K-Spectral Sets and Functions of Nonnormal Matrices

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Abstract

For normal matrices, the study of norms of functions of matrices is made simple through the study of its eigenvalues. However, for nonnormal matrices, eigenvalues do not paint the entire picture, and alternative sets in the complex plane may give a better understanding of the behavior of these matrices, such as K-spectral sets. For a fixed constant $K > 0$, a set $\Omega \subset \mathbb{C}$ is said to be a K-spectral set for A if the spectrum $\sigma(A)$ is contained in Ω, and $\|f(A)\| \leq K\|f\|_\Omega$ holds for every f analytic on Ω. The primary goal of my dissertation is to investigate K-spectral sets that may be of use in finding analytic bounds for norms of functions of nonnormal matrices. Sets such as the ϵ-pseudospectrum and numerical range have been studied for this purpose, but there are still other possible sets in the complex plane that could be utilized as K-spectral sets.

1 Introduction

Many problems in applied mathematics are concerned with estimating $\|f(A)\|$, where A is a matrix and f is a complex-valued function defined on a subset of the complex plane. For instance, the stability of a system of differential equations $x'(t) = Ax(t)$ is determined by $\|e^{tA}\|$, and the stability of the finite difference scheme $x_k = Ax_{k-1}$ depends on $\|A^k\|$. Throughout this paper, $\|\cdot\|$ denotes the 2-norm and the corresponding induced operator norm. Eigenvalues are the most common tool in practice to answer these stability questions, and are indeed very useful in the asymptotic regime. Indeed, if the spectrum $\sigma(A)$ lies in the left half-plane (for e^{tA}) or in the open unit disk (for A^k), then the solution must eventually decay as $t, k \to \infty$. However, one finds that for non-normal matrices, the asymptotic behavior of these functions suggested by the eigenvalues does not agree well with the short-time or transient behavior.

If A is a normal matrix, then it is unitarily diagonalizable, i.e. $A = Q\Lambda Q^*$ where Λ is a diagonal matrix and Q is a unitary matrix. As an example, suppose that A is diagonalizable so

that $A = V\Lambda V^{-1}$, and consider the system $x'(t) = Ax(t)$. Then we have

$$\begin{aligned}\|x(t)\| &= \|e^{tA}x(0)\| \\ &\leq \|e^{tA}\|\|x(0)\| \\ &\leq \|Ve^{t\Lambda}V^{-1}\|\|x(0)\| \\ &\leq \|V\|\|V^{-1}\| \max_{\lambda\in\sigma(A)} e^{\lambda t}\|x(0)\|\end{aligned}$$

Notice that if A were normal, then V would be unitary so that $\|V\| = \|V^{-1}\| = 1$, and we have a good upper bound on the behavior of $\|e^{tA}\|$ based on the spectrum.

For a function f analytic in a neighborhood of $\sigma(A)$ and diagonalizable $A = V\Lambda V^{-1}$, we have a similar bound based on the decomposition $f(A) = Vf(\Lambda)V^{-1}$, namely

$$\|f(A)\| \leq \kappa(V) \max_{\lambda\in\sigma(A)} |f(\lambda)| \tag{1.1}$$

When A is highly nonnormal, in the sense that the condition number $\kappa(V) = \|V\|\|V^{-1}\| \gg 1$, then this bound becomes significantly weaker, especially in short-time and transient regimes. Thus, alternative means of computing bounds for $\|f(A)\|$ are necessary for nonnormal matrices.

2 Functions of matrices

As we wish to study norms of functions of matrices, let us recall the various definitions of a matrix function $f(A)$; see, for example, [14]. First, we note that any $A \in \mathbb{C}^{n\times n}$ can be expressed in the Jordan canonical form $A = PJP^{-1}$, where J is a block diagonal matrix of Jordan blocks $J = \text{diag}(J_1, J_2, \ldots, J_p)$ of the form

$$J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix} \in \mathbb{C}^{m_k\times m_k}$$

where $m_1 + m_2 + \cdots + m_p = n$. We can use the Jordan form for functions as well, so long as f is sufficiently smooth on $\sigma(A)$ so that we have

$$f(A) = Pf(J)P^{-1} = P\text{diag}(f(J_k))P^{-1}$$

where

$$f(J_k) = \begin{bmatrix} f(\lambda_k) & f'(\lambda_k) & \dots & \frac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ & f(\lambda_k) & \ddots & \dots \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{bmatrix}$$

This can be derived from Taylor series considerations.

Another useful definition uses a generalization of the Cauchy integral theorem,

$$f(A) = \frac{1}{2\pi i} \int_\Gamma f(z)(zI - A)^{-1} dz, \tag{2.1}$$

where f is analytic on and inside a closed contour Γ that encloses $\sigma(A)$. The Jordan form approach to matrix functions and spectral theory is algebraic in nature, while the Cauchy integral approach involving the resolvent is more analytic, which makes it more suitable for infinite dimensional operators on Hilbert or Banach spaces. Even just for finite-dimensional matrices, the Cauchy integral approach is still a convenient definition to use numerically and for analytic bounds.

