

Non-Self-Adjoint Operators and Pseudospectra

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Abstract

The theory of pseudospectra has grown rapidly since its emergence from within numerical analysis around 1990. We describe some of its applications to the stability theory of differential operators, to WKB analysis and even to orthogonal polynomials. Although currently more a way of looking at non-self-adjoint operators than a list of theorems, its future seems to be assured by the growing number of problems in which the ideas are clearly of relevance.

1 Introduction

Those attending this meeting will hardly need persuading that interesting problems and techniques can enter mathematics from physics or probability, but it is less usual for a major new idea in spectral theory to originate in numerical analysis. This paper is an introduction to the theory of pseudospectra, a way of imposing some order on the chaos of non-self-adjoint (NSA) phenomena.

Since 1990 this subject has developed rapidly, and has been shown to give substantial insights into the properties of NSA matrices and operators, including second order differential operators. It is relevant to the study of resonances if one uses the method of complex scaling, and also models involving ‘optical potentials’ which replace certain channels by dissipative terms in the Schrödinger operator, but it has many other applications. Michael Berry has a series of papers on the importance of NSA 2×2 matrices in physics. I am happy to be able to announce on this occasion that as the result of my collaboration with Barry Simon, it has recently proved useful in resolving an outstanding question about orthogonal polynomials on the unit circle. However, most of the talk will be a description of the basic ideas, to be

found in three recent books on the subject. The most important is by Trefethen and Embree, the first of whom is responsible for the explosion of activity in the field; the authors illustrate it with a wealth of applications and numerical examples which demonstrate its relevance; [14]. The second, by Böttcher and Silbermann, is about Toeplitz operators, but makes substantial use of pseudospectral ideas; [1]. The third, by the author, covers many topics, some related to pseudospectra, and some not; [5]. Everything written here may be found in the last of these books, except where explicit references are given.

2 The Basic Ideas

If one wishes to compute the spectrum of a NSA linear operator, or even a large NSA matrix, one quickly comes up against problems which make one suspect that one has mistakes in the code. Although some of the eigenvalues appear where one expects, others may be in completely wrong positions. The reason is spectral instability: the fact that

$$\|Af - \lambda f\| < \varepsilon \|f\|$$

for $\varepsilon = 10^{-16}$ (say) does not imply that λ is close to the spectrum of A . It is best to describe the problem in terms of the resolvent norms. It is easy to prove that

$$\|R(z, A)\| \geq \text{dist}(z, \text{Spec}(A))^{-1}.$$

The converse is not necessarily true for NSA operators, nor is it even close to being true in general. Since z is an approximate eigenvalue in the sense described above if and only if $\|R(z, A)\| > \varepsilon^{-1}$, this implies that there might be large regions of the complex plane far from the spectrum which are associated with approximate eigenvalues. The graphics package EigTool enables one to compute the pseudospectral regions

$$\text{Spec}_\varepsilon(A) := \{z : \|R(z, A)\| > \varepsilon^{-1}\}$$

very efficiently; see [15]. The alternative definition

$$\text{Spec}_\varepsilon(A) := \bigcup \{\text{Spec}(A + B) : \|B\| < \varepsilon\}$$

provides the very helpful insight that one cannot hope to distinguish numerically between $\text{Spec}(A)$ and $\text{Spec}_\varepsilon(A)$ if ε is the rounding error of one's computer.

This is not just theory. The NSA harmonic oscillator $H := P^2 + c^2 Q^2$ acting in $L^2(\mathbf{R})$ has compact resolvent and its eigenvalues are $\lambda_n := c(2n + 1)$ where $n = 0, 1, \dots$. Its pseudospectral diagram is given in Figure 1, and started my interest in the subject. For every complex c the norms of the spectral projections P_n increase at an exponential rate as $n \rightarrow \infty$, and the precise constant is given in [7].

