = P_m(T-z)^* P_{k_m}(T-z)|_{P_m\mathcal{H}} - \epsilon I,$$
  
$$\tilde{T}_{\epsilon,m,k_m}(z) = P_m(T-z) P_{k_m}(T-z)^*|_{P_m\mathcal{H}} - \epsilon I.$$

Thus, by the last part of (5.3) it follows that

$$0 \in \sigma(T_{\epsilon,m,k_m}(z)), \qquad z = 0 \quad \forall m \in \mathbb{N} \setminus \{1\}.$$

In particular,  $0 \in \Gamma_{m,k_m}(\{x_{ij}\})$  for all m > 1. This, together with (5.5) contradicts (5.4), and we are done.

Although, as the previous proposition suggest, clever choices of sub sequences are not going to help, extra structure on the operators does help. This is documented in the next theorem.

**Theorem 5.4.** [27] Let  $\{e_j\}_{j\in\mathbb{N}}$  be a basis for the Hilbert space  $\mathcal{H}$  and let d be a positive integer. Define

$$\mathcal{E} = \{ T \in \mathcal{B}(\mathcal{H}) : \langle Te_{j+l}, e_j \rangle = \langle Te_j, e_{j+l} \rangle = 0, \quad l > d \}.$$

Let  $\epsilon > 0$  and  $n \in \mathbb{Z}_+$  and  $\Xi_1, \Xi_2, \Xi_3 : \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi_1(T) = \overline{\sigma_{n,\epsilon}(T)}$ ,  $\Xi_2(T) = \overline{\omega_{\epsilon}(\sigma(T))}$  and  $\Xi_3(T) = \sigma(T)$ . Then

$$SCI(\Xi_1) = 1,$$
  $SCI(\Xi_2) \le 2,$   $SCI(\Xi_3) \le 2.$ 

The proof of this theorem is a little involved and we refer to [27] for details, however, we will sketch the ideas. To prove the theorem one defines a set of estimating function for  $\Xi_1$  (containing only one element) as follows. For  $T \in \mathcal{E}$ ,  $x_{ij} = \langle Te_j, e_i \rangle$  and  $\Theta_k$  defined as in (4.1), with  $k \in \mathbb{N}$ , we let

where  $T_{\epsilon,k,2^nd+k}(z)$  and  $\widetilde{T}_{\epsilon,k,2^nd+k}(z)$  are defined in (5.2).

#### 6 The Unbounded Case

So far we have only considered bounded operators, however, in quantum mechanics it is really the unbounded operators that have the most impact. In particular, we are interested in determining spectra of Schrödinger operators

$$H = -\Delta + V,$$

and more specifically we are interested in non-self-adjoint Schrödinger operators. The reason why we need non-self-adjointness in Quantum Mechanics is threefold:

(i) Open Systems: If the system is open, meaning that particles will enter or exit (or both) on cannot have energy preservation. Thus the time evolution operator  $e^{-itH}$  cannot be unitary and hence H cannot be self-adjoint.

- (ii) Closed Systems (PT-symmetry, alternative inner products) [9]: Physicists have recently considered the possibility that the usual inner product on  $L^2(\mathbb{R}^d)$  can be replaced by a different inner product. Thus a Schrödinger operator on  $L^2(\mathbb{R}^d)$  may be self-adjoint with the usual inner product, however, non-self adjoint with another inner product, and vice versa.
- (iii) Resonances [48]: This is a well know phenomenon in Quantum Mechanics that yield non-self-adjoint operators.

Fortunately, we have bounds on the Solvability Complexity Index also for unbounded operators.

**Theorem 6.1.** [27] Let  $\{e_j\}_{j\in\mathbb{N}}$  and  $\{\tilde{e}_j\}_{j\in\mathbb{N}}$  be bases for the Hilbert space  $\mathcal{H}$  and let

$$\tilde{\mathcal{E}} = \{ T \in \mathcal{C}(\mathcal{H} \oplus \mathcal{H}) : T = T_1 \oplus T_2, T_1, T_2 \in \mathcal{C}(\mathcal{H}), T_1^* = T_2 \}$$

$$\mathcal{E} = \{ T \in \tilde{\mathcal{E}} : \operatorname{span}\{e_j\}_{j \in \mathbb{N}} \text{ is a core for } T_1, \operatorname{span}\{\tilde{e}_j\} \text{ is a core for } T_2 \}.$$

Let 
$$\epsilon > 0$$
,  $\Xi_1 : \mathcal{E} \to \mathcal{F}$  and  $\Xi_2 : \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi_1(T) = \overline{\sigma_{\epsilon}(T_1)}$  and  $\Xi_2(T) = \sigma(T_1)$ . Then  $SCI(\Xi_1) \leq 2$ ,  $SCI(\Xi_2) \leq 3$ .