3 K-spectral sets

Having defined suitable interpretations of $f(A)$, we now define K-spectral sets and determine some of their basic properties. While we mostly only consider finite-dimensional matrices corresponding to the Hilbert space $\mathbb{C}^n$ with the standard inner product throughout this paper, it is natural to work in a general complex Hilbert space H.

Suppose that $A \in \mathcal{L}(H)$ is a bounded linear operator on H. Let Ω be a closed set in the complex plane. For a constant $K > 0$, the set X is a K-spectral set for A if the spectrum $\sigma(A)$ of A is included in Ω and we have

$$\|f(A)\| \leq K \|f\|_\Omega \tag{3.1}$$

for every $f \in \mathcal{R}(\Omega)$, the set of complex-valued rational functions defined on Ω. Here, $\|\cdot\|_\Omega$ denotes the ∞-norm of f on Ω. In particular, Ω is a spectral set for A if it is a K-spectral set with $K = 1$. Spectral sets were first introduced by John von Neumann [25], who proved the inequality

$$\|f(A)\| \leq \|f\|_{\mathbb{D}}, \tag{3.2}$$

where f is a polynomial (more generally, a rational function with poles off the closed unit disk $\mathbb{D}$, or any function that is analytic in $\mathbb{D}$) and A is a Hilbert space contraction, meaning $\|A\| \leq 1$. In other words, the unit disk is a spectral set for a contraction. If A is a normal matrix, then the spectrum $\sigma(A)$ is a minimal spectral set, i.e. a spectral set having no proper closed subset which is spectral.

3.1 Numerical range

The numerical range (also called the field of values) of a matrix $A \in \mathbb{C}^{n\times n}$ is the set

$$W(A) = \{\langle Av, v\rangle : \|v\| = 1\} \tag{3.3}$$

Clearly $\sigma(A) \subset W(A)$, as we can simply take v to be normalized eigenvector, and $v^*Av = v^*v\lambda = \lambda$. It is a closed, convex subset of $\mathbb{C}$ [15] that contains the convex hull of the spectrum $\sigma(A)$, and if A is normal, then this containment is an identity. As A becomes more non-normal, the numerical range deviates further and further away from the minimal convex set containing the spectrum, to the point where it may no longer resemble the original spectrum and potentially give extra information about the matrix.

We first note some basic properties of the numerical range and discuss its use in estimating norms of functions of matrices; see, for example, [13] and [23]. Note that if $z \in W(A)$, then

$$\text{Re } z = \frac{z + \bar{z}}{2} = x^* \left(\frac{A + A^*}{2}\right) x$$

One can then show that the real part of the numerical range is

$$\text{Re } (W(A)) = \left[\lambda_{min}\left(\frac{A + A^*}{2}\right), \lambda_{max}\left(\frac{A + A^*}{2}\right)\right]$$

The rightmost part of the numerical range is an important quantity in applications, so we define the numerical abscissa as

$$\omega(A) = \max_{z\in W(A)} \text{Re } z \tag{3.4}$$

This idea can also be used to determine the intersection of $W(A)$ with any line in the complex plane, forming the basis of the algorithm used to compute points on the boundary of the numerical range [15].

The numerical range is useful in the context of estimating functions of matrices, especially for initial short-time behavior. As an example, we note that one can show that if $\|x_0\| = 1$, then

$$\frac{d}{dt}\|e^{tA}x_0\|\Big|_{t=0} = x_0^* \left(\frac{A + A^*}{2}\right) x_0$$

Thus, the rightmost point in $W(A)$ determines the initial slope of $\|e^{tA}\|$ at $t = 0$. In fact, for all $t \geq 0$, it can be shown that

$$\|e^{tA}\| \leq e^{t\omega(A)}$$

Note that $\|e^{tA}\| \leq 1$ for all $t \geq 0$ if and only if $\omega(A) \leq 0$.

We can also define the numerical radius

$$\mu(A) = \sup_{z \in W(A)} |z| \tag{3.5}$$

This satisfies the following power inequality

$$\|A^k\| \leq 2(\mu(A))^k,$$

a result due to Berger [5]. While the downside of the numerical range is that it may be much larger than the spectrum for nonnormal operators and can give significant overestimates after initial or transient behavior, it does have the advantage of being robust to perturbations, due to the fact [23]:

$$W(A + E) \subset W(A) + \overline{\mathbb{D}}_{\|E\|}$$

where $\overline{\mathbb{D}}_{\|E\|}$ denotes the closed disk about 0 of radius $\|E\|$.