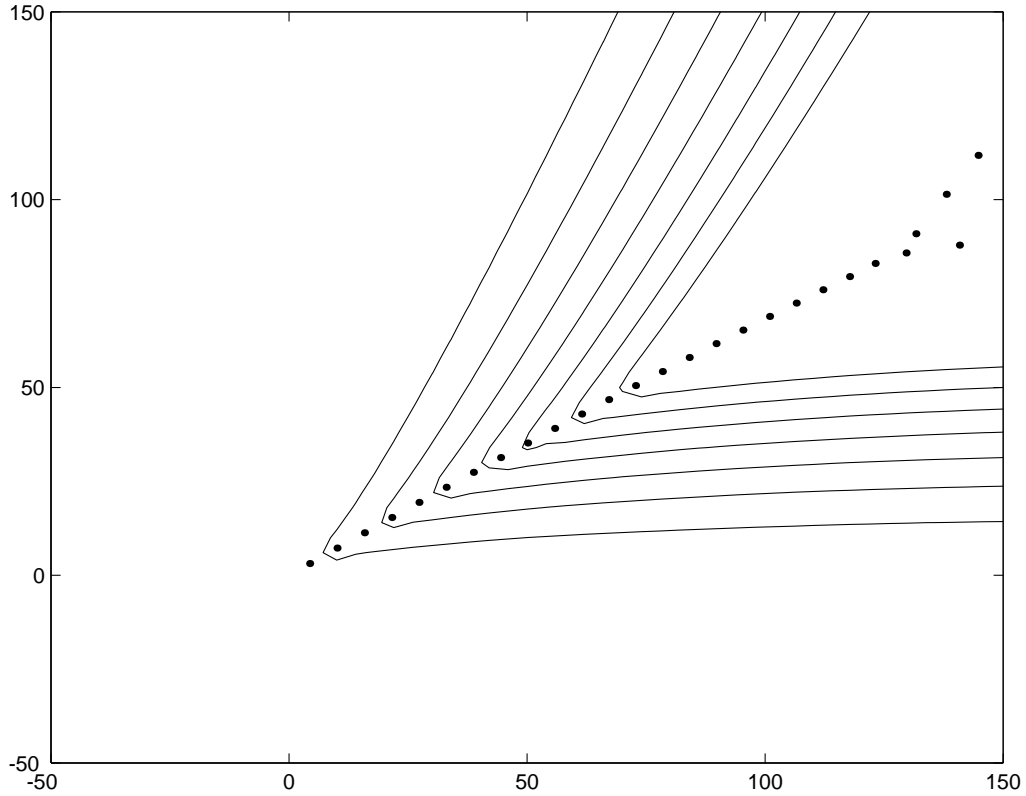


Figure 1 Pseudospectra of the NSA Harmonic Oscillator

Although e^{-Ht} is compact for all $t > 0$ and its kernel is given by Mehler's formula, the expansion

$$e^{-Ht} = \sum_{n=0}^{\infty} e^{-\lambda_n t} P_n,$$

where P_n are the spectral projections, is only norm convergent for t greater than a certain positive critical constant; [7].

Understanding the pseudospectra of this example depended on the development of NSA WKB analysis; [2, 3]. The basic idea is to use WKB methods to produce explicit approximate eigenfunctions associated with points in the (real) phase space which satisfied a certain inequality expressed in terms of the classical Hamiltonian. The approximate eigenvalue is the (complex) value of the classical Hamiltonian at the relevant point, and the error vanishes as $h \rightarrow 0$. It was realized by Zworski that the idea was applicable to general pseudodifferential operators and was simply a new way of looking at an old theorem of Hörmander; [16]. It has inspired a number of new theorems on the subject; [10, 4].

Example 1 The standard $n \times n$ Jordan matrix J_n is defined by

$$(J_n)_{r,s} := \begin{cases} 1 & \text{if } s = r + 1, \\ 0 & \text{otherwise.} \end{cases}$$

The resolvent norm is most easily computed if one uses the l^1 norm on \mathbf{C}^n . Starting from the formula

$$((zI - J_n)^{-1})_{r,s} = \begin{cases} z^{r-s-1} & \text{if } r \leq s, \\ 0 & \text{otherwise.} \end{cases}$$

one immediately obtains

$$\|(zI - J_n)^{-1}\|_1 = \frac{|z|^{-n} - 1}{1 - |z|}.$$

This diverges at an exponential rate as $n \rightarrow \infty$ for every z satisfying $|z| < 1$. The same phenomenon occurs if one uses the standard l^2 (Euclidean) norm on \mathbf{C}^n and the pseudospectra are again rotationally invariant in \mathbf{C} . One says that the pseudospectra fill up the unit circle at an exponential rate even though $\text{Spec}(J_n) = \{0\}$ for every n .

The following theorem may be used two ways. If one only knows an operator A to within an error $\delta > 0$ then its pseudospectra $\text{Spec}_\varepsilon(A)$ do not have any significance for $\varepsilon < \delta$, although they are numerically stable for substantially larger ε . Conversely if one is only interested in the shape of the pseudospectra of A for $\varepsilon > \delta$, one may add any perturbation of norm significantly less than δ to A before carrying out the computation.

