PSEUDOSPECTRAL RADII OF LARGE SCALE MATRICES

by
Zuhal Demireli

A Thesis Submitted to the
Graduate School of Sciences and Engineering
in Partial Fulfillment of the Requirements for
the Degree of Master of Science

in
Mathematics
Koç University
February 2016

Koç University
Graduate School of Sciences and Engineering

This is to certify that I have examined this copy of a master's thesis
by
Zuhal Demireli

and have found that it is complete and satisfactory in all respects,
and that any and all revisions required by the final
examining committee have been made.

Thesis Committee Members:

Assoc. Prof. Dr. Emre Mengi (Advisor) .....

Assoc. Prof. Dr. Mine Çağlar .....

Assoc. Prof. Dr. Ahmet Duran .....

Date: February 2016

Abstract

The ε-pseudospectral radius of a square matrix A is the maximal modulus attained among the points that belong to its ε-pseudospectrum, the set consisting of the eigenvalues of all matrices within the ε neighborhood of A with respect to the matrix 2-norm. We present a numerical algorithm to estimate this quantity for a large scale matrix, and provide some analysis of it. We tackle the problem by viewing it as a nonsmooth eigenvalue optimization problem, and constructing piecewise quadratic overestimators for the eigenvalue functions. Overall algorithm is an extension of a recent work by Meerbergen, Mengi, Michiels and Van Beeumen, which concerns the ε-pseudospectral abscissa in the more general nonlinear eigenvalue problem setting. The approach presented benefits from a subspace and a restart idea introduced by Kressner and Vandereycken, and Meerbergen et al. in other contexts. We observe convergence to a point with largest modulus locally at a superlinear rate.

Keywords: Optimization, overestimator, pseudospectral radius, piecewise quadratic, restart, subspace methods, singular value, local convergence.

ÖZET

Bir kare matris A için ε yaklaşık spektal yarıçapı, ε yaklaşık spektrumundaki noktalar arasında erişilen en büyük modulüs olarak tanımlı. Burada ε yaklaşık spektrumu, A matrisinin matris 2-normuna göre ε komşuluğunda bulunan matrislerin özdeğerlerinden oluşan küme. Bu çalışmada ε yaklaşık yarıçapının hesabı için sayısal bir yöntem sunuyoruz, ve yöntemi bir miktar analiz ediyoruz. Problemi her yerde türevlenemeyen bir özdeğer optimizasyonu problemi olarak ele alıyoruz, çözümü için özdeğer fonksiyonlarının üzerinde yatan kuadratik fonksiyonlar oluşturuyoruz. Yöntem yakın zamanda Meerbergen, Mengi, Michiels ve Van Beeumen tarafından ε yaklaşık spektral absisa hesabı için önerilen yaklaşımın adapte edilmiş hali. Kressner ve Vandereycken tarafından ortaya sürülen bir alt uzay fikrinden, ve Meerbergen vd. tarafından önerilen alt uzayı yeniden başlatma fikrinden faydalanıyoruz. Yerel olarak en büyük modulüse sahip bir noktaya süper lineer bir hızla yakınsama gözlemliyoruz.

Acknowledgement

Without the support,patience and guidance of the following people and foundations,this thesis would not have been completed.
Firstly, I would like to thank my advisor Dr. Emre Mengi for his patience, guidance and criticism throughout this process.
I express special thanks to the committee members, Dr. Mine Çağlar and Dr. Ahmet Duran for their careful reading.
I would like to thank Koç University and TÜBİTAK for their financial supports.
I owe my thanks to my father Zeki Demireli whose love and patience are always with me during my life. I also thank to my sisters Melike and Sara.I could not carry on writing this thesis without their sisterly love.
Finally, I want to express my deepest gratitudes to my fellow Gamze Kuruk whose real support is unforgettable since our first acquaintance at Yeditepe University.

