**Pseudospectra of the
Convection-Diffusion Operator**

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Abstract. The spectrum of the simplest 1D convection-diffusion operator is a discrete subset of the negative real axis, but the pseudospectra are regions in the complex plane that approximate parabolas. Put another way, the norm of the resolvent is exponentially large as a function of the Péclet number throughout a certain parabolic region. These observations have a simple physical basis, and suggest that conventional spectral analysis for convection-diffusion operators may be of limited value in some applications.

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CONTENTS

1. Introduction...	1
2. Eigenfunctions and pseudo-eigenfunctions...	5
3. The limiting case $d = \infty$...	8
4. Estimates of the pseudospectra...	11
5. Symmetrizability and a further estimate...	16
6. Finite difference and spectral discretizations...	19
7. Applications...	22
Appendix: formulas for arbitrary convection and diffusion coefficients...	28
References...	30

1. Introduction

Figure 1 illustrates the phenomenon that is the subject of this paper. Let $\mathcal{L}$ denote the convection-diffusion operator*

$$\mathcal{L}u = u'' + u', \quad u(0) = u(d) = 0, \quad (1.1)$$

acting in the Hilbert space $L^2[0, d]$.[†] For $d = 40$, the solid dots in the figure show the first 27 eigenvalues of $\mathcal{L}$, a set of numbers on the negative real axis. These eigenvalues are the points $\lambda \in \mathbb{C}$ where the resolvent of $\mathcal{L}$, $(\lambda I - \mathcal{L})^{-1}$, has a pole, which we may write as

$$\|(\lambda I - \mathcal{L})^{-1}\| = \infty.$$

This much is standard, but now consider the behavior of $\|(\lambda I - \mathcal{L})^{-1}\|$ at other points λ . Counting from the outside in, the figure plots the following contour lines in the complex λ -plane:

$$\|(\lambda I - \mathcal{L})^{-1}\| = 10^1, 10^2, 10^3, \dots, 10^7.$$

(Section 6 explains how these curves were computed.) Outside the shaded region Π bounded by the dashed “critical parabola,” $\|(\lambda I - \mathcal{L})^{-1}\|$ is small. Inside that region, however, it is huge, attaining values as great as 10^7 at points λ that are far from the eigenvalues. In fact, for any λ in the interior of the shaded region, $\|(\lambda I - \mathcal{L})^{-1}\|$ grows exponentially as $d \rightarrow \infty$. If d were 400 instead of 40, the figure would look much the same but with the contours representing $10^{10}, 10^{20}, \dots, 10^{70}$.

It is common practice in both pure and applied mathematics to analyze an operator by investigating its spectrum. However, Figure 1 shows that in the case of convection-diffusion operators, there may be a great deal of structure in the surface $\|(\lambda I - \mathcal{L})^{-1}\|$ that is not revealed by the points where its height is infinite. This is a reflection of the fact that these operators are *non-normal*.

*Convection-diffusion operators are often written with explicit convection and/or diffusion parameters, e.g., $\mathcal{L}u = \nu u'' + cu'$. The results of this paper carry over to this alternative formulation if d is replaced by the *Péclet number* $= dc/\nu$. Details are given in the Appendix.

[†]To be precise, the domain of $\mathcal{L}$ is the subset of $L^2[0, d]$ of continuous functions on $[0, d]$ which satisfy the boundary conditions and possess a second derivative in $L^2[0, d]$. Similar remarks apply to the operators $\mathcal{L}^{[0, \infty)}$ and $\mathcal{L}^{(-\infty, \infty)}$ defined in Section 3.

Figure 1. Contour plot of the resolvent norm surface $\|(\lambda I - \mathcal{L})^{-1}\|$ in the complex λ -plane ($d = 40$). The contours represent levels $10^1, 10^2, \dots, 10^7$, and the dots are the eigenvalues. At each point λ in the interior of the region Π (shaded), $\|(\lambda I - \mathcal{L})^{-1}\|$ grows exponentially as $d \rightarrow \infty$. Equivalently, this can be interpreted as a depiction of ϵ -pseudospectra of $\mathcal{L}$ for $\epsilon = 10^{-1}, 10^{-2}, \dots, 10^{-7}$.

This means that they cannot be unitarily diagonalized, or to put it another way, their eigenfunctions are not orthogonal. For the convection-diffusion problem, the degree of non-normality grows exponentially with d . It follows that any attempt to make quantitative estimates of the behavior of $\mathcal{L}$ by means of its eigenfunctions or eigenvalues is likely to lead to exponentially large constants. Such estimates are of little use when d is large, and have no content at all that is uniformly valid as $d \rightarrow \infty$. Indeed, as far as spectra are concerned, the limit $d \rightarrow \infty$ is a singular one. For each $d < \infty$, the spectrum of $\mathcal{L}$ is a discrete subset of the negative real axis, but for the analogous operator $\mathcal{L}^{[0, \infty)}$ on a semi-infinite interval, the spectrum is the entire shaded region Π .

This paper is devoted to an alternative analysis of convection-diffusion operators: the investigation of their *pseudospectra*, which are robust with respect

to the limit $d \rightarrow \infty$. Here is the definition:

DEFINITION. Let $\mathcal{L}$ be a closed linear operator in a Hilbert space $\mathcal{H}$ and let $\epsilon \geq 0$ be arbitrary. The ϵ -pseudospectrum $\Lambda_\epsilon(\mathcal{L})$ is the set of all $\lambda \in \mathbb{C}$ such that

$$(i) \|(\lambda I - \mathcal{L})^{-1}\| \geq \epsilon^{-1},$$

or equivalently,

$$(ii) \text{ For any } \epsilon' > \epsilon, \lambda \text{ belongs to the spectrum of } \mathcal{L} + \mathcal{E} \text{ for some bounded operator } \mathcal{E} \text{ on } \mathcal{H} \text{ with } \|\mathcal{E}\| \leq \epsilon'.$$

By convention we write $\|(\lambda I - \mathcal{L})^{-1}\| = \infty$ if $(\lambda I - \mathcal{L})^{-1}$ is unbounded or non-existent, i.e., if λ is in the spectrum $\Lambda(\mathcal{L})$. An equivalent formulation of condition (ii) is to consider $\|\mathcal{E}\| \leq \epsilon$ and then take the closure of the resulting set.

In words: the pseudospectrum is the set of all points where the resolvent norm is large, or equivalently, which are spectral values of a slightly perturbed operator. Thus Figure 1 can be described as a depiction of the boundaries of the pseudospectra

$$\Lambda_{10^{-1}}(\mathcal{L}), \Lambda_{10^{-2}}(\mathcal{L}), \dots, \Lambda_{10^{-7}}(\mathcal{L}),$$

and illustrates that the pseudospectra of $\mathcal{L}$ are approximately parabolas. If $\mathcal{L}$ were normal, the ϵ -pseudospectrum for each ϵ would be just the union of the closed ϵ -balls about each eigenvalue.

The analysis of linear operators by means of the resolvent and its norm is an old technique, especially among theoreticians; see, e.g., [24]. The specific idea of considering the sets that we call pseudospectra was perhaps first introduced by H. J. Landau in 1975 [26,27], and has been subsequently and for the most part independently employed by others including Varah [43], Wilkinson [45], Demmel [9], Chatelin [7], and especially Godunov, Kostin, Malyshev, and their colleagues in Novosibirsk [16,28]. Apart from the work by Landau, these applications have been primarily concerned with the effect of rounding errors on matrix computations. Most recently, the work in this vein by Trefethen and Reddy and their colleagues has followed Landau's original view that pseudospectra also provide information about the behavior of non-normal matrices and operators of a more fundamental kind, unrelated to rounding errors or indeed to perturbations of

any sort. Applications of this nature have been investigated in numerical linear algebra [14,32,39], the numerical solution of differential equations [11,23,36], and fluid dynamics [35,42]. For introductions to these ideas, see [34,37,40]. A survey of the theory and applications of pseudospectra is in preparation [41].