Theorem 2 *Let A_1, A_2 be two bounded operators on \mathcal{B} satisfying $\|A_1 - A_2\| < \delta$. If we put*

$$\sigma_r(z) := \begin{cases} 0 & \text{if } z \in \text{Spec}(A_r), \\ \|R(z, A_r)\|^{-1} & \text{otherwise,} \end{cases}$$

for $r = 1, 2$ then

$$\text{Spec}_\varepsilon(A_r) = \{z : \sigma_r(z) < \varepsilon\}$$

and

$$|\sigma_1(z) - \sigma_2(z)| \leq \delta$$

for all $z \in \mathbf{C}$.

3 Generalized Pseudospectra

The standard theory of pseudospectra is a study of properties of the operator family $z \rightarrow (zI - A)$ where A is a bounded or unbounded linear operator; see [14]. However, the key ideas and theorems extend to other operator families. The parameter space need not be \mathbf{C} , and in [4] it is the set of all points in the phase space associated with the differential operator. Even if we restrict to $z \in \mathbf{C}$ as the parameter one may consider polynomial operator pencils such as

$$A(z) := \sum_{r=1}^n A_r z^r$$

where A_r are operators on some Banach space \mathcal{B} . Whole books have been devoted to this subject, but we mention just one example.

Example 3 Given bounded operators A, B on some space \mathcal{B} one seeks solutions of an abstract telegraph equation

$$\frac{\partial^2 f}{\partial t^2} + B \frac{\partial f}{\partial t} + Af = 0$$

that are of the form $f_t := e^{zt}g$. Assuming that suitable technical conditions are satisfied this leads one directly to

$$Ag + zBg + z^2g = 0.$$

This can be rewritten as a conventional eigenvalue equation for the 2×2 block matrix

$$X := \begin{pmatrix} -B & I \\ -A & 0 \end{pmatrix}$$

The eigenvalue problem for the general 2×2 block matrix

$$Y := \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is often reformulated as a generalized eigenvalue problem for the analytic family

$$M(z) := C(zI - A)^{-1}B + D - zI$$

where one assumes that $z \notin \text{Spec}(A)$.

For simplicity of exposition we assume below that the parameter is a complex number and that the operators concerned are bounded, although many of the theorems hold in more generality. The theorems below are taken from [5], but

their proofs are obvious adaptations of the same results for the standard notion of pseudospectra.

By definition the spectrum of an operator family is the set

$$\text{Spec}((A(\cdot))) := \{z : A(z) \text{ is not invertible}\}.$$

The pseudospectra are the sets

$$\text{Spec}_\varepsilon((A(\cdot))) := S \cup \text{Spec}(A(\cdot))$$

where S is the set of z for which there exists an ‘approximate eigenvector’ $f \in \mathcal{B}$ satisfying $\|A(z)f\| < \varepsilon\|f\|$.

Note that if A and B are bounded invertible operators the equations $Af = zBf$, $B^{-1}Af = zf$ and $f = zA^{-1}Bf$ have the same eigenvalues z , but the pseudospectra may look very different, depending on the norms of the inverse operators (among other things).

Theorem 4 *The following three conditions on an operator family $A(\cdot)$ are equivalent.*

- (i) $z \in \text{Spec}_\varepsilon(A(\cdot))$;
- (ii) *There exists a bounded operator $D : \mathcal{B}_1 \rightarrow \mathcal{B}_2$ for which $\|D\| < \varepsilon$ and $A(z) + D$ is not invertible;*
- (iii) *Either $z \in \text{Spec}(A(\cdot))$ or $\|A(z)^{-1}\| > \varepsilon^{-1}$.*

Some information about the shape of the pseudospectra is provided by the next theorem.

Theorem 5 *Given an analytic operator-valued family $A(\cdot)$ acting on a Hilbert space put*

$$\sigma(z) := \begin{cases} \|A(z)^{-1}\|^{-1} & \text{if } A(z) \text{ is invertible,} \\ 0 & \text{otherwise.} \end{cases}$$

Then σ is continuous and its local minima all lie in $\text{Spec}(A(\cdot))$.