LIST OF SYMBOLS/ABBREVIATIONS

$\mathbb{R}$	real numbers
$\mathbb{C}$	complex numbers
$\mathbb{Z}$	integers
$\mathbb{R}^+$	nonnegative real numbers
$\mathbb{C}^+$	complex numbers with nonnegative real parts
$\mathbb{C}^n$	vectors of complex numbers of size n
$\mathbb{R}^n$	vectors of real numbers of size n
$\mathbb{R}^n_-$	vectors of nonnegative real numbers of size n
$\mathbb{C}^{n\times m}$	complex $n \times m$ matrices
$\mathbb{R}^{n\times m}$	real $n \times m$ matrices
$H(A)$	Hermitian part $\left(\frac{A+A^*}{2}\right)$ of the matrix A
$N(A)$	skew-Hermitian part $\left(\frac{2A-A^*}{2}\right)$ of the matrix A
$\det(A)$	determinant of the matrix A
$\|A\|$	2-norm of the matrix A
$\Lambda(A)$	spectrum of the matrix A
$\Lambda_\varepsilon(A)$	ε-pseudospectrum of the matrix A
$\sigma(A)$	set of singular values of the matrix A
$\lambda_{max}(A)$	largest eigenvalue of the matrix A
$\lambda_{min}(A)$	smallest eigenvalue of the matrix A
$\lambda_j(A)$	jth largest eigenvalue of a Hermitian matrix A
$\sigma_{min}(A)$	minimum singular value of the matrix A
$\alpha(A)$	spectral abscissa of the matrix A
$\rho(A)$	spectral radius of the matrix A
$\alpha_\varepsilon(A)$	ε-pseudospectral abscissa of the matrix A
$\rho_\varepsilon(A)$	ε- pseudospectral radius of the matrix A
$\Re z$	real part of the complex number z
$\Im z$	imaginary part of the complex number z
$\|z\|$	modulus of the complex number z
$A \otimes B$	Kronecker product of the matrices A and B
I	identity matrix

SPECIAL CLASS OF MATRICES

Symmetric matrix	$A^T = A$
Hermitian matrix	$A^* = A$
Normal matrix	$A^*A = AA^*$
Unitary matrix	$Q \in \mathbb{C}^{n\times n}$ and $Q^*Q = I$

Contents

List of Figures

List of Tables

Chapter 1

INTRODUCTION

This thesis work concerns the computation of an outermost point in the subset of the complex plane commonly referred as the ε-pseudospectrum for a given square matrix and for a given real number $\varepsilon > 0$. Formally, the ε-pseudospectrum of a square matrix A is the set consisting of the eigenvalues of all matrices within the ε neighborhood of the matrix A with respect to the matrix 2-norm, and the main theme of this thesis is the ε-pseudospectral radius of A, the modulus of an outermost point in the ε-pseudospectrum of A. This set and its outermost points are computationally difficult objects because of their nonconvex and nonsmooth nature. In this chapter, we first summarize the background, and give basic definitions. This is followed by a motivation for why this set has drawn considerable attention for the last twenty years, a discussion of what is the significance of their outermost points, and a literature survey. The outline of this thesis work is provided at the end of the chapter.

1.1 Background

1.1.1 Eigenvalue problem

Eigenvalues are precious tools in mathematics and various engineering disciplines. For instance they play a prominent role in the analysis of vibrations, and when analyzing the stability of certain dynamical systems. For a given matrix $A \in \mathbb{C}^{n\times n}$, we call a scalar

$\lambda \in \mathbb{C}$ an eigenvalue of A if

$$Ax = \lambda I \tag{1.1.1}$$

holds for some nonzero $x \in \mathbb{C}^n$, which is referred as an eigenvector associated with λ. Eigenvalues of A correspond to the roots of the characteristic polynomial $p_A(\lambda) = \det(A - \lambda I)$. In other words, λ is an eigenvalue of A if and only if $\det(A - \lambda I) = 0$. Therefore, there are exactly n eigenvalue of A counting the multiplicities.

Definition 1.1.1 (Spectrum [26]). *The set of eigenvalues of $A \in M_n$ is called the spectrum of A, and is denoted by $\Lambda(A)$, that is*

$$\Lambda(A) := \{\lambda \in \mathbb{C} : det(A - \lambda I) = 0\}. \tag{1.1.2}$$

Definition 1.1.2 (Eigenspace [26]). *The set of all vectors satisfying $Ax = \lambda x$ is called the eigenspace of A corresponding to the eigenvalue λ. Every nonzero element of this eigenspace is an eigenvector of A corresponding to λ.*

Definition 1.1.3 (Geometric and Algebraic Multiplicities [10]). *The dimension of the eigenspace of $A \in \mathbb{C}^{n\times n}$ corresponding to the eigenvalue λ is called the geometric multiplicity of the eigenvalue λ. On the other hand, the multiplicity of λ as a zero of the characteristic polynomial $p_A(\lambda)$ is called the algebraic multiplicity of the eigenvalue λ.*

1.1.2 Asymptotic stability of linear autonomous systems

Various engineering applications, for instance mechanical vibrations, electrical networks, lead to eigenvalue problems. Eigenvalues are also closely to related to the stability of dynamical systems. Our work here specifically concerns the stability of linear time-invariant dynamical systems., which arise in fields such as signal processing and communications. In a broad sense, they are classified into *continuous time* and *discrete time* linear time-invariant dynamical systems.