The results of the present paper can be summarized as follows. Though the spectrum of $\mathcal{L}$ is a subset of the negative real axis, its pseudospectra are large regions in the left half-plane bounded approximately by parabolas, as depicted in Figure 1. Any point λ at a distance $\text{dist}(\lambda, \Pi)$ outside the critical parabola lies outside all of the pseudospectra $\Lambda_\epsilon(\mathcal{L})$ with $\epsilon < \text{dist}(\lambda, \Pi)$, independently of d ; equivalently, $\|(\lambda I - \mathcal{L})^{-1}\| \leq 1/\text{dist}(\lambda, \Pi)$ (Theorem 4). Any point λ inside the parabola is an ϵ -pseudo-eigenvalue for a value of ϵ that decreases exponentially as a function of d ; equivalently, $\|(\lambda I - \mathcal{L})^{-1}\|$ grows exponentially as $d \rightarrow \infty$ (Theorem 5). Overall, although $\Lambda(\mathcal{L}) \not\rightarrow \Lambda(\mathcal{L}^{[0,\infty)})$ as $d \rightarrow \infty$, $\Lambda_\epsilon(\mathcal{L}) \rightarrow \Lambda_\epsilon(\mathcal{L}^{[0,\infty)})$ as $d \rightarrow \infty$ for every $\epsilon > 0$ (Theorem 6). Finally, the condition number of the basis of eigenfunctions of $\mathcal{L}$ grows exponentially as $d \rightarrow \infty$ (eq. (5.3)). Pseudospectra of finite-difference and spectral discretizations of the convection-diffusion operator are considered in Section 6, and Section 7 discusses some applications.

Convection-diffusion operators have a long history in applied mathematics and numerical analysis. They are the canonical examples of non-self-adjoint operators, or after discretization, of nonsymmetric matrices. For $d \rightarrow \infty$, (1.1) becomes the simplest example of a singular perturbation problem, with a solution involving a boundary layer at $x = 0$ (relative to the length of the full interval). Such problems pose a natural challenge to analytical methods and to numerical algorithms. Finite difference and finite element strategies for solving them, proposed as early as 1955, have been continuously defined and refined since then, resulting in the almost overwhelming selection of methods available today [1,2,3,6,10,30]. In recent years convection-diffusion equations have also assumed a new role in numerical analysis, emerging as favorite test problems for nonsymmetric iterative linear solvers and preconditioners [8,12,13,14,15,18,22]. Our results imply that in any of these applications, when convection is dominant, predictions based on the exact spectrum are likely to be misleading, and numerical methods based on the exact spectrum are likely to be suboptimal.

2. Eigenfunctions and pseudo-eigenfunctions

If we ignore for the moment the matter of boundary conditions, the operator $\mathcal{L}$ multiplies the function $e^{\alpha x}$ by the factor

$$\lambda = \alpha^2 + \alpha. \quad (2.1)$$

Conversely, for each $\lambda \in \mathbb{C}$, there are two functions $e^{\alpha x}$ that $\mathcal{L}$ multiplies by λ , namely those given by the roots of (2.1),*

$$\alpha_{\pm} = -\frac{1}{2} \pm \frac{1}{2}\sqrt{1+4\lambda}. \quad (2.2)$$

In stating these observations we are making implicit use of the factorization

$$\mathcal{L} - \lambda I = (\mathcal{D} - \alpha_+ I)(\mathcal{D} - \alpha_- I), \quad (2.3)$$

where $\mathcal{D}$ is the differentiation operator (cf. [33]).

For any λ and corresponding α_+ and α_- , the function

$$\phi(x) = \frac{e^{\alpha_+ x} - e^{\alpha_- x}}{\alpha_+ - \alpha_-} \quad (2.4)$$

satisfies the condition for an eigenfunction with eigenvalue λ in the interior of $[0, d]$ and the boundary condition at $x=0$. It satisfies the boundary condition at $x=d$ too provided $e^{\alpha_+ d} = e^{\alpha_- d}$, that is, $(\alpha_+ - \alpha_-)d = 2\pi i n$ for some nonzero $n \in \mathbb{Z}$. By (2.2), this amounts to the condition $d\sqrt{1+4\lambda} = 2\pi i n$, and upon squaring we obtain the following eigenvalues:

THEOREM 1. The spectrum of $\mathcal{L}$ is $\Lambda(\mathcal{L}) = \cup_{n>0} \{\lambda_n\}$, with

$$\lambda_n = -\frac{1}{4} - \frac{\pi^2 n^2}{d^2}, \quad n = 1, 2, 3, \dots \quad (2.5)$$

Thus $\Lambda(\mathcal{L})$ is a discrete set of negative real numbers in the interval $(-\infty, -\frac{1}{4})$.[†]

*In the confluent case $\alpha_{\pm} = -\frac{1}{2}$, the second function becomes $x e^{-x/2}$. All of our results carry over continuously to this confluent point, so in the remainder of this paper, for simplicity, we shall ignore this case and speak as if α_+ and α_- are always distinct.

†The calculation above does not prove Theorem 1 completely, but by more careful reasoning it can be shown that each number λ_n is a simple eigenvalue of $\mathcal{L}$ and that there are no other points in the spectrum.

Figure 2. The first two eigenfunctions of $\mathcal{L}$ ($d=5$). The non-normality of $\mathcal{L}$ can be seen in the fact that u_1 and u_2 are not orthogonal.

By (2.2), the eigenfunctions (2.4) can be written (after rescaling by a constant)

$$u_n(x) = e^{-x/2} \sin(\pi n x / d), \quad n = 1, 2, 3, \dots \quad (2.6)$$

This is a sine wave times an exponentially decaying envelope, and the cases $n = 1, 2$ are plotted for $d = 5$ in Figure 2. The boundary layer at the left of the domain can be interpreted as the result of leftward convection introduced by the term u' . Note that this figure confirms that $\mathcal{L}$ is non-normal, since the eigenfunctions are obviously not orthogonal.

If $\mathcal{L}$ were purely a diffusion operator, the term $-\frac{1}{2}$ would be absent from (2.2), α_+ and α_- would be negatives of each other, and for every λ , one of $e^{\alpha_+ x}$ and $e^{\alpha_- x}$ would be decreasing as a function of x and the other would be increasing. For our problem, however, there are choices of λ for which both α_+ and α_- lie in the left half-plane and thus both $e^{\alpha_+ x}$ and $e^{\alpha_- x}$ are decreasing functions. For the eigenfunctions (2.6), this occurs with $\operatorname{Re} \alpha_+ = \operatorname{Re} \alpha_- = -\frac{1}{2}$. More generally, it occurs if and only if α belongs to the strip

$$S = \{\alpha \in \mathbb{C} : -1 \leq \operatorname{Re} \alpha \leq 0\}, \quad (2.7)$$

since if α is one solution of (2.2), the other is $-1 - \alpha$. The corresponding region

Figure 3. The algebra of the critical parabola P . The value λ belongs to Π if and only if both of the corresponding values $\alpha_{\pm}$ lie in the left half-plane, or equivalently, if and only if either one lies in the strip S .

in the λ -plane is the image of S under the function $\lambda = \alpha + \alpha^2$, which we denote by Π :

$$\Pi = \{\lambda \in \mathbb{C} : \lambda = \alpha^2 + \alpha, -1 \leq \operatorname{Re} \alpha \leq 0\}. \quad (2.8)$$

The “critical parabola” that bounds Π is the image of the boundary of S under the same function, which we can represent simply by

$$P = \{\lambda \in \mathbb{C} : \lambda = \alpha^2 + \alpha, \operatorname{Re} \alpha = 0\} \quad (2.9)$$

since $\operatorname{Re} \alpha = -1$ maps onto the same parabola as $\operatorname{Re} \alpha = 0$. See Figure 3.

Suppose now that λ is any complex number in the interior of Π , so that $\operatorname{Re} \alpha_+ < 0$ and $\operatorname{Re} \alpha_- < 0$. Then $\phi(x)$ decreases exponentially with x , so if d is reasonably large, it follows that the boundary condition $u(d) = 0$ is *nearly* satisfied, with an error of order $e^{\mu d}$, where

$$\mu = \max\{\operatorname{Re} \alpha_+, \operatorname{Re} \alpha_-\} = -\frac{1}{2} + \left| \operatorname{Re} \alpha_{\pm} + \frac{1}{2} \right|. \quad (2.10)$$

See Figure 4. Thus $\phi(x)$ is “nearly an eigenfunction” of $\mathcal{L}$, though λ may be far from any of the exact eigenvalues.* This phenomenon is the essence of the

*The term “pseudo-eigenfunction” in the heading of this section is generally applied not to a function like $\phi(x)$ that nearly satisfies the prescribed boundary conditions, but to a function that satisfies the boundary conditions exactly and thus belongs to the domain of the operator under investigation. It is a straightforward matter to add a small correction $\Delta\phi$ to ϕ so as to construct a perturbed function $\tilde{\phi} \approx \phi$ of this kind, with $\|(\lambda I - \mathcal{L})^{-1} \tilde{\phi}\| / \|\tilde{\phi}\|$ of order approximately $e^{-\mu d}$; $\tilde{\phi}$ is then an ϵ -pseudo-eigenfunction of $\mathcal{L}$ with ϵ of order approximately $e^{\mu d}$.