Finally, we note that there is a fascinating open conjecture by Michel Crouzeix [7] concerning the numerical range as a K-spectral set that would be helpful for determining the norm of matrix functions. Let f be a function analytic on $W(A)$. Crouzeix has proved [8] that then

$$\|f(A)\| \leq K \max_{z \in W(A)} |f(z)|, \tag{3.6}$$

with $K = 11.08$. He has conjectured that $K = 2$ holds. Of course, there are better estimates for normal matrices, for which we know $\sigma(A)$ is a spectral set, but lowering the constant K in Crouzeix's conjecture would provide estimates for nonnormal matrices. Some progress has been made in simple cases; for example if $W(A)$ is a disk, then it is 2-spectral [3]. Also, the dimension $n = 2$ case has been proved [7], which can be used to show that it holds when A is a quadratic matrix as well. Numerical experiments, such as those done by Crouzeix using numerical conformal maps and Blaschke products [9], or by Overton et al. using sophisticated optimization routines [12], have all suggested that the conjecture is true. However, beyond two dimensions far less has been proven beyond some matrices with very special structure.

3.2 ϵ-pseudospectrum

Another spectral set commonly employed in applied mathematics is the ϵ-pseudospectrum, which was introduced and popularized by Nick Trefethen in the 1990s - see [23] for a comprehensive review on the subject. There are several equivalent definitions of pseudospectra σ_ϵ for a given $\epsilon > 0$ and

matrix $A \in \mathbb{C}^{n\times n}$:

$$\begin{aligned}\sigma_\epsilon(A) &= \{z \in \mathbb{C} : z \in \sigma(A+E), \text{ for some } E \text{ with } \|E\| < \epsilon\} \\ &= \{z \in \mathbb{C} : \|(zI - A)^{-1}\| > 1/\epsilon\} \\ &= \{z \in \mathbb{C} : z \in \sigma(A) \text{ or } \|Av - zv\| < \epsilon \text{ for some unit vector } v\}\end{aligned}$$

These different definitions can be useful in different contexts, but the second definition based on the resolvent norm is the most useful definition for the purpose of investigating the behavior of functions of matrices.

To illustrate the use of pseudospectra as an alternative to the traditional spectrum for bounding functions of matrices, we list some basic results below. The ϵ-pseudospectral abscissa of A measures the rightmost extent of $\sigma_\epsilon(A)$:

$$\alpha_\epsilon(A) = \sup_{z\in\sigma_{\epsilon(A)}} \text{Re } z \tag{3.7}$$

and the ϵ-pseudospectral radius of A measures the maximum magnitude in $\sigma_\epsilon(A)$:

$$\rho_\epsilon(A) = \sup_{z\in\sigma_{\epsilon(A)}} |z| \tag{3.8}$$

Also, $\alpha(A)$ and $\rho(A)$ denote the traditional spectral abscissa and spectral radius respectively. For any function f analytic in a neighborhood of $\sigma(A)$, we have

$$\|f(A)\| \leq \max_{\lambda\in\sigma(A)} |f(\lambda)|$$

for which equality holds when A is normal. Thus:

$$\|e^{tA}\| \geq e^{t\alpha(A)}, \quad \|A^k\| \geq \rho(A)^k$$

For a simple upper bound using pseudospectra, we have the following theorem. Let Γ_ϵ be the boundary of the ϵ-psuedospectrum for some $\epsilon > 0$, and suppose f is an analytic function on Γ_ϵ and its interior. Then,

$$\|f(A)\| \leq \frac{L_\epsilon}{2\pi\epsilon} \max_{z\in\Gamma} |f(z)| \tag{3.9}$$

where L_ϵ denotes the arc length of Γ_ϵ - this can be shown using the Cauchy integral form of $f(A)$ and the resolvent definition of pseudospectra. Note that this implies that the closure of the ϵ-pseudospectrum is a K-spectral set for $K = L_\epsilon/(2\pi\epsilon)$. For the special cases considered above we also have

$$\|e^{tA}\| \leq \frac{L_\epsilon}{2\pi\epsilon} e^{t\alpha_\epsilon(A)}, \quad \|A^k\| \leq \frac{L_\epsilon}{2\pi\epsilon}\rho_\epsilon(A)^k$$

Different values of ϵ can give better bounds for different t and k. Typically, larger values of ϵ are

better for small t and k, while smaller values are better for larger t and k. In a sense, we can think of pseudospectra as interpolating between the spectrum (which gives asymptotic behavior and corresponds to $\epsilon \to 0$) and the numerical range (which gives a better indication of initial behavior, and corresponds to larger values of ϵ).

3.3 Other K-spectral sets

There are still many other K-spectral sets that can be derived for a given operator A. For example, if Ω is a K-spectral set for B and if $A = f(B)$, then $f(\Omega)$ is a K-spectral set for A. There are also many K-spectral sets with simple geometries. For example, the closed disk $\{z \in \mathbb{C} : |z - \alpha| \leq r\}$ is a 1-spectral set if and only if $\|A - \alpha I\| \leq r$, and any closed half-plane is a 1-spectral set for A if and only if it contains the numerical range $W(A)$ [25]. For matrices with special structure we also obtain simple spectral sets - for example, the unit circle $\mathbb{T}$ is a spectral set for A if and only if A is unitary, and the real axis $\mathbb{R}$ is a spectral set for A if and only if A is Hermitian.