4 Truncation

If L is the standard convection-diffusion operator

$$(Lf)(x) := -f''(x) + f'(x)$$

acting in $L^2(\mathbf{R})$ then L is normal and its spectrum is the parabola

$$\{(x, y) : x = y^2\}.$$

If one restricts the same operator to $L^2(0, a)$ and imposes Dirichlet boundary conditions. then the operator L_a has compact resolvent, and its spectrum is

$$\{1/4 + \pi^2 n^2 / a^2 : n = 1, 2, \dots\}.$$

It follows that the spectrum of L_a converges as $a \rightarrow \infty$ to $[1/4, \infty)$, and has no connection with the spectrum of L . In this particular case one can get the right limit by using periodic boundary conditions rather than Dirichlet boundary conditions. However, there is no theorem which states that this always works for operators with variable coefficients in one dimension, and if one replaces the intervals by an increasing sequence of regions in \mathbf{R}^n periodic boundary conditions may not make sense. To add to the complexity of this problem the spectrum of L restricted to $L^2(0, \infty)$ and subject to Dirichlet boundary conditions at 0 is equal to the boundary plus interior of the parabola.

If one adopts the pseudospectral point of view the situation is immediately clarified. Although the spectrum of L_a remains within $[1/4, \infty)$ as a increases, the resolvent norms $\|R(z, A_a)\|$ diverge rapidly provided z is inside the parabola, but they remain uniformly bounded for z outside the parabola. In fact the pseudospectra of L_a converge to the pseudospectra of the half-line operator as $a \rightarrow \infty$.

A similar problem also exists for self-adjoint operators if there is a gap between two parts of the essential spectrum. If one uses standard finite element packages to compute the spectrum, one finds a large number of eigenvalues in the spectral gap. This does not happen for eigenvalues below the bottom of the essential spectrum, because of variational theorems. The phenomenon is called spectral pollution, and there are various ad hoc procedures for avoiding it. There is also a rigorous way of doing so, but at substantially greater computational cost. See [8] for a ‘geometrical’ account of the rigorous numerical procedures involved.

5 Numerical Range and Functional Calculus

The material in this section is to appear in [6]. Let A be a bounded operator on a Banach space \mathcal{B} and let γ be a closed curve surrounding the spectrum of A . If f is an analytic function in the interior of γ which extends continuously to γ then one may define

$$f(A) = \frac{1}{2\pi i} \int_{\gamma} f(z) R(z, A) \, dz,$$

and deduce the estimate

$$\|f(A)\| \leq \frac{c}{2\pi} |\gamma| \|f\|_{\infty}.$$

provided $\|R(z, A)\| \leq c$ for all $z \in \gamma$, $|\gamma|$ is the length of γ and $\|f\|_{\infty}$ is the maximum value of $|f|$ on γ . Unfortunately the resolvent norm may be very large

on γ even if γ remains at a considerable distance from the spectrum of A . If A is an $n \times n$ matrix with n distinct eigenvalues λ_r then the alternative formula

$$f(A) := \sum_{r=1}^n f(\lambda_r) P_r$$

where P_r are the rank one spectral projections of A may run into related problems – the norms of spectral projections can be arbitrarily large even for 2×2 matrices, and for larger matrices this problem is commonplace. Dismissing non-diagonalizable Jordan matrices because they form a set of zero Lebesgue measure is a serious mistake: in many problems one may indeed write $A = SDS^{-1}$ where D is diagonal, but the condition number $\kappa(S) = \|S\| \|S^{-1}\|$ of the diagonalization is so large that the procedure is computationally infeasible. It is argued in [6] that the usefulness of diagonalization depends on how small $\kappa(S)\varepsilon + \|B\|$ can be made, where $A = SDS^{-1} + B$, ε is the rounding error of the computations, B is a small perturbation and D is diagonal. Numerical experiments suggest that the answer is frequently of order $\varepsilon^{1/2}$, and this has been proved for certain types of Jordan matrix A which cannot themselves be diagonalized.

The problem of computing $f(A)$ can sometimes be resolved by using the concept of numerical range. The set

$$\text{Num}(A) := \overline{\{\langle Af, f \rangle : \|f\| = 1\}}.$$

is always convex, and satisfies

$$\text{Spec}(A) \subseteq \text{Num}(A) \subseteq \{z : |z| \leq \|A\|\}.$$

It is easy to compute, but not by evaluating $\langle Af, f \rangle$ for a large collection of unit vectors! There is a theorem stating that

$$\|R(z, A)\| \leq \text{dist}(z, \text{Num}(A))^{-1}$$

so that if γ encloses $\text{Num}(A)$ rather than just $\text{Spec}(A)$, and $\text{dist}(\gamma, \text{Num}(A))$ is not too small, then one obtains a useful estimate on $\|f(A)\|$.