Figure 4. For any λ in the interior of Π , the function $\phi(x) = (e^{\alpha_+ x} - e^{\alpha_- x})/(\alpha_+ - \alpha_-)$ satisfies the eigenvalue condition and the boundary condition at $x = 0$, and it satisfies the boundary condition at $x = d$ up to an error that decreases exponentially with d . Thus $\phi(x)$ behaves nearly like an eigenfunction.

reason why the pseudospectra of $\mathcal{L}$ approximate parabolic regions in the left half-plane.

Equation (2.10) suggests the back-of-the-envelope estimate

$$\Lambda_{e^{\mu d}}(\mathcal{L}) \approx \Pi_\mu, \quad -1 \leq \mu < 0, \quad (2.11)$$

where Π_μ denotes the region of the λ -plane bounded by the parabola P_μ that is the image of the strip in the α -plane bounded by the lines $\operatorname{Re} \alpha = \mu$ and $\operatorname{Re} \alpha = -1 - \mu$. Sections 4 and 5 will make this estimate more precise.

3. The limiting case $d = \infty$

Before estimating the pseudospectra of $\mathcal{L}$ more carefully, it is instructive to consider the analogous operators defined on the intervals $[0, \infty)$ and $(-\infty, \infty)$. Intuitively speaking, the boundary conditions become $u(0) = u(\infty) = 0$ and $u(-\infty) = u(\infty) = 0$, respectively. Since we are working in L^2 spaces, however, the boundary conditions at $\pm\infty$ are taken care of automatically and need not be imposed explicitly. Thus formally, the two operators in question are $\mathcal{L}^{[0, \infty)}$, acting in $L^2[0, \infty)$ with boundary condition $u(0) = 0$, and $\mathcal{L}^{(-\infty, \infty)}$, acting in $L^2(-\infty, \infty)$ with no boundary conditions.

The operator $\mathcal{L}^{(-\infty, \infty)}$ is normal, and its spectrum and pseudospectra are easily determined. In the following theorem Δ_ϵ denotes the closed disk $\{\lambda \in \mathbb{C} :$

$|\lambda| \leq \epsilon\}$ and the sum of two sets $A, B \subseteq \mathbb{C}$ has the usual meaning: $A+B = \{\lambda \in \mathbb{C} : \lambda = \lambda_a + \lambda_b, \lambda_a \in A, \lambda_b \in B\}$.

THEOREM 2. The spectrum of $\mathcal{L}^{(-\infty, \infty)}$ is

$$\Lambda(\mathcal{L}^{(-\infty, \infty)}) = P, \quad (3.1)$$

and for each $\epsilon \geq 0$, the ϵ -pseudospectrum is

$$\Lambda_\epsilon(\mathcal{L}^{(-\infty, \infty)}) = P + \Delta_\epsilon. \quad (3.2)$$

Equivalently, for $\lambda \notin P$ the resolvent norm satisfies

$$\|(\lambda I - \mathcal{L}^{(-\infty, \infty)})^{-1}\| = \frac{1}{\text{dist}(\lambda, P)}. \quad (3.3)$$

In words, the ϵ -pseudospectrum of $\mathcal{L}^{(-\infty, \infty)}$ is the parabola P together with a cushion of thickness ϵ .

Proof of Theorem 2. This result is standard (see e.g. [17]), but since the proof is easy we shall give it. Suppose $(\lambda I - \mathcal{L}^{(-\infty, \infty)})u = f$ for some $\lambda \in \mathbb{C}$ with $u, f \in L^2(-\infty, \infty)$. Then by taking Fourier transforms we obtain

$$(\lambda + \omega^2 - i\omega)\hat{u}(\omega) = \hat{f}(\omega).$$

The Fourier variable $i\omega$ corresponds to α in (2.1), and by (2.6), the factor $\lambda + \omega^2 - i\omega = \lambda - \alpha^2 - \alpha$ is zero for some $\omega \in \mathbb{R}$ if and only if λ lies on the critical parabola P . If this is so, then $\lambda I - \mathcal{L}^{(-\infty, \infty)}$ annihilates the corresponding function $e^{i\omega x} = e^{\alpha x}$, and thus $\lambda \in \Lambda(\mathcal{L}^{(-\infty, \infty)})$. On the other hand for $\lambda \notin P$, we calculate

$$\begin{aligned} \|(\lambda I - \mathcal{L}^{(-\infty, \infty)})^{-1}\| &= \sup_{\omega \in \mathbb{R}} \left| \frac{\hat{u}(\omega)}{\hat{f}(\omega)} \right| \\ &= \sup_{\omega \in \mathbb{R}} \frac{1}{|\lambda + \omega^2 - i\omega|} = \frac{1}{\text{dist}(\lambda, P)}. \end{aligned}$$

This proves (3.1) and (3.3), and the equivalence of (3.2) and (3.3) follows from the definition of pseudospectra. ■

On the semi-infinite interval, P is replaced by Π :

THEOREM 3. The spectrum of $\mathcal{L}^{[0,\infty)}$ is

$$\Lambda(\mathcal{L}^{[0,\infty)}) = \Pi, \quad (3.4)$$

and for each $\epsilon \geq 0$, the ϵ -pseudospectrum is

$$\Lambda_\epsilon(\mathcal{L}^{[0,\infty)}) = \Pi + \Delta_\epsilon. \quad (3.5)$$

Equivalently, for $\lambda \notin \Pi$ the resolvent norm satisfies

$$\|(\lambda I - \mathcal{L}^{[0,\infty)})^{-1}\| = \frac{1}{\text{dist}(\lambda, \Pi)}. \quad (3.6)$$

Moreover, if $W(\mathcal{L}^{[0,\infty)})$ denotes the numerical range of $\mathcal{L}^{[0,\infty)}$, then

$$\text{cl}\{W(\mathcal{L}^{[0,\infty)})\} = \Pi. \quad (3.7)$$

The numerical range $W(\mathcal{L}^{[0,\infty)})$ is defined as the set of all Rayleigh quotients $(u, \mathcal{L}^{[0,\infty)}u)/(u, u)$ for u in the domain of $\mathcal{L}^{[0,\infty)}$, and $\text{cl}\{\cdot\}$ denotes set closure.

Proof of Theorem 3. For any λ in the interior of Π , the function $\phi(x)$ of (2.4) satisfies both boundary conditions and belongs to $L^2[0, \infty)$. Thus $\phi(x)$ is an eigenfunction of $\mathcal{L}^{[0,\infty)}$ with eigenvalue λ . Since the spectrum is closed and contained in the closure of the numerical range [21, problem 214], this implies $\Pi \subseteq \Lambda(\mathcal{L}^{[0,\infty)}) \subseteq \text{cl}\{W(\mathcal{L}^{[0,\infty)})\}$.

We now establish the converse inclusion $W(\mathcal{L}^{[0,\infty)}) \subseteq \Pi$, which implies $\text{cl}\{W(\mathcal{L}^{[0,\infty)})\} = \Lambda(\mathcal{L}^{[0,\infty)}) = \Pi$ and thus completes the proof of both (3.4) and (3.7). By standard arguments to be found for example in [24], (3.7) is also equivalent to (3.6), and as in the proof of Theorem 2, the equivalence of (3.6) and (3.5) follows from the definition of pseudospectra.