Other K-spectral sets have also been studied beyond simple geometries like disks and half-planes, such as lemniscates [19]. If p is a polynomial with distinct roots with $\|p(A)\| \leq R$ for some $R \geq 0$ and the lemniscate $\{z \in \mathbb{C} : |p(z)| = R\}$ contains no critical points of p, then $\{z \in \mathbb{C} : |p(z)| \leq R\}$ is a K-spectral set for A. Intersections of K-spectral sets can also yield interesting geometries, such as a sector, strip, convex lens, nonconvex lens, or an annulus; these intersections can yield K-spectral sets (though not necessarily with the same constant K) and are investigated by Badea, Beckermann, and Crouzeix in [2]. Still other sets were investigated by considering certain convex sets Ω containing the numerical range $W(A)$ of a given matrix A. Some examples of such sets studied by Beckermann and Crouzeix include when Ω is a convex sector $\mathcal{S}_\alpha = \{z \in \mathbb{C} : z \neq 0,\ |\arg(z)| < \alpha\}$, which is K-spectral with $K = 2 + \frac{2}{\sqrt{3}}$, when the boundary $\partial\Omega$ is a parabola or the branch of a hyperbola ($K = 2 + \frac{2}{\sqrt{3}}$), and when the boundary of Ω is an ellipse with eccentricity $e \leq 1$ ($K = 2 + \frac{2}{\sqrt{4-\epsilon^2}}$) [4].

It would be interesting to continue the investigation of different candidate sets in the complex plane to study $\|f(A)\|$. For instance, one may wish to see how far left can the rightmost part of a 2-spectral set be pushed in order to give bounds on $\|e^{tA}\|$. One could numerically investigate this by starting with a half-plane $\{z :\ \mathrm{Re}(z) \leq c\}$ where c is initially set to be the spectral abscissa, checking to see if the numerical radius of the mapped matrix $\mu(g(A)) \leq 1$ so that $g(A)$ is 2-similar to a contraction, and moving this half-plane to the right until the condition is verified. Alternatively, one can directly check if $\|X^{-1}g(A)X\| \leq 1$ for some X with $\kappa(X) \leq 2$; note that this can hold even if $\mu(g(A)) > 1$.This is just one type of function to investigate using one type of candidate set, so there are definitely opportunities for numerical exploration here.

As a simple example, let us consider a 2×2 upper-triangular matrix A, with real eigenvalues

and complex off-diagonal entry a, i.e.

$$A = \begin{bmatrix} \lambda_1 & a \\ 0 & \lambda_2 \end{bmatrix}, \quad \lambda_1, \lambda_2 \in \mathbb{R}, a \in \mathbb{C}$$

Let us assume that $a \neq 0$ so that $W(A)$ is either an elliptical or circular disk and does not degenerate to a line segment, as in the case of a diagonal 2×2 matrix. Using the ideas sketched above, we can analytically determine a 2-spectral half-plane Π_c for A such that the largest real part of the half-plane is pushed as far left as possible while still satisfying $\mu(g(A)) \leq 1$. The conformal map from a half-plane $\Pi_c = \{z : \text{ Re } (z) < c\}$ to the unit disk is given by $g(z) = (z - c + 1)/(z - c - 1)$, so we compute

$$g(A) = (A - cI + I)(A - cI - I)^{-1} = \begin{bmatrix} \frac{\lambda_1 - c + 1}{\lambda_1 - c - 1} & -\frac{2a}{(\lambda_1 - c - 1)(\lambda_2 - c - 1)} \\ 0 & \frac{\lambda_2 - c + 1}{\lambda_2 - c - 1} \end{bmatrix} = \begin{bmatrix} \mu_1 & b \\ 0 & \mu_2 \end{bmatrix}$$

For a 2×2 matrix, the numerical range is explicitly known, and when the eigenvalues are real, we can easily determine the numerical radius of the mapped matrix $g(A)$. Since the eigenvalues μ_1 and μ_2 of the mapped matrix $g(A)$ are real, we can write the numerical radius in terms of the semi-major axis of the ellipse. If the trace of $g(A)$ is nonnegative, then we have

$$\mu(g(A)) = \frac{\mu_1 + \mu_2}{2} + \frac{1}{2}\sqrt{(\mu_1 - \mu_2)^2 + |b|^2}$$

otherwise,

$$\mu(g(A)) = \frac{1}{2}\sqrt{(\mu_1 - \mu_2)^2 + |b|^2} - \frac{\mu_1 + \mu_2}{2}$$

Focusing on the case where $\text{trace}(g(A)) \geq 0$ and writing $\mu(g(A)) \leq 1$ in terms of λ_1 and λ_2, simplification yields

$$\gamma^2 - \text{trace}(A)\gamma + \det(A) - \frac{|a|^2}{4} \geq 0 \implies \mu(g(A)) \leq 1 \tag{3.10}$$

for $\gamma = 1 + c$. Hence, the farthest left we can push the half-plane Π_c such that it is guaranteed by the condition $\mu(g(A)) \leq 1$ to remain 2-spectral for A is

$$c = -1 + \frac{\text{trace}(A)}{2} + \frac{1}{2}\sqrt{[\text{trace}(A)]^2 - 4\det(A) + |a|^2} \tag{3.11}$$