Corollary 6.2. Let  $\{e_j\}_{j\in\mathbb{N}}$  be a basis for the Hilbert space  $\mathcal{H}$  and let

$$\mathcal{E} = \{ A \in \mathcal{SA}(\mathcal{H}) : \operatorname{span}\{e_j\}_{j \in \mathbb{N}} \text{ is a core for } A \}.$$

Let 
$$\epsilon > 0$$
 and  $\Xi_1, \Xi_2 : \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi_1(T) = \sigma(T)$  and  $\Xi_2(T) = \overline{\omega_{\epsilon}(\sigma(T))}$ . Then  $SCI(\Xi_1) \leq 3$ ,  $SCI(\Xi_2) \leq 2$ .

## 7 Polynomial numerical hulls

Polynomial numerical hulls were defined in [34] with an extension to convergence properties of approximations in [35]. Basic properties and related later work are highlighted in [20], see also [18, 23]. The original definitions for polynomial numerical hulls were for bounded operators in Banach space but we here carry the discussion within a unital Banach algebra  $\mathcal{A}$ . Given an element  $a \in \mathcal{A}$  and a monic polynomial p we set

$$V_p(a) = \{ z \in \mathbb{C} : |p(z)| \le ||p(a)|| \}. \tag{7.1}$$

It follows from the *spectral mapping theorem* that such a set is always an inclusion set for the spectrum

$$\sigma(a) \subset V_p(a)$$
.

The set  $V_p(a)$  can have at most d components where d denotes the degree of the polynomial. It follows from the maximum principle that each component is simply connected and as a consequence possible holes in the spectrum cannot be uncovered with this tool. On the other hand, denoting by  $\hat{\sigma}(a)$  the polynomially convex hull of the spectrum, it is well known that the following holds.

**Proposition 7.1.** The spectrum of  $a \in A$  considered as an element in the subalgebra it generates is  $\hat{\sigma}(a)$ .

**Example 7.2** If  $S \in \mathcal{B}(l^2(\mathbb{Z}))$  denotes the bilateral shift, then the spectrum is the unit circle but within the subalgebra generated by it it is the whole closed disc.

Let us denote by  $\mathbb{P}^0$  the set of all monic polynomials and by  $\mathbb{P}^0_d$  the set of monic polynomials of degree at most d.

Theorem 7.3. We have

$$\bigcap_{p \in \mathbb{P}^0} V_p(a) = \hat{\sigma}(a). \tag{7.2}$$

For a proof see [34] or [20]. The polynomial numerical hull of order k is the set

$$V^k(a) := \bigcap_{p \in \mathbb{P}^0_k} V_p(a).$$

If  $T \in \mathcal{B}(\mathcal{H})$  then denote by W(T) the numerical range of T. Recall that the numerical range may not be closed in infinite dimensional cases.

**Theorem 7.4.** For  $T \in \mathcal{B}(\mathcal{H})$  we have

$$V^1(T) = \overline{W(T)}.$$

The proof is in [34]. The theorem has actually a simple form also for operators in Banach spaces. For results on higher order numerical hulls we refer to [20].

## 8 Results based on polynomial numerical hull techniques

The discussion here is formulated in unital Banach algebras. For basic properties of spectral theory we refer to [5]. When we deal with operators in Hilbert or Banach spaces spectral information often enters naturally via a black box of the form: input a vector, output the image under the operator. So, in particular, the boundary of the spectrum is a subset of the approximate point spectrum, which is determined exactly by operator vector multiplication. More specifically, for  $T \in \mathcal{B}(\mathcal{X})$ , we have

$$\sigma_{ap}(T) = \{ z \in \mathbb{C} : \inf_{\|x\|=1} \|(T-z)x\| = 0 \}.$$
 (8.1)