Let u be a function in the domain of $\mathcal{L}^{[0,\infty)}$ normalized by $\|u\| = 1$. By integration by parts we calculate

$$(u, \mathcal{L}^{[0,\infty)}u) = \int_0^\infty \bar{u}(x)(u'' + u') dx = -\int_0^\infty |u'(x)|^2 dx + \int_0^\infty \bar{u}(x)u'(x) dx.$$

The first term is real, and another integration by parts shows that the second is imaginary, so by the Cauchy-Schwarz inequality we obtain

$$\operatorname{Re}(u, \mathcal{L}^{[0,\infty)}u) = -\|u'\|^2, \quad |\operatorname{Im}(u, \mathcal{L}^{[0,\infty)}u)| \leq \|u\| \|u'\| = \|u'\|.$$

Therefore

$$\operatorname{Re}(u, \mathcal{L}^{[0,\infty)}u) \leq -|\operatorname{Im}(u, \mathcal{L}^{[0,\infty)}u)|^2,$$

or by (2.9), $(u, \mathcal{L}^{[0,\infty)}u) \subseteq \Pi$. Thus $W(\mathcal{L}^{[0,\infty)}) \subseteq \Pi$, as claimed. ■

Figure 5 summarizes the results of Theorems 2 and 3.

Figure 5. Spectra of $\mathcal{L}^{(-\infty, \infty)}$ and $\mathcal{L}^{[0, \infty)}$.

4. Estimates of the pseudospectra

Our first theorem concerning the pseudospectra of $\mathcal{L}$ asserts that outside the parabolic region Π , the resolvent norm of $\mathcal{L}$ decreases inverse-linearly with constant 1 in the numerator—i.e., the “Kreiss constant” is 1 (cf. [11]).

THEOREM 4. For each $\epsilon \geq 0$, the ϵ -pseudospectrum of $\mathcal{L}$ satisfies

$$\Lambda_\epsilon(\mathcal{L}) \subseteq \Pi + \Delta_\epsilon. \quad (4.1)$$

Equivalently, for $\lambda \notin \Pi$ the resolvent norm satisfies

$$\|(\lambda I - \mathcal{L})^{-1}\| \leq \frac{1}{\text{dist}(\lambda, \Pi)}, \quad (4.2)$$

and the numerical range satisfies

$$W(\mathcal{L}^{[0, \infty)}) \subseteq \Pi. \quad (4.3)$$

Proof. By changing the upper limit of integration from ∞ to d in the proof of Theorem 3, we obtain a proof of (4.3), and this implies (4.2) and equivalently (4.1). ■

We now turn to the problem of estimating the resolvent norm and hence the pseudospectra inside Π . To motivate our estimates, note that the resolvent is the solution operator for the inhomogeneous problem

$$(\lambda I - \mathcal{L})u = f, \quad u(0) = u(d) = 0 \quad (4.4)$$

for $f \in L^2[0, d]$. For each fixed λ and y , the Green's function $G(x, y)$ for this problem is the solution $u(x)$ corresponding to $f(x) = \delta(x - y)$, and it can be written

$$G(x, y) = a\phi(x) + \phi([x - y]_+), \quad (4.5)$$

where $\phi(x)$ is the function (2.4) illustrated in Figure 4, $[x - y]_+$ denotes 0 for $x - y \leq 0$ and $x - y$ for $x - y \geq 0$, and a is a constant. The term $\phi([x - y]_+)$ would be a solution to (4.4) if there were no right-hand boundary condition, and the term $a\phi(x)$ is a correction added to enforce that boundary condition. Figure 6 sketches $G(x, y)$ for $d = 20$, $y = 10$, and three values of λ . The figure reveals that in the case $\lambda = -0.2$, this correction term is exponentially large in $0 < x < y$.

For general functions $f(x)$ in (4.4), we can make an analogous decomposition of $u(x)$ into two terms. Assuming that λ is in the interior of Π , write

$$(\lambda I - \mathcal{L})^{-1} = R_\infty + R_d, \quad (4.6)$$

Figure 6. Green's functions $G(x, y)$ for three values of λ on the interval $[0, d]$, $d = 20$, $y = 10$, normalized by $G(y, y) = 1$. The value $\lambda = -0.2$ lies in the interior of Π , and this explains the exponentially large lobe of $G(x, y)$ for $0 < x < y$ in the first plot.

where R_∞ is the operator on $L^2[0, d]$ defined as follows: extend the data by zero to $L^2(-\infty, \infty)$, apply $(\lambda I - \mathcal{L}^{(-\infty, \infty)})^{-1}$, then restrict the result to $[0, d]$. By construction $\|R_\infty\| \leq \|(\lambda I - \mathcal{L}^{(-\infty, \infty)})^{-1}\|$, so by (3.3) we have

$$\|R_\infty\| \leq \frac{1}{\text{dist}(\lambda, P)}. \quad (4.7)$$

This quantity is small compared with the exponentials of interest, and thus (4.6) and (4.7) effectively reduce the estimation of $\|(\lambda I - \mathcal{L})^{-1}\|$ to the estimation of $\|R_d\|$, which we can carry out with the aid of explicit representations of R_∞ and

R_d . First, by integrating the term $\phi([x-y]_+)$ in (4.5) against $f(y)$, we obtain the following formula for $v = R_\infty f$:

$$v(x) = \int_0^x \phi(x-y)f(y) dy. \quad (4.8)$$

In particular,

$$v(d) = \int_0^d \phi(d-y)f(y) dy. \quad (4.9)$$

Since R_d is designed to enforce the boundary condition $(R_\infty f + R_d f)(d) = 0$, we have the following formula for $w = R_d f$:

$$w(x) = -v(d) \frac{\phi(x)}{\phi(d)}. \quad (4.10)$$

Combining (4.9) and (4.10) gives

$$\|R_d\| = \sup_f \frac{\|w\|}{\|f\|} = \frac{\|\phi\|}{|\phi(d)|} \sup_f \frac{|v(d)|}{\|f\|}. \quad (4.11)$$

By the Cauchy-Schwarz inequality applied to (4.9), the second supremum in (4.11) is $\|\phi\|$, attained with $f(y) = \bar{\phi}(d-y)$, and thus we have

$$\|R_d\| = \frac{\|\phi\|^2}{|\phi(d)|}. \quad (4.12)$$

Estimates for $\|(\lambda I - \mathcal{L})^{-1}\|$ can now be obtained by combining (4.7) and (4.12) with the inequality

$$\|R_d\| - \|R_\infty\| \leq \|(\lambda I - \mathcal{L})^{-1}\| \leq \|R_d\| + \|R_\infty\|, \quad (4.13)$$

a consequence of (4.6).

The following theorem presents several estimates of this kind. Note that (4.16) shows that the back-of-the-envelope estimate (2.11) got the leading exponential behavior right but missed an algebraic factor of size $O(|\alpha_\pm|^{-1}) = O(|\lambda|^{-1/2})$ as $\lambda \rightarrow \infty$.

THEOREM 5. Let λ be an arbitrary point in the interior of Π , with $\alpha_{\pm}$ and $\phi(x)$ defined by (2.2) and (2.4), and write $\alpha_+ - \alpha_- = \sqrt{1+4\lambda} = \sigma + i\tau$. Then

$$\|(\lambda I - \mathcal{L})^{-1}\| \sim \frac{\|\phi\|^2}{\phi(d)} \quad (4.14)$$

and

$$\|\phi\|^2 \sim \frac{2}{(1-\sigma^2)(1+\tau^2)} \quad (4.15)$$

as $d \rightarrow \infty$. If in addition $\lambda \notin (-\infty, -\frac{1}{4}]$, then $\phi(d) \sim e^{\mu d}/|\alpha_+ - \alpha_-|$ and therefore

$$\|(\lambda I - \mathcal{L})^{-1}\| \sim \frac{2e^{-\mu d}(\sigma^2 + \tau^2)^{1/2}}{(1-\sigma^2)(1+\tau^2)}, \quad (4.16)$$

where $\mu = \max\{\operatorname{Re}\alpha_+, \operatorname{Re}\alpha_-\} < 0$ as in (2.10).

Proof. By (4.7), $\|R_{\infty}\|$ is bounded independently of d as $d \rightarrow \infty$, whereas it follows from (4.12) that $\|R_d\|$ grows without bound. Therefore (4.14) follows from (4.12) and (4.13). Note that if $\lambda \in (-\infty, -\frac{1}{4})$, the terms on either side of (4.14) oscillate through ∞ between large positive and negative values each time d passes through a zero of $v(d)$ (making λ an eigenvalue of $\mathcal{L}$). Nevertheless, the ratio of the two converges to 1 as $d \rightarrow \infty$, as the “ $\sim$ ” requires.