As a specific example, consider the matrix

$$A = \begin{bmatrix} -1 & 4 \\ 0 & -1 \end{bmatrix} \tag{3.12}$$

The numerical radius of this matrix is $\mu(A) = 1$, so we have $\|e^{tA}\| \leq e^t$ for all $t \geq 0$. Asymptotically, as $t \to \infty$, we know that $\|e^{tA}\|$ decays like te^{-t}. We can use these estimates to give a good indication of initial and asymptotic behavior, but what about for intermediate times t? Does $\|e^{tA}\|$ first grow over several orders of magnitude before starting to decay as the spectrum suggests? For this matrix, the answer is no, and we can find bounds on transient growth using the above analysis. Below is a plot of the region in the eigenvalue plane (λ_1, λ_2) with $a = 4$, $c = 0$ for which the condition $\mu(g(A)) \leq 1$ is satisfied:

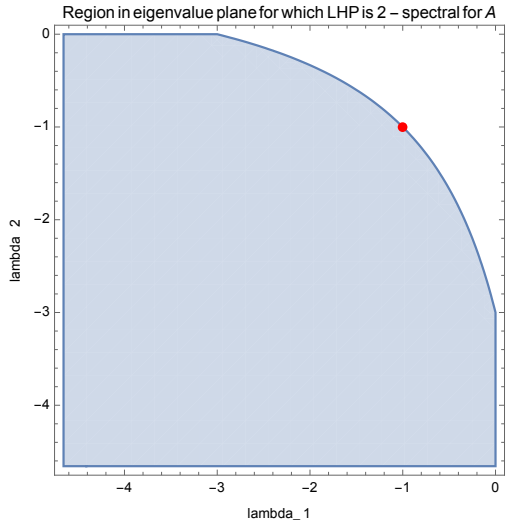
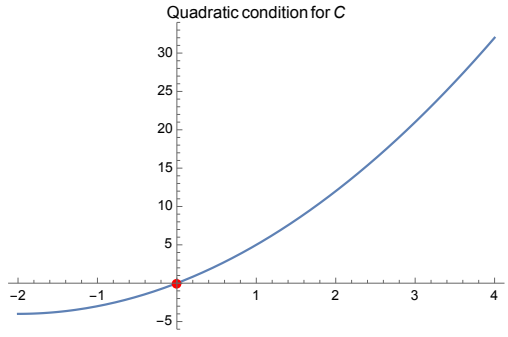


Figure 1: Region in the (λ_1, λ_2)-plane for which the left half-plane Π_0 is a 2-spectral set for A with off-diagonal entry $a = 4$. When $|a| \leq 2$, all values $\lambda_1, \lambda_2 < 0$ work, but for $|a| > 2$, a hyperbola branch forms a boundary in the lower left quadrant of the complex plane.

Notice that the eigenvalue pair corresponding to our choice of A, namely $\lambda_1 = \lambda_2 = -1$, appears on the boundary of the hyperbola branch for which $\mu(g(A)) = 1$. We can also show that for this matrix A, $c = 0$ indeed corresponds to the root of the quadratic in (3.10):



Hence, the left half-plane Π_0 corresponding to $c = 0$ in (3.11) is a 2-spectral set for A and we have

the bound

$$\|e^{tA}\| \leq 2 \quad \forall\, t > 0 \tag{3.13}$$

In my dissertation, I plan to investigate - analytically and numerically - which half-planes are 2-spectral sets for various classes of matrices, i.e. determine matrix properties which ensure that the left-half plane is a 2-spectral set. Other values of K may prove useful as well, and it would be interesting to find other conditions that would ensure that $g(A)$ is K-similar to a contraction for $K \neq 2$, the way $\mu(g(A)) \leq 1$ ensures that $g(A)$ is 2-similar to a contraction.

Another related question of interest is: when is the unit disk $\mathbb{D}$ a 2-spectral (or K-spectral for some moderate size K) set for A. This is important for studying norms of powers of matrices since $\|A^j\| \leq K$ for all $j = 1, 2, \ldots$, if the unit disk is a K-spectral set for A. It is known that any disk containing $W(A)$ is a 2-spectral set for A ([1], [20]), but other disks that do not contain all of $W(A)$ may be 2-spectral sets as well. One approach that can be used numerically, and perhaps analytically, is to determine if A is 2-similar to a contraction.

4 Related Problems

In this section, some problems related to the study of spectral sets and Crouzeix's conjecture are discussed. While the task of estimating $\|f(A)\|$ may seem to lie solely in the realm of numerical linear algebra and functional analysis, there are several interesting connections to problems from disparate fields, such as complex analysis and approximation theory. Here we describe some of the ways that ideas from complex analysis can be applied to the study of spectral sets, as well as some work done related to Crouzeix's conjecture and nonnormal matrices.