This allows us to search for points in the spectrum given that we can carry out operator vector multiplication. The situation in an abstract Banach algebra is very different. In short: for  $a \in \mathcal{A}$ , in order to determine the spectrum, we are supposed to search for complex numbers z such that the resolvent does not exist. This is not a very useful starting point for computations. The picture reverses itself almost automatically: it is more natural to search for z such that

$$(z-a)^{-1}$$

exists, allowing the possibility for a constructive approach. Clearly, this happens if and only if there is a  $b(z) \in \mathcal{A}$  such that

$$||(z-a)b(z)-1|| < 1.$$

In this formulation it is also clear that if such an element b(z) in the subalgebra generated by a is constructed, we know that the point is not in the spectrum, and also we can write down the inverse. A typical algorithm in this type of case tries to find such an element and terminates after it has been found, and otherwise it runs for ever. In this sense deciding whether a given complex number z is outside of  $\hat{\sigma}(a)$  appears easier than deciding whether  $z \in \hat{\sigma}(a)$ . In some contexts people speak of semi-decidable situations. We start by stating a "metatheorem". In what follows we shall assume that the following operations are available.

- (i) Given  $a \in \mathcal{A}$  one can form powers of a and combine them into polynomials  $p(a) = \sum_{j=0}^{d} \alpha_j a^j$  with complex coefficients.
- (ii) Given  $p(a) \in \mathcal{A}$  we can evaluate its norm ||p(a)||.
- (iii) Normal computations with complex numbers are assumed, for example we can ask for given  $z \in \mathbb{C}$  whether

(iv) What we are *not* assuming is the operation of inversion for invertible elements:

$$a \mapsto a^{-1}$$
.

**Proposition 8.1.** "Metatheorem" Suppose you could compute, with a finite number of operations of (i)-(iii), for given  $a \in A$ , compact sets  $K_n(a) \subset \mathbb{C}$  (where  $n \in \mathbb{N}$ ) such that

(v) testing whether a complex number is inside  $K_n(a)$  requires only a finite number of steps,

(vi)

$$K_{n+1}(a) \subset K_n(a)$$

(vii)

$$\hat{\sigma}(a) = \bigcap_{n \ge 1} K_n(a).$$

Then the question, whether

$$z \in \hat{\sigma}(a)$$
,

would be answered in finite number of steps if the answer is negative, and otherwise the process would run for ever.

Remark 8.2 Observe that since the compact sets are in inclusion, (vii) immediately implies the convergence in the Hausdorff metric

$$d_H(K_n(a), \hat{\sigma}(a)) \to 0.$$

The next result contains an actual construction of such compacts sets  $K_n(a)$ .

**Theorem 8.3.** [36] There exists a recursive procedure which uses only (i)-(iii) and creates (v)-(vii). The sets  $K_n(a)$  are of the form

$$V_{p_n}(a) = \{ z \in \mathbb{C} : |p_n(z)| \le ||p_n(a)|| \}, \tag{8.2}$$

where  $p_n$  are monic polynomials.

Thus, in particular, testing whether z is in or out of  $V_p$  is easy. The heart of the process is in computing the sequence of polynomials. For each polynomial the procedure terminates in finite number of steps, but in addition to (i)-(iii) a "step" contains a finite number of minimization problems on norms of polynomials of fixed degree. The construction of the polynomials is rather complicated with quite a lot of effort needed to guarantee that the sets are in inclusion. As a byproduct, the degrees of the polynomials grow rather rapidly. Next we present another result, which is weaker in conclusions but much simpler in construction.

**Theorem 8.4.** [36] Let  $p_j$  be a monic polynomial such that for all monic polynomials p of degree j one has

$$||p_j(a)|| \le ||p(a)||.$$
 (8.3)

Denoting

$$Z = \bigcap_{j \ge 1} V_{p_j}(a)$$

and

$$Z_n = \bigcap_{j=1}^n V_{p_j}(a),$$

we have

$$\hat{\sigma}(a) \subset Z \tag{8.4}$$

and

$$\sup_{z \in \partial \hat{\sigma}(a)} \operatorname{dist}(z, \ \mathbb{C} \setminus Z_n) \longrightarrow 0, \qquad n \to \infty.$$
 (8.5)