To derive (4.15), we compute

$$\begin{aligned} \int_0^d |e^{\alpha_+ x} - e^{\alpha_- x}|^2 dx &\sim \int_0^{\infty} |e^{\alpha_+ x} - e^{\alpha_- x}|^2 dx \\ &= \int_0^{\infty} (e^{\alpha_+ x} - e^{\alpha_- x})(e^{\bar{\alpha}_+ x} - e^{\bar{\alpha}_- x}) dx \\ &= \int_0^{\infty} (e^{(\alpha_+ + \bar{\alpha}_+)x} + e^{(\alpha_- + \bar{\alpha}_-)x} - e^{(\alpha_- + \bar{\alpha}_+)x} - e^{(\bar{\alpha}_- + \alpha_+)x}) dx \\ &= -\frac{1}{\alpha_+ + \bar{\alpha}_+} - \frac{1}{\alpha_- + \bar{\alpha}_-} + \frac{1}{\alpha_- + \bar{\alpha}_+} + \frac{1}{\bar{\alpha}_- + \alpha_+} \\ &= \frac{1}{1-\sigma} + \frac{1}{1+\sigma} - \frac{1}{1+i\tau} - \frac{1}{1-i\tau} \end{aligned}$$

$$= \frac{2}{1-\sigma^2} - \frac{2}{1+\tau^2} = \frac{2(\sigma^2 + \tau^2)}{(1-\sigma^2)(1+\tau^2)}.$$

Since $\phi(x) = (e^{\alpha_+ x} - e^{\alpha_- x})/(\alpha_+ - \alpha_-)$ and $|\alpha_+ - \alpha_-|^2 = \sigma^2 + \tau^2$, this establishes (4.15). From here, the derivation of $\phi(d) \sim e^{\mu d}/|\alpha_+ - \alpha_-|$ and then (4.16) is trivial. ■

When d is reasonably large, the estimate (4.16) is a very good one. For example, if Figure 1 is redrawn to plot contours of (4.16) instead of $\|(\lambda I - \mathcal{L})^{-1}\|$, all the curves except the outermost one ($\epsilon = 10^{-1}$) remain unchanged to plotting accuracy.

Theorems 4 and 5 imply as a corollary that for each $\epsilon > 0$, $\Lambda_\epsilon(\mathcal{L})$ behaves continuously in the limit $d \rightarrow \infty$. The following theorem to this effect is analogous to Theorem 3.3 of [37].

THEOREM 6. For each $\lambda \in \mathbb{C}$,

$$\|(\lambda I - \mathcal{L})^{-1}\| \rightarrow \|(\lambda I - \mathcal{L}^{[0,\infty)})^{-1}\| \quad \text{as } d \rightarrow \infty. \quad (4.17)$$

Proof. If λ is in the interior of Π , the right-hand side of (4.17) is ∞ by Theorem 3, and by Theorem 5, the left-hand side converges to ∞ as $d \rightarrow \infty$. Suppose on the other hand that λ is in the exterior of Π or on the boundary P . The right-hand side of (4.17) is now $1/\text{dist}(\lambda, \Pi)$, and by Theorem 4, the left-hand side is $\leq 1/\text{dist}(\lambda, \Pi)$ for all d . To derive a reverse inequality, for any $\delta_1 > 0$ and $\delta_2 > 0$, let λ' be a point in the interior of Π with $|\lambda' - \lambda| < \text{dist}(\lambda, \Pi) + \delta_1$, and take d large enough so that $\|(\lambda' I - \mathcal{L})^{-1}\| > \delta_2^{-1}$. Then it is easily seen that there exists a perturbation $\mathcal{L}'$ with $\|\mathcal{L}' - \mathcal{L}\| < |\lambda' - \lambda| + \delta_2 < \text{dist}(\lambda, \Pi) + \delta_1 + \delta_2$ such that λ is in the spectrum of $\mathcal{L}'$, which implies $\|(\lambda I - \mathcal{L})^{-1}\| > 1/(\text{dist}(\lambda, \Pi) + \delta_1 + \delta_2)$. Taking $\delta_1 \rightarrow 0$ and $\delta_2 \rightarrow 0$ completes the proof. ■

5. Symmetrizability and a further estimate

For each fixed d , the operator $\mathcal{L}$ is *symmetrizable*: similar by a diagonal similarity transformation to a self-adjoint operator with, of course, the same

real eigenvalues. This is pointed out in Example III.6.11 of [24]* and is also suggested by the form of the eigenfunctions (2.6).

To carry out the symmetrization we define $u(x) = e^{-x/2}v(x)$, which implies

$$u' = e^{-x/2}(-\frac{1}{2}v + v'), \quad u'' = e^{-x/2}(\frac{1}{4}v - v' + v'')$$

and therefore

$$\mathcal{L}u = u'' + u' = e^{-x/2}(v'' - \frac{1}{4}v).$$

Thus if we define

$$\mathcal{K}v = v'' - \frac{1}{4}v, \quad \mathcal{M}v = e^{-x/2}v, \quad (5.1)$$

then we have

$$\mathcal{L} = \mathcal{M}\mathcal{K}\mathcal{M}^{-1}. \quad (5.2)$$

Here $\mathcal{K}$ is a self-adjoint operator and $\mathcal{M}$ is a diagonal operator with $\|\mathcal{M}\| = 1$, $\|\mathcal{M}^{-1}\| = e^{d/2}$, and consequently

$$\kappa(\mathcal{M}) = \|\mathcal{M}\|\|\mathcal{M}^{-1}\| = e^{d/2}. \quad (5.3)$$

The notation $\kappa(\mathcal{M})$ comes from numerical analysis, where $\|\mathcal{M}\|\|\mathcal{M}^{-1}\|$ is interpreted as a condition number. On the face of it $\kappa(M)$ is just the condition number of the symmetrizing transformation M , but a little thought shows that it is also equal to the condition number of the basis of eigenfunctions (2.6) if they are normalized to satisfy $\|u_n\| = 1$, for these eigenfunctions are related by the same transformation M to an orthonormal set of eigenfunctions of $\mathcal{K}$, namely the suitably normalized sine functions.

Since $\mathcal{K}$ is self-adjoint, its resolvent norm is

$$\|(\lambda I - \mathcal{K})^{-1}\| = \frac{1}{\text{dist}(\lambda, \Lambda(\mathcal{K}))} = \frac{1}{\text{dist}(\lambda, \Lambda(\mathcal{L}))}.$$

On the other hand the resolvents of $\mathcal{L}$ and $\mathcal{K}$ are related by

$$(\lambda I - \mathcal{L})^{-1} = (\lambda I - \mathcal{M}\mathcal{K}\mathcal{M}^{-1})^{-1} = \mathcal{M}(\lambda I - \mathcal{K})^{-1}\mathcal{M}^{-1}.$$

Combining these formulas yields the following new bound:

*A good deal of information about convection-diffusion operators can be found in [24]. See Section III.2.3 and Examples III.5.32, III.6.11, III.6.20, VIII.1.19.

THEOREM 7. For any $d > 0$ and $\lambda \in \mathbb{C}$,

$$\|(\lambda I - \mathcal{L})^{-1}\| \leq \frac{e^{d/2}}{\text{dist}(\lambda, \Lambda(\mathcal{L}))} \leq \frac{e^{d/2}}{|\text{Im} \lambda|}. \quad (5.4)$$

It is interesting to compare this result with Theorem 5. That theorem, as well as Figure 1 and our discussion up to this point, suggested that the pseudospectra of $\mathcal{L}$ approximate parabolas. Theorem 7 reveals that although this may be true in a large part of the λ -plane, it cannot be true as $|\lambda| \rightarrow \infty$. Instead, for any fixed ϵ and d , $\Lambda_\epsilon(\mathcal{L})$ must be contained in a strip of finite (though typically very large) width:

$$\Lambda_\epsilon(\mathcal{L}) \subseteq \{\lambda \in \mathbb{C} : |\text{Im} \lambda| \leq \epsilon e^{d/2}\}. \quad (5.5)$$

With hindsight we can see that this deviation from a parabola was foreshadowed in the presence of the algebraic factors $O(|\lambda|^{-1/2})$ in (4.16), and is visible in Figure 1.