One area of complex analysis that has proven fruitful in the study of nonnormal matrices is conformal mapping. Assuming that the interior of the numerical range of a given matrix A is nonempty but not all of $\mathbb{C}$, then the Riemann mapping theorem states that there is a bijective holomorphic mapping from the interior of $W(A)$ to the unit disk $\mathbb{D}$. Furthermore, due to Carathéodory's theorem, this map can be extended continuously to the boundary, yielding a homeomorphism from the closure of the numerical range $\overline{W(A)}$ to the closed unit disk $\overline{\mathbb{D}}$. Hence, we can always transfer the study of functions defined on the numerical range (or, more generally, any simply connected set with nonempty interior that is not all of $\mathbb{C}$) to the unit disk.

There are some simplifications in the study of Crouzeix's conjecture that result from changing from the potentially complicated geometry of $W(A)$ to the unit disk. Suppose first that A is diagonalizable, so that $A = V\Lambda V^{-1}$. Then $f(A) = g(A)$ if and only if $f(\Lambda) = g(\Lambda)$. Given a set S, one can find a function $g \in \mathcal{H}^\infty(S)$ such that $f(\Lambda) = g(\Lambda)$ and $\|g\|_{\mathcal{L}^\infty(S)}$ is minimal, where $\mathcal{H}^\infty(S)$ denotes the space of bounded analytic functions in S. When $S = \mathbb{D}$, this is a Pick-Nevanlinna interpolation problem, and the minimal interpolating function is known to be a scalar multiple of a finite Blaschke product [10]. Hence, by transferring the problem to the unit disk via conformal

mapping, one can then restrict the class of functions to finite Blaschke products. Crouzeix uses this method to study bounds for $\|f(A)\|$ in various convex domains both analytically and numerically [7], [9]. In particular, his arguments in the study of 3×3 matrices involve a computational part [9](see the section on numerical conformal mapping).

Another way in which conformal maps can be used is as an alternative method of testing Crouzeix's conjecture. If one first constructs a bijective conformal map g from $W(A)$ to $\mathcal{D}$, then one can check if

$$\min_{\kappa(X)\leq 2} \|Xg(A)X^{-1}\| \leq 1$$

where $\kappa(X)$ is the condition number of X. Equivalently, one could maximize $\kappa(X)$ subject to the constraint $\|Xg(a)X^{-1}\| \leq 1$ and see if $\kappa(X) \leq 2$. This technique was used by Greenbaum and Choi [6] to show that Crouzeix's conjecture holds for matrices A of the form PD, where P is a permutation matrix and D is diagonal. Additionally, this can be used as a numerical means of verifying Crouzeix's conjecture for a particular matrix A, as one can construct the conformal mapping numerically and use an optimization routine to search for the corresponding similarity transformation.

4.1 Numerical conformal mapping

As noted in the previous section, conformal mapping has played a vital part in various methods of attack for investigating the numerical range and other sets as candidate K-spectral sets. However, aside from simpler geometries, the conformal mapping from a given candidate set S to the unit disk may be too complicated to be useful analytically, and one must construct such a map numerically or approximate it via other means, such as asymptotic expansion. Hence, it is fruitful to look at various ways these conformal maps can be constructed.

One method of constructing conformal maps is via Schwarz-Christoffel mappings, which provide transformations of the upper half-plane or the unit disk onto the interior of a simple polygon. By approximating the numerical range $W(A)$ with a polygon and using a numerical package such as the SC toolbox, developed by Driscoll and Trefethen, one can obtain an approximation to the desired mapping $g(A)$. This method would work best when the sets to be mapped are nearly polygonal, such as for the numerical range of a diagonal matrix. However, in the context of nonnormal matrices, we are mostly interested in sets with more generic geometries. For instance, the boundary of the numerical range $\partial W(A)$ may be some combination of smooth parts and straight line segments, and for most generic matrices the boundary is analytic. Other means of constructing these conformal maps based on integral equations take advantage of this smoothness and yield a more efficient numerical procedure.

In Crouzeix's numerical experiments for 3×3 matrices [9], he employs a modification of Symm's method, which involves solving an integral equation of the first kind to obtain the boundary corre-

spondence function between $\partial W(A)$ and the unit circle. This is done by writing $g(z) = z\exp(u+iv)$, where $u(z)$ and $v(z)$ are harmonic real-valued functions and noting that $u(z) = -\log|z|$ on $\partial W(A)$. Parameterizing the boundary as $\sigma(\theta);\ \theta \in [0, 2\pi]$ and noting that there exists a real-valued density function q such that

$$(u+iv)(z) = \int_0^{2\pi} q(\theta)\log(\sigma(\theta) - z)d\theta, \quad \int_0^{2\pi} q(\theta)d\theta = -1, \tag{4.1}$$

Crouzeix then solves the boundary equation $u = -\log|z|$ by approximating $q(\theta)$ by a degree n trigonometric polynomial and using the trapezoidal rule with $2n+1$ collocation points. So long as the boundary is analytic, this method is very efficient, with super-algebraic convergence due to the trapezoidal rule, though there are some difficulties dealing with non-generic geometries with corners and cusps.