Above we denote  $\operatorname{dist}(z, W) = \inf_{w \in W} |z - w|$ . Observe that the conclusion (8.5) is weaker than convergence in the Hausdorff metric

$$d_H(\hat{\sigma}(a), Z_n) \longrightarrow 0, \qquad n \to \infty.$$

We can simplify the statements above, based on Theorem 8.3. In fact, since there is a constructive way to create a sequence of polynomials  $\{p_n\}$  such that the sets  $\{V_{p_n}(a)\}$  are in inclusion and satisfy

$$\bigcap_{n>1} V_{p_n}(a) = \hat{\sigma}(a), \tag{8.6}$$

we could in principle do the following: enumerate all polynomials with coefficients having rational real and imaginary parts. Start computing the sets  $V_p(a)$  and keep in memory only the smallest set so far computed. By Theorem 8.3 this trivial (but of course impractically slow) procedure creates a converging sequence and the essential requirements are:

- (viii) one is given the enumeration of monic polynomials with rational coefficients,
- (ix) one can test whether  $V_p(a) \subset V_q(a)$  for any two polynomials p and q.

Observe that since the boundaries of  $V_p(a)$  are given by lemniscates (ix) reduces to checking whether given lemniscates intersect and if not, each one has only finitely many components and one has to check which one is subset of what. Clearly all this is relatively easy to do. We summarize:

Algorithm 8.5 (based on enumeration). Assume (i)-(iii) and (viii)-(ix).

- Find an enumeration  $\{p_n\}_{n\in\mathbb{N}}$  of all monic polynomials with rational coefficients.
- Compute  $V_{p_1}(a)$  and set  $K_1(a) = V_{p_1}(a)$ .
- When  $K_m(a)$  has been defined with  $K_m(a) = V_{p_{n_m}}(a)$  keep computing  $V_{p_n}(a)$  for  $n = n_m + 1, \ldots$  and define  $K_{m+1}(a)$  when you first time meet a subset of  $K_m(a)$ .

**Theorem 8.6.** The Algorithm based on enumeration satisfies the assumptions of Proposition 8.1.

**Remark 8.7** If the norm of any element in the algebra can be computed with a countable number of elementary steps, then if the solvability complexity index would be defined for this type of general algorithm, the index would be at most 2.

## 9 Representing the resolvent

We shall now assume that we have a monic polynomial p, which could come from one of the procedures discussed in the previous section. Suppose

$$z \notin V_p(a)$$

where  $V_p(a)$  is given by (8.2). Suppose  $p \in \mathbb{P}_d$  is of the form

$$p(z) = z^d + \alpha_1 z^{d-1} + \dots + \alpha_d.$$
 (9.1)

We put for  $j = 0, 1, \dots, d-1$ 

$$Q_j(z) = z^j + \alpha_1 \lambda^{j-1} + \dots + \alpha_j \tag{9.2}$$

and then, with  $a \in \mathcal{A}$ ,

$$q(z,a) = \sum_{j=0}^{d-1} Q_{d-1-j}(z)a^{j}.$$
(9.3)

One checks easily that then

$$(a-z)q(z,a) = p(a) - p(z). (9.4)$$

Since we assume (8.2), p(a) - p(z) has an inverse in the form of a convergent power series and we obtain from (9.4) a representation for the resolvent in an explicit form:

**Proposition 9.1.** Let  $a \in \mathcal{A}$  and  $z \notin V_p(a)$ , then

$$(z-a)^{-1} = \frac{q(z,a)}{p(z)} \sum_{j=0}^{\infty} \frac{p(a)^j}{p(z)^j}.$$
 (9.5)

What is remarkable here is that this *single* representation works everywhere outside a computed set  $V_p(a)$  and one does *not* have to know the spectrum of  $a \in \mathcal{A}$  in order to apply it.