Because of the equivalence of conditions (i) and (ii) in the definition of pseudospectra, (5.4) can be interpreted as a statement about the sensitivity of the spectrum $\Lambda(\mathcal{L})$: if $\mathcal{L}$ is perturbed to $\mathcal{L} + \mathcal{E}$, each eigenvalue changes by at most $e^{d/2} \|\mathcal{E}\|$. In numerical analysis this bound is known as the *Bauer-Fike theorem*. To see how close it is to sharp, one can calculate the (absolute) condition number of an individual eigenvalue λ_n , equal to the inverse of the absolute value of the inner product of the corresponding normalized eigenvectors of $\mathcal{L}$ and its adjoint. Such a calculation shows that the condition numbers are $\sim e^{d/2}/d$ for fixed d as $n \rightarrow \infty$, so (5.5) is sharp up to a factor asymptotic to d .

One might be tempted to conclude from the above observations that since $\mathcal{L}$ is symmetrizable, with a spectrum whose sensitivity to perturbations is finite, there is no need to pay attention to non-normality of convection-diffusion operators or to distinguish spectra and pseudospectra. Relatedly, the symmetrization (5.2) amounts to the observation that $\mathcal{L}$ is a self-adjoint operator in a space with an exponentially weighted inner product, and thus one might argue that since non-normality is a norm-dependent property, it is of no consequence. However, arguments like these miss a great deal. Theoretically, they miss the point that

the quantities in question are finite only for each fixed d ; $\mathcal{L}$ is by no means uniformly symmetrizable as $d \rightarrow \infty$, nor are the eigenvalue condition numbers uniformly bounded. Practically, they miss the point that even for fixed d , these quantities are huge, so that ignoring them is asking for trouble. Norm-independence may seem an attractive property mathematically, but quantities that are measurable in the laboratory are rarely norm-independent. Indeed, one might take that as a principle: if it's norm-independent, it's probably non-physical.

6. Finite difference and spectral discretizations

Pseudospectra of differential operators can be computed numerically by finite difference, finite element, or spectral methods. In future work we hope to prove convergence of some of these numerical approximations. Here, we shall just present two examples.

The simplest finite-difference discretizations of (1.1) involve 3-point approximations to the first and second derivatives. In practice it may be better to use an irregular grid in the convection-dominated case, but for simplicity, consider the regular grid

$$x_j = jh, \quad h = \frac{d}{N}, \quad j = 0, 1, \dots, N \quad (6.1)$$

for some $N > 1$ and the centered difference approximations

$$u''(x_j) \approx \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2}, \quad u'(x_j) \approx \frac{v_{j+1} - v_{j-1}}{2h}$$

with $v_j \approx u(x_j)$. With this discretization and our homogeneous boundary conditions, $\mathcal{L}$ is approximated by the tridiagonal Toeplitz matrix $L^{(N)}$ of dimension $N - 1$ with entries

$$L_{j,j}^{(N)} = -2h^{-2}, \quad L_{j,j\pm 1}^{(N)} = h^{-2} \pm (2h)^{-1}. \quad (6.2)$$

Figure 7 plots numerically computed pseudospectra of $L^{(N)}$ for $d = 40$ and $N = 30$. The parameters and contour lines are the same as in Figure 1, and the

Figure 7. A finite-difference approximation to Figure 1 with $N = 30$.

Figure 8. A Chebyshev spectral approximation to Figure 1 with $N = 30$. Six real eigenvalues lie off-scale to the left of the figure.

reader should compare these figures. Evidently $\Lambda_\epsilon(L^{(N)})$ approximates $\Lambda_\epsilon(\mathcal{L})$ well near the origin of the λ -plane, corresponding to smooth modes that are well resolved by the discretization. For larger λ the approximation deteriorates quickly and it is clear that one would have to take $N \gg 200$ to achieve a good match throughout the region displayed. As it happens, quite a bit is known about the pseudospectra of Toeplitz matrices [37]. In particular, the fact that the pseudospectra $\Lambda_\epsilon(L^{(N)})$ approximate ellipses is related to the fact that the symbol of a tridiagonal Toeplitz matrix maps circles about the origin onto ellipses.

Better approximations to $\Lambda_\epsilon(\mathcal{L})$ can be achieved with spectral methods. In Figure 8, the same pseudospectra are plotted for the case of a spectral collocation approximation $L_{\text{sp}}^{(N)}$ based on the Chebyshev grid

$$x_j = \frac{1}{2}d(1 + \cos(\frac{j\pi}{N})), \quad j = 0, 1, \dots, N. \quad (6.3)$$

For the details of such approximations see [5]. It is obvious at a glance that the approximation $\Lambda_\epsilon(L_{\text{sp}}^{(N)}) \approx \Lambda_\epsilon(\mathcal{L})$ is accurate over a larger region of the λ -plane than in the finite-difference case. Indeed it appears to be “spectrally accurate” over a sizable portion of the plane. Note that this effect happens automatically when the differential operator is discretized; in no sense is the discretization an explicit attempt to capture pseudospectra.

The spectral structure of $L_{\text{sp}}^{(N)}$ is complicated, by contrast, and in fact, there are three real pairs of additional eigenvalues off-scale to the left of Figure 8, with absolute values approximately 7, 17, and 95. The properties of the eigenvalues of spectral discretization matrices are of some importance, for sometimes the location of the outlying eigenvalues determines the allowable step size in discretization of time-dependent problems. A comparison of Figure 8 with Figure 1 suggests, however, that the location of the higher eigenvalues in the spectrum is almost an accidental matter, with the essential approximation phenomenon taking place in the pseudospectra. There is a natural reason for this. If a discrete operator approximates a continuous operator to a certain accuracy τ , it is reasonable to expect that the ϵ -pseudospectra with $\epsilon \geq O(\tau)$ may be approximated meaningfully, at least in regions near eigenvalues whose eigenfunctions are well resolved by the grid, but there is little reason to expect

accurate approximations “below the level of truncation error,” i.e., for $\epsilon \ll \tau$ and in particular for $\epsilon = 0$.

A fine point that comes up in computations such as these is the question of norms. The quantity $\|(\lambda I - \mathcal{L})^{-1}\|$ is defined with respect to the norm of $L^2[0, d]$, whereas $\|(\lambda I - L^{(N)})^{-1}\|$ and $\|(\lambda I - L_{\text{sp}}^{(N)})^{-1}\|$ would appear to be defined with respect to the discrete ℓ^2 norms on the grid (6.1) and (6.3), respectively. To correct for this discrepancy, in our computation $L^{(N)}$ is actually replaced by $W^{(N)}L^{(N)}(W^{(N)})^{-1}$ and $L_{\text{sp}}^{(N)}$ by $W_{\text{sp}}^{(N)}L_{\text{sp}}^{(N)}(W_{\text{sp}}^{(N)})^{-1}$, where $W^{(N)}$ and $W_{\text{sp}}^{(N)}$ are appropriate weighting matrices. As the effect on the plots is in the end slight, we omit the details.

We can now explain how Figure 1 was computed. Experiments indicate that for each λ , after weighting as described above, both $\|(\lambda I - L^{(N)})^{-1}\|$ and $\|(\lambda I - L_{\text{sp}}^{(N)})^{-1}\|$ converge to the correct value $\|(\lambda I - \mathcal{L})^{-1}\|$ as $N \rightarrow \infty$. To produce Figure 1 we used spectral discretizations $L_{\text{sp}}^{(N)}$ and chose values of N adaptively for each λ until convergence to four relative digits seemed to be achieved. The values of λ used for this picture lay on a grid of 150×70 points in the complex upper half-plane, so $O(10^4)$ such computations were involved altogether. The largest value of N required for the range of λ in Figure 1 was 72, with a more typical value being 32. The whole computation required approximately 1.2×10^9 floating-point operations as measured by Matlab (four hours on a SPARC 2 workstation).

7. Applications

In this final section we briefly examine applications of the pseudospectra of $\mathcal{L}$, and relatedly, some of the limitations of spectral analysis for convection-diffusion problems.