A continuous linear time-invariant dynamical system has the form

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{1.1.3}$$

where $t \in \mathbb{R}$ denotes the time, $x : \mathbb{R} \to \mathbb{R}^n$ is the state function, $u : \mathbb{R} \to \mathbb{R}^m$, $y : \mathbb{R} \to \mathbb{R}^p$ are the input and output functions, respectively. The matrices $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$ and $D \in \mathbb{R}^{p\times m}$ are given and do not vary in time. The dynamical system above with no input and output, that is $x'(t) = Ax(t)$, is called *autonomous*. The autonomous dynamical system $\dot{x} = Ax$ is asymptotically stable, if solutions $x(t)$ tend to zero as t approaches infinity for any initial condition $x(0)$. It is well known that this definition of asymptotic stability is equivalent to the inclusion of all eigenvalues of A on the left half of the complex plane. For an asymptotically stable system, the rate at which the solution decays to zero depends the *spectral abscissa* of A defined by

$$\alpha(A) := \max\{\Re\lambda : \lambda \in \Lambda(A)\}. \tag{1.1.4}$$

Thus the system is asymptotically stable if and only if $\alpha(A) < 0$. Moreover, for a stable system, the smaller values of $\alpha(A)$ gives rise to systems decaying to zero more rapidly.

On the other side, a discrete-time linear dynamical system has the form

$$\begin{aligned} x^{(k+1)} &= Ax^{(k)} + Bu^{(k)} \\ y^{(k)} &= Cx^{(k)} + Du^{(k)}. \end{aligned} \tag{1.1.5}$$

The matrices A, B, C, D are as before with real entires, and of size $n \times n$, $n \times m$, $p \times n$ and $p \times m$, respectively. Above, $\{x^{(k)}\}, \{u^{(k)}\}, \{y^{(k)}\}$ denote the state, input and output sequences in $\mathbb{R}^n, \mathbb{R}^m, \mathbb{R}^p$, respectively. This system without any input and output simplifies to the autonomous discrete system $x^{(k+1)} = Ax^{(k)}$. It is called stable if $x^{(k)} \to 0$ as $k \to \infty$ for all $x^{(0)}$, and this is equivalent to the strict inclusion of all eigenvalues of A inside the unit circle. For an asymptotically stable system, the decay rate to zero is

determined by the *spectral radius* of A given by

$$\rho(A) := \max\{|\lambda| : \lambda \in \Lambda(A)\}. \tag{1.1.6}$$

Clearly, a system is asymptotically stable if and only if $\rho(A) < 1$, and the smaller $\rho(A)$ is, the faster the system decays to zero.

1.1.3 Polar and singular value decomposition

A fundamental matrix decomposition that plays a key role throughout this thesis work is the singular value decomposition. Recall that an orthogonal eigenvalue decomposition exists only for normal matrices. An eigenvalue decomposition exists only for matrices with a complete set of linearly independent eigenvectors spanning the whole space. A Jordan factorization always exists, but cannot be computed accurately in the presence of the rounding errors. In contrast to all these decompositions that reveal eigenvalues, the singular value decomposition always exists and can be computed reliably even in the presence of rounding errors. It is closely related to the polar decomposition, which enjoys the same nice properties.

Recall that a Hermitian matrix A is called positive semidefinite if and only if $v^*Av \geq 0$ for all $v \in \mathbb{C}^n$.

Theorem 1.1.4 ([15]). *A Hermitian matrix $A \in \mathbb{C}^{n\times n}$ is positive semidefinite if and only if it has a positive semidefinite square root A_0 such that $A = A_0^2$. Moreover* $\operatorname{rank}(A_0) = \operatorname{rank}(A)$.

Any complex number $z \in \mathbb{C}$ has the polar representation $z = re^{i\theta}$ where r is a nonnegative real number and $e^{i\theta}$ for some $\theta \in [0, 2\pi)$ has unit modulus. Polar decomposition, whose existence is asserted by the next theorem proven in [15], is a generalization of this polar representation for matrices.

Theorem 1.1.5 ([15]). *Any matrix $A \in \mathbb{C}^{n\times n}$ can be represented of the form*

$$A = HU \tag{1.1.7}$$

where H is positive semidefinite and U is unitary. Moreover, the matrix H in Equation 1.1.7 is unique and given by $H = (AA^*)^{\frac{1}{2}}$

The existence of the singular value decomposition stated below is immediate from the polar decomposition by exploiting the orthogonal eigenvalue decomposition $H = Q\Sigma Q^*$ where H is as in (1.1.7), that is as in the polar decomposition of A. We remark that the middle diagonal factor Σ consists of nonnegative eigenvalues along its diagonal, since H is positive semidefinite.