**Example 9.2** Suppose you want to compute  $\log(a)$ . The approach requires the following. You first run some version of the algorithms of producing polynomials, e.g. the one in Theorem 8.3, and you keep checking whether

$$0 \notin V_p(a). \tag{9.6}$$

If this never happens, it means that either  $0 \in \sigma(a)$  or the spectrum separates 0 from  $\infty$ , and in these cases  $\log(a)$  cannot be consistently defined. If, on the other hand, (9.6) holds for some p then, as  $V_p(a)$  is polynomially convex, one could cut the plane from 0 to  $\infty$  outside of  $V_p(a)$  and thus have a single valued logarithm, say  $\log(z)$ . Let  $\gamma$  be a contour around  $V_p(a)$  such that  $\log(z)$  is well defined along it. Then one can simply use the Cauchy integral formula to obtain

$$\log(a) = \sum_{j=0}^{\infty} c_j(a)p(a)^j$$
(9.7)

where

$$c_j(a) = \frac{1}{2\pi i} \int_{\gamma} \text{Log}(z) \frac{q(z, a)}{p(z)^{j+1}} dz.$$
 (9.8)

Observe that the representation of the resolvent gives rational approximations if we truncate the series expansion. Thus the approximations are analytic and the values of the integrals are path independent. This is in contrast to more standard approximations of the resolvent which are often created around selected discrete points along  $\gamma$ . Then the local approximations are typically only piecewise analytic, at best, and one continues to compute the integrals using suitable quadrature formulas. Here the integrals can be evaluated using the residue calculus at the zeros of the polynomial p. We shall now shortly discuss the resulting algorithmic approach for holomorphic functional calculus.

## 10 Multicentric decompositions and holomorphic calculus

Let f be analytic in a domain  $\Omega \subset \mathbb{C}$ . We assume the following on f and  $\Omega$ . Given a monic polynomial p with roots  $z_i \in \Omega$  and an element a in a Banach algebra

- (x) we can test whether  $V_p(a) \subset \Omega$ ,
- (xi) we can evaluate the derivatives of all orders of f at the roots  $z_i$ .

The algorithmic approach starts by searching for a polynomial p satisfying

$$V_p(a) \subset \Omega.$$
 (10.1)

By Theorem 8.3 such a polynomial  $p_n$  is found after a finitely many steps if and only if

$$\hat{\sigma}(a) \subset \Omega. \tag{10.2}$$

In fact, if U is open such that

$$\bigcap_{j\geq 1} K_j \subset U,$$

where the compact sets  $K_j$  are in inclusion, then there exists also an integer n such that

$$K_n \subset U$$
.

Assume then that a monic p of degree d has been found, satisfying (10). We may further assume that p has only simple zeros. Denote by  $\delta_k(z)$  the interpolating polynomial of degree d-1:

$$\delta_k(z) = \frac{p(z)}{p'(z_k)(z - z_k)}.$$

One checks easily that q in (9.3) can be written as

$$q(z,a) = \sum_{k=1}^{d} p'(z_k)\delta_k(a)\delta_k(z). \tag{10.3}$$

We could represent f in a multicentric power series or Jacobi series as in (9.7)

$$f(z) = \sum_{j=0}^{\infty} c_j(z)p(z)^j,$$
(10.4)

where the coefficients  $c_j$  are polynomials of at most degree d-1. However, we prefer to proceed to the multicentric decomposition of f. Given f there are unique analytic functions  $f_k$  such that

$$f(z) = \sum_{k=1}^{d} \delta_k(z) f_k(p(z)).$$
 (10.5)

**Proposition 10.1.** If  $\gamma$  is a contour surrounding all zeros  $z_k$  and staying inside  $\Omega$  then  $f \in H(\Omega)$  has a unique multicentric decomposition (10.5), where each function  $f_k$  has a power series

$$f_k(w) = \sum_{j=0}^{\infty} \alpha_{kj} w^j$$

with

$$\alpha_{kj} = \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z - z_k} \frac{dz}{p(z)^j}.$$

Since  $f_k$  has an explicit Taylor series at the origin, it is easy to come up with effective estimates for the coefficients allowing one to control the accuracy in truncating the series. We refer to [38] for details, but remark at the end that the coefficients can be computed recursively. Also, [38] contains references to the history of these expansions. It is clear that we could also write the expressions in the form

$$f(z) = \sum_{j=0}^{\infty} c_j(z)p(z)^j$$
 (10.6)

where  $c_j$  are polynomials of degree at most d-1. Some authors call (10.6) Jacobi series and, in fact, C. G. J. Jacobi [29] studied such expansions, without the use of the Cauchy integral.