One common application of spectral analysis is to simplify a problem by expressing it in the basis of eigenmodes, where the equation becomes diagonal. The limitation of this idea for convection-diffusion problems is apparent from (5.3): the basis of eigenmodes is exponentially ill-conditioned. If a function of norm $O(1)$ is expanded in this basis, then as a rule the expansion coefficients

will be of order $e^{d/2}$, and the time evolution will be largely determined by the evolving patterns of cancellation among these coefficients. This is an indication that the eigenfunction basis is a poor one. It may be simpler and more natural to work with a basis chosen for its approximation properties, unrelated to eigenmodes. If $e^{d/2}$ is greater than the inverse of machine precision on the computer, one will be forced to do so, or else the computation will fail because of rounding errors.

Another application of spectra is the estimation of norms of evolution processes. Suppose one wishes to study energy growth or decay for the time-dependent linear problem

$$u_t = \mathcal{L}u, \quad u(0) = u_0. \quad (7.1)$$

The solution is $u(t) = e^{t\mathcal{L}}u_0$, with norm governed by the quantity $\|e^{t\mathcal{L}}\|$. From spectral analysis we expect that $\|e^{t\mathcal{L}}\|$ should be related to $\alpha(\mathcal{L})$, the *spectral abscissa* of $\mathcal{L}$, whose value we know from Theorem 1:

$$\alpha(\mathcal{L}) = \sup_{\lambda \in \Lambda(\mathcal{L})} \operatorname{Re} \lambda = -\frac{1}{4} - \frac{\pi^2}{d^2}. \quad (7.2)$$

However, a precise connection between $\|e^{t\mathcal{L}}\|$ and $\alpha(\mathcal{L})$ again requires the introduction of the exponentially large factor $\kappa(M) = e^{d/2}$ of (5.3):

$$e^{t\alpha(\mathcal{L})} \leq \|e^{t\mathcal{L}}\| \leq \kappa(M)e^{t\alpha(\mathcal{L})}, \quad (7.3)$$

or by combining (7.2) and (7.3),

$$e^{-t/4 - t\pi^2/d^2} \leq \|e^{t\mathcal{L}}\| \leq e^{d/2 - t/4 - t\pi^2/d^2}. \quad (7.4)$$

Figure 9 plots the three quantities of (7.4) for the case $d = 40$. What we see is a great difference between the transient and the asymptotic behavior of $\|e^{t\mathcal{L}}\|$. In the transient phase, of length $O(d)$, $\|e^{t\mathcal{L}}\|$ is nearly constant. Only after that does the curve bend around to match the slope predicted by the spectrum. Physically, it is easy to see the explanation for this behavior. A broad pulse that begins at the upstream end of the interval may convect downstream with

Figure 9. Comparison of $\|e^{t\mathcal{L}}\|$ with upper and lower bounds based on the spectrum. Spectral information is meaningful asymptotically as $t \rightarrow \infty$, but fails to capture the transient.

relatively little diffusion for a time period $O(d)$, decaying rapidly in energy only when it nears the downstream end.

This gap between transient and asymptotic behavior can be captured better if one considers the pseudospectra of $\mathcal{L}$ as well as the spectra. One has the following relationships:

$$\|e^{t\mathcal{L}}\| \text{ for } t \rightarrow \infty \leftrightarrow \Lambda_\epsilon(\mathcal{L}) \text{ for } \epsilon \rightarrow 0, \quad (7.5a)$$

$$\|e^{t\mathcal{L}}\| \text{ for } t \rightarrow 0 \leftrightarrow \Lambda_\epsilon(\mathcal{L}) \text{ for } \epsilon \rightarrow \infty, \quad (7.5b)$$

$$\|e^{t\mathcal{L}}\| \text{ for finite } t \leftrightarrow \Lambda_\epsilon(\mathcal{L}) \text{ for finite } \epsilon. \quad (7.5c)$$

The first of these statements is the association just discussed between the asymptotic behavior of $\|e^{t\mathcal{L}}\|$ as $t \rightarrow \infty$ and the spectrum of $\mathcal{L}$. The second can be justified by the equation

$$e^{t\beta(\mathcal{L})-o(t)} \leq \|e^{t\mathcal{L}}\| \leq e^{t\beta(\mathcal{L})} \quad (7.6)$$

as $t \rightarrow 0$, where $\beta(\mathcal{L})$ is the the *numerical abscissa* of $\mathcal{L}$, i.e., the largest real part of the numerical range, which is very close to 0. It can be shown that the

numerical range is determined by the behavior of $\Lambda_\epsilon(\mathcal{L})$ in the limit $\epsilon \rightarrow \infty$, and this implies (7.5b). Finally, (7.5c) can be made precise in various ways with the aid of the contour integral

$$e^{t\mathcal{L}} = \frac{1}{2\pi i} \int_{\Gamma} e^{t\lambda} (\lambda I - \mathcal{L})^{-1} d\lambda, \quad (7.7)$$

where Γ is any contour enclosing $\Lambda(L)$. From (7.7) one can derive bounds on $\|e^{t\mathcal{L}}\|$ that depend on the location of the pseudospectra in the complex plane; an example is the Kreiss Matrix Theorem. We shall not give details here, but refer the reader to [11,35,42,44].

Can one do better than loose bounds and predict $\|e^{t\mathcal{L}}\|$ as a function of t exactly? Certainly not, based on the spectrum and/or the numerical range alone. With the knowledge of all the pseudospectra $\Lambda_\epsilon(\mathcal{L})$, however, the answer may be yes. In [19] it has been conjectured that for any two matrices or operators $\mathcal{L}_1$ and $\mathcal{L}_2$ with $\Lambda_\epsilon(\mathcal{L}_1) = \Lambda_\epsilon(\mathcal{L}_2)$ for all $\epsilon > 0$, one has $\|f(\mathcal{L}_1)\| = \|f(\mathcal{L}_2)\|$ for all functions f analytic in a neighborhood of the spectra. As of this writing, this conjecture remains unresolved.

All of these remarks apply to the purely linear, constant-coefficient problem (7.1). Another limitation of spectral analysis is that as a rule it is not robust with respect to the introduction of complications such as

- nonlinearity,
- variable coefficients,
- inhomogeneous forcing data,
- other perturbations.

If (7.1) is modified in any of these ways, the effect will typically be that the transient part of Figure 9 remains approximately unchanged, but the long-time part of the figure—precisely the part related to eigenvalues—may change entirely. Such modification of a linear constant-coefficient problem is more the rule than the exception, for many simple problems in the mathematical sciences arise from more complicated problems by the familiar sequence of steps of linearization, freezing of coefficients, and diagonalization:

$$\begin{array}{ccccccc} \textit{nonlinear} & \rightarrow & \textit{linear} & \rightarrow & \textit{linear problem with} & \rightarrow & \textit{collection of} \\ \textit{problem} & & \textit{problem} & & \textit{constant coefficients} & & \textit{scalar problems} \end{array} \quad .$$

In general, the first two of these simplifications are valid for short times and the third is valid for $t \rightarrow \infty$. When these time scales fail to overlap, spectral analysis may be of little value, even though there may be nothing wrong with the linearized approximation or with analyzing its behavior by pseudospectra.

Among the complications just listed, the easiest to make precise is the introduction of inhomogeneous forcing data. Suppose (7.1) is changed from an initial-value problem on $[0, \infty)$ to a problem on $(-\infty, \infty)$ driven by a periodic forcing term:

$$u_t = \mathcal{L}u + e^{\lambda t} \mathbf{v}, \quad -\infty < t < \infty \quad (7.8)$$

for some $\lambda \notin \Lambda(\mathcal{L})$ and some fixed function $\mathbf{v}$ in the domain of $\mathcal{L}$. (Values of λ on the imaginary axis correspond to forcing the system at a real frequency.) It is easily verified that the response will be

$$u(t) = e^{\lambda t} \mathbf{u}, \quad \mathbf{u} = (\lambda I - \mathcal{L})^{-1} \mathbf{v}. \quad (7.9)$$

Thus the resolvent $(\lambda I - \mathcal{L})^{-1}$ transforms “inputs” $\mathbf{v}$ in (7.8) to corresponding “outputs” $\mathbf{u}$, and the degree of amplification that may occur in the process is given by

$$\sup_{\mathbf{v} \neq 0} \frac{\|\mathbf{u}\|}{\|\mathbf{v}\|} = \|(\lambda I - \mathcal{L})^{-1}\|. \quad (7.10)$$

This equation implies that the resonant or “pseudo-resonant” response of a non-normal system to inputs at a frequency λ may be large when $\lambda \in \Lambda_\epsilon(\mathcal{L})$ for small ϵ , regardless of whether or not λ is close to the spectrum. In particular, a convection-diffusion problem may have a large-amplitude response to low-frequency input, even though the spectrum lies to the left of the line $\operatorname{Re} \lambda = -\frac{1}{4}$.