In some of our numerical experiments (see the section on near normal dilations), we employed the approach of Kerman and Trummer [17], who used the Kerzman-Stein integral equation based on the Szegö kernel [16]. This is an integral equation of the second kind, which yields a much better conditioned system of linear equations. The Szegö kernel $S(z,a)$ satisfies the relation

$$g'(z) = \frac{2\pi}{S(a,a)}S^2(z,a), \quad z \in \overline{\Omega}$$

where $g : \Omega \to \mathcal{D}$ is the desired Riemann mapping function with $g(a) = 0$. One can then find $g(z)$ without any integration via

$$R(z) = \frac{T(z)}{i}\frac{g'(z)}{|g'(z)|}, \quad z \in \partial\Omega$$

where $T(z)$ denotes the unit tangent to $\partial\Omega$ at z. To compute $S(z,a)$, Kerzmann and Trummer [17] solve the integral equation

$$f(z) + \int_{w\in\partial\Omega} A(z,w)f(w)d\sigma_w = g(z), \quad z \in \partial\Omega, \tag{4.2}$$

where $f(z) = S(z,a)$, $d\sigma$ denotes arc length on $\partial\Omega$,

$$g(z) = \frac{1}{2\pi i}\frac{\overline{T(z)}}{a-z}, \quad z \in \partial\Omega$$

and

$$A(w,z) = H(z,w) - H(w,z), \quad w \neq z \ (0 \text{ for } w = z)$$

where

$$H(w,z) = \frac{1}{2\pi i}\frac{T(z)}{z-w}$$

This yields a system of linear equations of the form $(I+K)x = y$, where K is skew-hermitian

and $I + K$ is very well-conditioned. The method works surprisingly well even when $\partial\Omega$ contains corners, even though the theory behind the method assumes a smooth boundary [18], [24]. The well-conditioned system of equations to be solved due to the smooth kernel combined with the super-algebraic convergence of the trapezoidal method make this an ideal method for numerically constructing maps from sets with (mostly) smooth boundaries to the unit disk.

4.2 Blaschke products

Here, we briefly describe the use of Blaschke products in studying $\|f(A)\|$. As noted above, we are able to transfer the study of A from the original set Ω containing $\sigma(A)$ to the unit disk $\mathcal{D}$ via a conformal mapping g, either analytically in the case of simple geometries or numerically in more generic cases.

To motivate why Blaschke products are a useful class of functions to look at, we note that we are trying to relate $\|f(A)\|$ to the size of f on a set $\Omega \subset \mathbb{C}$. However, there are infinitely many functions g such that $g(A) = f(A)$, i.e.

$$\tilde{f}(z) = f(z) + \chi(z)h(z),$$

where χ is the minimal polynomial of A and h is analytic. Such a function $\tilde{f}$ will match f at the eigenvalues of A, but will differ on other sets $\Omega \subset \mathbb{C}$. Since we are investigating estimates of the form $\|f(A)\| \leq K \max_{z\in S} |f(z)|$, it is natural to choose $\tilde{f}$ such that the ∞-norm on Ω is minimized. When $\Omega = \mathbb{D}$, this gives rise to a Pick-Nevanlinna interpolation problem. If A is diagonalizable, then the function $\tilde{f}$ is known to be a scalar multiple of a finite Blaschke product and be written as

$$\tilde{f}(z) = \mu \prod_{k=1}^{n-1} \frac{z - \alpha_k}{1 - \overline{\alpha_k} z}, \quad |\alpha_k| < 1 \tag{4.3}$$

$$= \mu \frac{\gamma_0 + \gamma_1 z + \cdots + \gamma_{n-1} z^{n-1}}{\overline{\gamma_{n-1}} + \overline{\gamma_{n-2}} z + \cdots + \overline{\gamma_0} z^{n-1}}, \quad \gamma_{n-1} = 1 \tag{4.4}$$

One can find $\tilde{f}$ and its ∞-norm by solving an eigenvalue problem [10]. This idea also extends to nondiagonalizable matrices, for which the interpolation problem requires that $\tilde{f}$ not only matches f at the eigenvalues, but also the derivatives of order up to $t - 1$ must match those of f at the eigenvalues corresponding to a $t \times t$ Jordan block.

These minimal norm interpolating functions can thus be used to study an equivalent form of Crouzeix's conjecture - for an $n \times n$ matrix A, one can study if $\|B(g(A))\| \leq 2$ for a conformal mapping g from $W(A)$ to $\mathbb{D}$ and for all Blaschke products B of degree at most $n - 1$.