**Proposition 10.2.** [38] Based on p one can pre compute coefficients such that the following holds. Set first  $\alpha_{k0} = f(z_k)$ . Then each  $\alpha_{kj}$  can be computed by explicit substitution requiring the following input:  $f^j(z_k)$ , and already computed coefficients  $\alpha_{m,i}$  for  $m = 1, \ldots, d$ ,  $i = 0, \ldots, j-1$ .

Thus, after the polynomial p has been fixed one obtains a countable expression for f(a) such that each of the truncated expressions can be computed with a finite number of operations.

**Remark 10.3** The multicentric calculus above can be applied for bounded operators  $T \in B(\mathcal{X})$  to compute f(T)x for holomorphic f and a vector  $x \in \mathcal{X}$  in such a way that one has to create only vectors  $T^jx$  provided one can be sure that

$$V_p(T) \subset \Omega$$
.

Notice that this requires testing |p(z)| against ||p(T)||, whereas testing against ||p(T)x|| does not suffice.

### 11 Open Problems

The great open problem is to get a complete classification theory of the Solvability Complexity Index. However, before we can get that we must solve the following problem: Let  $\mathcal{E} = \mathcal{B}(\mathcal{H})$  and  $\Xi : \mathcal{E} \to \mathcal{F}$  be defined by  $\Xi(T) = \sigma(T)$ . Is

$$SCI(\Xi) > 1$$
?

We will not speculate on what kinds of techniques one should use to answer this question, but rather engage in some philosophical thinking about the problem. What if  $SCI(\Xi) = 1$ ? That means that there exists an (as of today unknown) construction that allows us to recover the spectrum of any operator by using only arithmetic operations and radicals and then taking *one* limit. Such a result would indeed be spectacular, however, a little too good to be true.

What if  $SCI(\Xi) > 1$ ? If that is the case, it means that the Solvability Complexity Index makes a jump going from finite to infinite dimensions, similar to the jump between dimensions four and five. But where does the jump occur? We have already shown that, at least, the jump cannot occur between finite rank operators and compact operators. Also, could it be that  $SCI(\Xi) > 2$ ? In that case Theorem 2.4 automatically gives us that  $SCI(\Xi) = 3$ . However, in this case there will be not only one jump, but two, and where will they occur?

We hope to report on these issues in the future, however, note that to show that the Solvability Complexity Index of the spectrum makes a jump between dimensions four and five is equivalent to showing the unsolvability of the quintic using radicals. This was done by using tools outside of analysis and we will not exclude the possibility that deep mathematics from other fields will yield the solution to the problem.

The results above which are based on the polynomial numerical hull techniques are written in a way which does not automatically relate to the solvability complexity index as there are operations which are defined on higher level of abstraction. However, as pointed out in Remark 8.7, if we would have effective ways to control the computation of

$$T \mapsto ||p(T)||$$

then we would have a different way of addressing these questions.

#### 12 Addendum

Up to this section the paper is unchanged, modulo small corrections, from its original form that was put online in 2011. Since the conference Operator Theory and Applications: Perspectives and Challenges (2010), where some of these ideas were presented, and that was the starting point of this paper, there have been substantial developments in the field. For example, in [40] the techniques for computing spectra and  $(n, \epsilon)$ -pseudospectra discussed in Section 5 were extended to Banach space operators. Moreover, in [37] the multicentric calculus was used as a basis for holomorphic functional calculus, allowing a nontrivial extension of the von Neumann theorem that for polynomials p and contractions A in a Hilbert space  $\mathcal H$  we have

$$||p(A)|| \le \sup_{|z| \le 1} |p(z)|.$$

Furthermore, in [39], to get a functional calculus for nonholomorphic functions working for all square matrices, a Banach algebra was constructed starting from continuous functions

$$f:M\subset\mathbb{C}\to\mathbb{C}^d$$

and formulating a product  $\odot$  such that the multicentric representation of a scalar function  $\varphi$  could be viewed as the Gelfand transformation of f in that algebra. That then led to a natural functional calculus, where for example, differentiability of the function  $\varphi$  is not necessary at eigenvalues corresponding to nontrivial Jordan blocks.

Finally, in [7, 8], and many of the open problems have been solved. For example, expressed informally, we have the following:

- (i) The SCI of computing spectra of operators in  $\mathcal{B}(l^2(\mathbb{N}))$  is equal to 3.
- (ii) The SCI of computing spectra of self-adjoint and normal operators in  $\mathcal{B}(l^2(\mathbb{N}))$  are both equal to 2.
- (iii) The SCI of computing spectra of banded normal operators in  $\mathcal{B}(l^2(\mathbb{N}))$  is equal to 1, however computing the essential spectrum has SCI equal to 2.