Whether or not this is possible depends on the domain of analyticity of f . Consider the calculation of A^t for the highly NSA matrix

$$A_{r,s} := \begin{cases} r/n & \text{if } s = r + 1, \\ c & \text{if } r = s, \\ 0 & \text{otherwise.} \end{cases}$$

Figure 2 plots $\|A^t\|$ against t for $n = 100$ and $c = 0.6$. Computing the square root of a NSA matrix may be a highly unstable procedure.

The computations were carried out by diagonalizing $A + B$, where B is a random matrix of norm 10^{-8} . This number was chosen because it is the square root of the rounding error in the numerical computations; the reason for this choice has already been mentioned. The stability of the computations for different choices of B was checked.

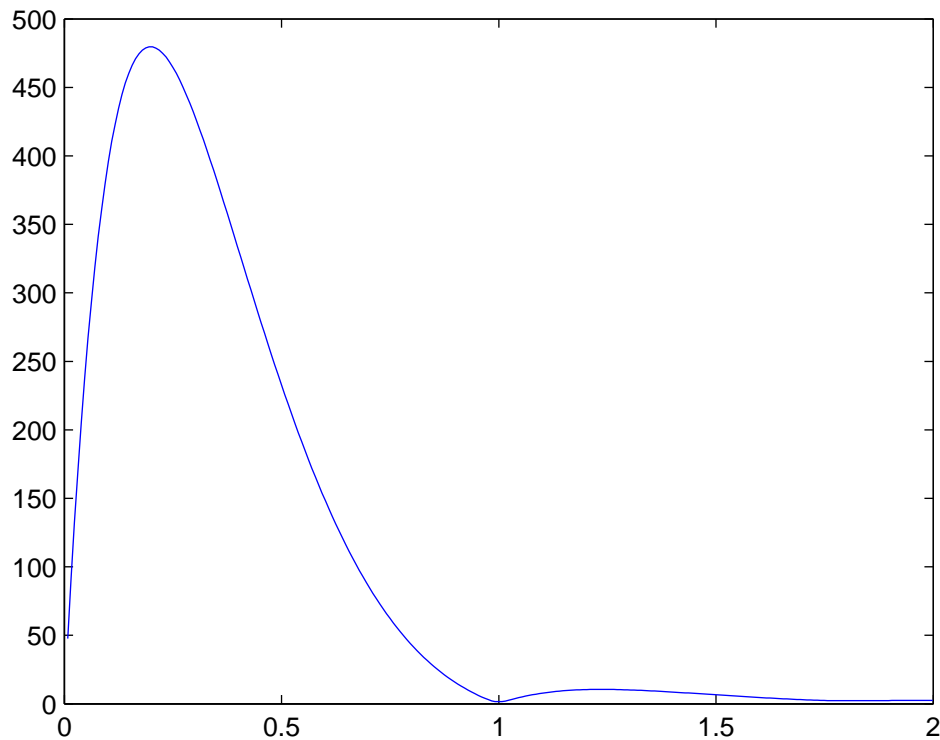


Figure 2 Graph of $\|A^t\|$ for $0 < t < 2$

This figure illustrates another point, that the short time behaviour of a one-parameter semigroup may be very different from the long time asymptotics. The latter is controlled by the spectrum of the operator, but the former is not. If

$$f'(t) = Af(t)$$

is obtained by linearizing a non-linear evolution equation around a stationary point, then one cannot assert the stability of the original problem just because the spectrum of the linearization A is in the left-hand half plane, unless one has proved that this is true in the particular context. See [14] for examples that demonstrate that ‘linear stability’ is not the same as stability.

Figure 3 provides a contour plot of the norms of the complex powers of the same matrix.