4.3 Near normal dilations of nonnormal matrices

In this section we describe some related work on the numerical construction of near-normal dilations for nonnormal matrices [11]. Let A be a linear operator on a Hilbert space H (e.g. a square matrix corresponding to $\mathbb{C}^n$). A dilation of A is a linear operator M on a larger space $K \supset H$ such that $A = P_H M|_H$, where P_H is the orthogonal projection onto H. If M^k is a dilation of A^k for all $k \in \mathbb{N}^+$, then M is said to be a power dilation of A. These dilations are potentially useful objects in the study of $\|f(A)\|$, since they may have nice properties that A does not have - if A is highly nonnormal, eigenvalues may be misleading for transient behavior of $\|f(A)\|$, but one can construct well-behaved (i.e. near normal) dilations that could be used instead to bound $\|f(A)\|$.

The Sz.-Nagy dilation theorem [22] states that every contraction C has a unitary power dilation U. In order for this to hold for all positive integer powers, an infinite matrix is required; however, one can construct a finite matrix form that is a unitary dilation up to a certain finite power [15]. If A is similar to a contraction via a well-conditioned similarity transformation, then the unitary dilations of C become near normal dilations of A.

To help explain where some of these dilation ideas come from, it is helpful to introduce the notion of a complete K-spectral set and the stronger version of Crouzeix's conjecture. A set $\Omega \subset \mathbb{C}$ is a complete K-spectral set for A if

$$\|P(A)\| \leq K \sup_{z \in \Omega} \|P(z)\| \tag{4.5}$$

for all matrix-valued polynomials P. By this we mean that $P(z)$ is an $\ell \times m$ matrix whose (i,j)-entry is $p_{ij}(z)$ for some polynomial p_{ij}, and $P(A)$ is an $\ell \times m$ array of operators whose (i,j)-block is $p_{ij}(A)$. Crouzeix was able to prove a completely bounded version [8] of his previous result on the numerical range:

$$\|P(A)\| \leq K \sup_{z \in W(A)} \|P(z)\| \tag{4.6}$$

for some K with $2 \leq K \leq 11.08$, for all $\ell \times m$ matrix-valued polynomials P and all positive integers ℓ and m.

Paulsen showed that if the unit disk $\mathbb{D}$ is a complete K-spectral set for A, then A is similar to a contraction via a similarity transformation with condition number K [21] . Assume that the interior of $W(A)$ is nonempty and not all of $\mathbb{C}$ and let g be a Riemann mapping from the interior of $W(A)$ to $\mathbb{D}$, extended continuously to the boundary. From Crouzeix's completely bounded result, $\mathbb{D}$ is a complete K-spectral set for $g(A)$. Thus, from Paulsen's theorem, $g(A) = XCX^{-1}$ with $\|C\| \leq 1$ and $\kappa(X) = K$. Sz.-Nagy's theorem then implies that C has a unitary power dilation U, and $g^{-1}(U)$ is then a normal power dilation of $g^{-1}(C)$ with spectrum around $\partial W(A)$. With an appropriate similarity transformation $S = \mathrm{diag}(\ldots, I, X, I, \ldots)$, $Sg^{-1}(U)S^{-1}$ is a power dilation of A with spectrum around $\partial W(A)$ that is similar to $g^{-1}(U)$ via the similarity transformation S

with condition number K. This means that every linear operator A whose numerical range has nonempty interior and is not all of $\mathbb{C}$ has a near normal power dilation with spectrum around $\partial W(A)$. For finite matrices, we can construct near normal dilations of A (whose powers up to a desired limit are dilations of the corresponding powers of A) with spectrum approximately around $\partial W(A)$, though this is best suited for small matrices due to storage concerns with high dimension and large powers.

Using the ideas above, we can construct near normal dilations M with spectrum on $\partial W(A)$ numerically and compare the behavior of $\|e^{tM}\|$ with $\|e^{tA}\|$. Interestingly, the dilated operator e^{tM} seems to have its own wave-like behavior that eventually dominates the behavior corresponding to the original operator A. In order to more closely match the behavior of the original matrix, one can form other dilations by noting that if M is a power dilation of A, then so is $\tilde{M} = \phi(M)$, where $\phi(z)$ is of the form $z + \chi_A(z)h(z)$, where χ_A is the minimal polynomial of A and h is an analytic function. Via the spectral mapping theorem, $\sigma(\phi(M)) = \phi(\sigma(M))$. Hence, one can try to choose h to minimize the largest real part of $\phi(\partial W(A))$ in order to minimize the spectral abscissa of $\phi(M)$ and obtain bounds for $\|e^{tA}\|$ using $\|e^{t\phi(M)}\|$.

5 Proposed work

The goal of this dissertation is to numerically and analytically investigate sets in the complex plane that can be used as K-spectral sets (in particular, with $K = 2$) for the purpose of estimating norms of functions of matrices. A great deal is known about the traditional spectrum $\sigma(A)$, ϵ-pseudospectrum $\sigma_\epsilon(A)$, and the numerical range $W(A)$. However, other sets in the complex plane may be useful 2-spectral sets in different contexts. For instance, asking how far left can the rightmost part of a 2-spectral be could give better bounds for $\|e^{tA}\|$. Similarly, asking how small can $\sup_{z\in S}|z|$ be made for a 2-spectral set S would be useful for the study of $\|A^k\|$.

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