Moreover, these results are true also when one removes the possibility of using radicals. In addition, the concept of the SCI can be generalized to arbitrary computational problems.

#### 12.1 The SCI hierarchy and Smale's program

In the 1980's S. Smale initiated [43, 42, 44] a comprehensive program for establishing the foundations of computational mathematics. In particular, he started by asking basic questions on the existence of algorithms. One of the fundamental algorithms in numerical analysis is Newtons method. However, the problem is that it may not converge, an issue that causes trouble in for example polynomial root finding. Thus, Smale [43] questioned whether there exists an alternative to Newton's method, namely, a purely iterative generally convergent algorithm (see [43] for definition). More precisely he asked: "Is there any purely iterative generally convergent algorithm for polynomial zero finding?" The problem was settled by C. McMullen in [31] as follows: yes, if the degree is three; no, if the degree is higher (see also [32]). However, in [22] P. Doyle and C. McMullen demonstrated a fascinating phenomenon: this problem can be solved in the case of the quartic and the quintic using several limits. In particular, they provide a construction such that, by using several rational maps and independent limits, a root of the polynomial can be computed. In other words, this is an example of a problem where the SCI is greater than one, but still finite.

It turns out that this phenomenon happens everywhere in scientific computing and Smale's questions and McMullens answers are indeed an example of classification problems in the SCI hierarchy that can be described as follows. Given a definition of what an algorithm can do, we have that

- (i)  $\Delta_0$  is the set of problems that can be computed in finite time.
- (ii)  $\Delta_1$  is the set of problems with SCI  $\leq 1$ , where one also has error control., i.e. the algorithm halts on an input parameter  $\epsilon$  and the output is no further away than  $\epsilon$  from the true solution.
- (iii)  $\Delta_2$  is the set of problems where SCI  $\leq 1$ , but error control may not be possible.
- (iv)  $\Delta_{m+1}$  is the set of problems where the SCI  $\leq m$ .

This hierarchy shows up in many basic computational problems, and below follow some examples.

**Example 12.1 (Spectral problems)** Assuming that an algorithm can do arithmetic operations and comparisons of real numbers (complex numbers are treated as a pair of real numbers), then the general computational spectral problem is in  $\Delta_4$ , but not in  $\Delta_3$ . The self-adjoint spectral problem is in  $\Delta_3$  but not in  $\Delta_2$ . The compact spectral problem is in  $\Delta_2$  but not in  $\Delta_1$ . The finite-dimensional spectral problem is in  $\Delta_1$ , but not in  $\Delta_0$ .

**Example 12.2 (Inverse Problems)** Assuming the same type of algorithm as in the previous example and suppose that  $b \in l^2(\mathbb{N})$  and  $A \in \mathcal{B}_{inv}(l^2(\mathbb{N}))$  (the set of bounded invertible operators), then solving

$$Ax = b$$

is in  $\Delta_3$  and not in  $\Delta_2$ . If A is self-adjoint, then the problem is still in  $\Delta_3$  and not in  $\Delta_2$ . However, if A is banded then the problem is in  $\Delta_2$  but not in  $\Delta_1$ . Finally, if A is finite-dimensional, then the problem is in  $\Delta_0$ .

**Example 12.3 (Optimization)** Assuming the same as above, we may consider a popular problem occurring in infinite-dimensional compressed sensing [1, 2]. In particular, given an  $A \in \mathcal{B}(l^2(\mathbb{N}))$  and  $y \in l^2(\mathbb{N})$  that are feasible, then the optimization problem of finding

$$x \in \underset{\eta \in l^p(\mathbb{N})}{\operatorname{argmin}} \|\eta\|_{l^1} \text{ subject to } \|A\eta - y\| \le \delta, \qquad \delta > 0$$

is not in  $\Delta_2$ , however, it is not known where in the SCI hierarchy this problem is.

An important result in [7, 8] is that the SCI hierarchy does not collapse regardless of the axioms on the algorithm. This demonstrates that any theory aiming at establishing the foundations of computational mathematics will have to include the SCI hierarchy.

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