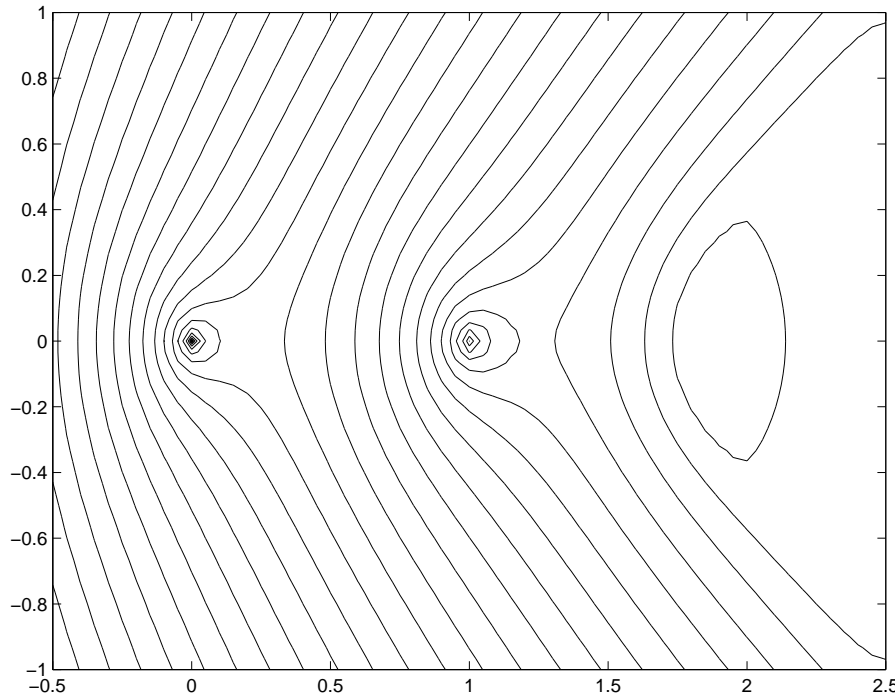


Figure 3
Contour plot of $\|A^{x+iy}\|$ for $-0.5 < x < 2.5$ and $-1 < y < 1$

6 Orthogonal Polynomials

If μ is a probability measure on the unit circle S , one can apply Gram-Schmidt to construct a sequence of monic polynomials Φ_n on S that are orthogonal within $L^2(S, d\mu)$. A certain sequence of contractions A_n on $L^2(S)$ lie at the centre of the theory of such orthogonal polynomials. They are defined by

$$A_n := P_n M_z P_n|_{L_n}$$

where M_z is the unitary operator of multiplication by z and P_n is the orthogonal projection with range

$$L_n := \text{lin}\{\Phi_r : 0 \leq r \leq n-1\}.$$

It is well-known that the zeros of Φ_n coincide with the eigenvalues of A_n .

Since $\|A_n\| = 1$, the spectrum and numerical range of A are contained in the unit circle. This section is a description of joint work with Barry Simon concerning the

existence of eigenvalues of A_n near the boundary S of the ball. In spite of the general problems described in earlier sections, we were able to prove that if A_n has an approximate eigenvalue z near S then z is close to a true eigenvalue, with precise estimates. This was a key ingredient in the study of the zeros of certain random orthogonal polynomials $\Phi_n(z, \omega)$, which also relies heavily on earlier work of Stoichiu; [12, 13].

The main theorem is

Theorem 6 [9] *Let A be an $n \times n$ matrix and suppose that $z \in \mathbf{C}$ satisfies $|z| \geq \|A\|$ and $z \notin \text{Spec}(A)$. Then*

$$\text{dist}(z, \text{Spec}(A)) \|R(z, A)\| \leq \cot\left(\frac{\pi}{4n}\right)$$

and the constant on the RHS is optimal.

The paper also contains a much more elementary proof in which the RHS is replaced by the weaker bound $2n$. A related but weaker result has been also proved by Nikolski in [11]. The theorem is applied as follows. If there exists $f \in \mathbf{C}^n$ and $\varepsilon > 0$ such that

$$\|Af - zf\| < \varepsilon \|f\|$$

then

$$\|R(z, A)\| > \varepsilon^{-1}$$

so

$$\text{dist}(z, \text{Spec}(A)) < \varepsilon \cot\left(\frac{\pi}{4n}\right).$$

The proof that the constant is optimal depends on identifying the ‘worst possible’ matrix, which is

$$M_n = \begin{pmatrix} 1 & 2 & \dots & 2 & 2 \\ 0 & 1 & \dots & 2 & 2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 2 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}$$

This matrix has a number of special properties and is a discretization of the standard Volterra integral operator. The proof of the theorem relies upon the fact that z is close to the boundary of the numerical range of A . Indeed there is a more general version.

Theorem 7 [9] *Let A be an $n \times n$ matrix and suppose that $z \in \mathbf{C}$ is not in the spectrum or the interior of the numerical range of A . Then*

$$\text{dist}(z, \text{Spec}(A)) \|R(z, A)\| \leq \cot\left(\frac{\pi}{4n}\right)$$

and the constant on the RHS is optimal.

I hope that I have persuaded you that NSA spectral theory has features quite foreign to those brought up in the SA tradition. It is unrealistic to guess what the theorems are without being prepared to do some numerical experimentation, but the starting point must be to forget everything you ever learned from the SA theory.

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