For further discussion of these matters, see [23], and for their application to the physical problem of hydrodynamic stability, see [42].

We shall close with a discussion of a different type of application of the ideas of this paper. Suppose we wish to solve a linear system of equations

$$L^{(N)} u = f \quad (7.11)$$

by a nonsymmetric Chebyshev iteration of the kind investigated by Manteuffel [29], where $L^{(N)}$ is a discrete approximation to $\mathcal{L}$ as considered in Section 6. Such an iteration depends upon a pair of parameters $a, b \in \mathbb{C}$, which define

an interval with respect to which a family of Chebyshev polynomials $\{p_n\}$ is implicitly constructed. The lemniscates $|p_n(z)| = \text{const.}$ of these polynomials approximate ellipses with foci a, b .

The conventional view is that a and b should be chosen so that the spectrum $\Lambda(L^{(N)})$ lies in one of these ellipses that is in an appropriate sense as small as possible. This view is supported by the estimate analogous to (7.2),

$$\frac{\|r_n\|}{\|r_0\|} \leq \|p_n\|_{\Lambda(L^{(N)})} \kappa(M), \quad (7.12)$$

where $\|r_n\|/\|r_0\|$ denotes the ratio of the n th to the initial residual norms, $\|p_n\|_{\Lambda(L^{(N)})}$ denotes the supremum of $|p_n(z)|$ for $z \in \Lambda(L^{(N)})$, and $\kappa(M)$ is the condition number of a transformation that makes $L^{(N)}$ diagonal or self-adjoint. The trouble with (7.12) is that the factor $\kappa(M)$ may be exponentially large [37]. An alternative bound can be based on the norm of p_n on a pseudospectrum, rather than the spectrum. For any $\epsilon > 0$ we have

$$\frac{\|r_n\|}{\|r_0\|} \leq \|p_n\|_{\Lambda_\epsilon(L^{(N)})} \frac{\ell_\epsilon}{2\pi\epsilon}, \quad (7.13)$$

where ℓ_ϵ denotes the arc length of $\partial\Lambda_\epsilon(L^{(N)})$; the proof is by a contour integral analogous to (7.7) [32]. When $\kappa(M)$ is large and ϵ is not too small, a comparison of (7.12) and (7.13) suggests that when $L^{(N)}$ is far from normal, the parameters of a nonsymmetric matrix iteration may be more appropriately based on the pseudospectra than on the spectrum. Experiments confirm this prediction dramatically for certain problems [39]. A striking related example is the phenomenon of direction-dependent convergence considered in [4,13,22]: a Gauss-Seidel or SOR iteration for a convection-diffusion problem may converge in far fewer steps if one sweeps with the convection rather than against it. This effect cannot be explained on the basis of spectra alone, which are typically independent of the sweep direction, but the explanation becomes clear when one looks at the pseudospectra. A similar gap between spectra and pseudospectra appears if one considers the numerical stability of discrete methods for convection-diffusion equations [20,31,36].

It is a curious phenomenon that choices of iteration parameters based on adaptive or automatic estimates of the spectrum $\Lambda(L^{(N)})$, such as those constructed by the Manteuffel algorithm, are often more reliable than the above

observations seem to suggest. The same is true of choices based on certain kinds of a priori analysis of $\Lambda(L^{(N)})$, as in a recent paper by Kellogg [25]. The explanation is that most approximate techniques for estimating spectra—both of matrices and of operators—are robust enough that they actually estimate pseudospectra instead, whether or not that was the intent of their authors. This remark applies for example to Gerschgorin’s theorem, the simplest of all eigenvalue estimates; to the Arnoldi process, one of the more sophisticated [14,38]; and to approximations based on energy methods, which are so robust that they are typically valid for the numerical range as well as the spectrum and the pseudospectra. Many numerical methods based on estimates of spectra of nonsymmetric matrices would become markedly less reliable if those estimates could magically be replaced by exact spectral information.

Appendix. Formulas for arbitrary convection and diffusion coefficients

The results in this paper have been stated for the nondimensionalized operator (1.1), with convection and diffusion coefficients both equal to 1. However, this is no essential restriction. Suppose we are given the fully dimensional equation

$$\frac{\partial U}{\partial \tau} = \mathcal{N}U = \nu \frac{\partial^2 U}{\partial \xi^2} + c \frac{\partial U}{\partial \xi}, \quad U(0, t) = U(\delta, t) = 0; \quad (\text{A.1})$$

we have introduced a time variable for motivation. Then the substitutions

$$\xi = \frac{\nu}{c}x, \quad \tau = \frac{\nu}{c^2}t, \quad U(\xi, \tau) = u(x, t) \quad (\text{A.2})$$

reduce the problem to

$$\frac{c^2}{\nu} \frac{\partial u}{\partial t} = \mathcal{N}u = \frac{c^2}{\nu} \frac{\partial^2 u}{\partial x^2} + \frac{c^2}{\nu} \frac{\partial u}{\partial x}, \quad u(0, t) = u(\delta c/\nu, t) = 0.$$

With the further substitutions

$$\mathcal{N} = \frac{c^2}{\nu} \mathcal{L}, \quad \delta = \frac{d\nu}{c} \quad (\text{A.3})$$

we obtain

$$\frac{\partial u}{\partial t} = \mathcal{L}u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x}, \quad u(0, t) = u(d, t) = 0, \quad (\text{A.4})$$

the time-dependent analogue of (1.1). These reductions show that any convection-diffusion problem (A.1) is equivalent to a problem that depends on a single parameter $d = \delta c / \nu$, the *Péclet number*.

By means of the transformations just described, the results of this paper can be extended to arbitrary convection-diffusion operators $\mathcal{N}$ of the form (A.1). One simply makes the following substitutions indicated by (A.2) and (A.3):

$$x = \frac{c}{\nu} \xi, \quad \mathcal{L} = \frac{\nu}{c^2} \mathcal{N}, \quad d = \frac{\delta c}{\nu}. \quad (\text{A.5})$$

(No other changes should be made; in particular $\alpha_{\pm}$ and λ do not change.) All of the results in this paper now apply to $\mathcal{N}$.

For example, Theorem 1 describes the spectrum of $\mathcal{L}$, i.e., the spectrum of $\nu \mathcal{N} / c^2$. Multiplying by c^2 / ν shows that the eigenvalues of $\mathcal{N}$ are the numbers

$$\mu_n = -\frac{c^2}{4\nu} - \frac{\pi^2 n^2 \nu}{\delta^2}.$$

The “critical parabola” $\Pi_{\mathcal{N}}$ for $\mathcal{N}$ is likewise obtained by multiplying by c^2 / ν :

$$\Pi_{\mathcal{N}} = \{\lambda \in \mathbb{C} : \lambda = \frac{c^2}{\nu}(\alpha^2 + \alpha), \operatorname{Re} \alpha = 0\}.$$

For another example, replacing $\mathcal{L}$ by $\nu \mathcal{N} / c^2$ in (4.2) and multiplying by ν / c^2 gives

$$\|(\lambda c^2 I / \nu - \mathcal{N})^{-1}\| \leq \frac{\nu / c^2}{\operatorname{dist}(\lambda, \Pi)},$$

which reduces to

$$\|(\mu I - \mathcal{N})^{-1}\| \leq \frac{1}{\operatorname{dist}(\mu, \Pi_{\mathcal{N}})}$$

if we set $\mu = c^2 \lambda / \nu$. As a final example, Theorem 5 likewise remains valid, now as a statement about the limit $\delta c / \nu \rightarrow \infty$. The exponential growth of $\|(\lambda I - \mathcal{L})^{-1}\|$ at each fixed point λ corresponds to exponential growth of $\|(\mu I - \mathcal{N})^{-1}\|$ at points $\mu = c^2 \lambda / \nu$.

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