Theorem 1.1.6 ([31]). *A matrix $A \in \mathbb{C}^{m\times n}$ can be represented of the form*

$$A = U\Sigma V^*$$

where $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ are unitary and $\Sigma \in \mathbb{R}^{m\times n}$ is diagonal with nonnegative entries along its diagonal.

The theorem above also establishes the existence of the singular values and singular vectors of A defined below.

Definition 1.1.7 ([31]). *For a matrix $A \in \mathbb{C}^{n\times m}$, a nonnegative scalar σ is called a singular value of A, if there exist vectors $u \in \mathbb{C}^m$ and $v \in \mathbb{C}^n$ such that $\|u\|_2 = \|v\|_2$ and*

$$Av = \sigma u \ \text{ and } \ u^*A = \sigma v^* \tag{1.1.8}$$

The vectors u, v are called the left and right singular vector corresponding to σ respectively.

Let us consider the singular value decomposition $A = U\Sigma V^*$. This can be rearranged as follows:

$$AV = U\Sigma \ \text{ and } \ U^*A = \Sigma V^*.$$

Moreover, let us denote the diagonal entry of Σ at position (j, j) by σ_j, the jth columns of U and V by u_j and v_j, respectively. It follows that, for each $j = 1, \ldots, \min(m, n)$, we

have

$$Av_j = \sigma_j u_j \text{ and } u_j^* A = \sigma_j v_j^*.$$

Thus, σ_j is a singular value of A, and u_j, v_j consist of a pair of unit left, unit right singular vectors corresponding to this singular value.

Since U, V are unitary matrices, the matrices A and Σ have the same rank. In particular, the rank of A is given by the number of nonzero singular values of A. Thus for a rank k matrix A, we have $\Sigma = \text{diag}(\sigma_1, ..., \sigma_k, 0, ..., 0)$, where $\sigma_1, \ldots, \sigma_k > 0$. The matrix A can be decomposed into a sum of k rank one matrices:

$$A = \sum_{j=1}^{k} \sigma_j u_j v_j^*.$$

Now, for any r such that $0 < r < k$, we have

$$\Delta A_* = \sum_{j=r+1}^{k} -\sigma_j u_j v_j^* \tag{1.1.9}$$

satisfying the properties

- $\text{rank}(A + \Delta A_*) = r$
- $\|\Delta A_*\| = \sigma_{r+1}(A)$

In the next result and throughout the rest of this text, $\sigma_j(A)$ denotes the jth largest singular value of A. The following theorem has various applications in control theory, signal processing, image processing, and will also be frequently used throughout this work.

Theorem 1.1.8 (Eckart-Young [31])**.** *Let $A = U\Sigma V^* = U\,diag(\sigma_1, ..., \sigma_k, 0, ..., 0)V^* \in \mathbb{C}^{m\times n}$ be a singular value decomposition. Then for any integer r with $0 < r < k$, we have*

$$\beta_r(A) := \min\{\|\Delta A\|_2 \mid \text{rank}(A + \Delta A) \leq r\} = \|\Delta A_*\|_2 = \sigma_{r+1}(A),$$

where ΔA_* is as in (1.1.9).

For an $n \times n$ non-singular matrix A, the distance $\beta_{n-1}(A)$ corresponds to the distance to a nearest singular matrix from A with respect to the matrix 2-norm. An application of the Eckart-Young theorem above leads to $\beta_{n-1}(A) = \sigma_{min}(A)$. This will be exploited in the next section.

Next we remind the relation between the singular values of a rectangular $m \times n$ matrix A and the eigenvalues of certain square matrices. First, let us suppose that $m \geq n$. Since the matrix A^*A is positive semidefinite, by Theorem 1.1.4, it has a positive semidefinite square root A_0 such that $(A^*A)^{\frac{1}{2}} = A_0$. It is straightforward to verify that

$$\sigma_j(A) = \lambda_j((A^*A)^{\frac{1}{2}})$$

for $j = 1, \ldots, n$, where $\lambda_j(\cdot)$ denotes the jth largest eigenvalue of its matrix argument. Similarly, when $m < n$, we have

$$\sigma_j(A) = \lambda_j((AA^*)^{\frac{1}{2}})$$

for $j = 1, \ldots, m$. Alternatively, given the singular value decomposition $A = U\Sigma V^*$, observe that

$$\underbrace{\begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix}}_{\mathcal{H}} = \begin{bmatrix} V & V \\ U & -U \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & -\Sigma \end{bmatrix} \begin{bmatrix} V & V \\ U & -U \end{bmatrix}^*,$$

which is an orthogonal eigenvalue decomposition of $\mathcal{H}$. Hence, the largest $\min(m, n)$ eigenvalues of $\mathcal{H}$ are the singular values of A. The next result is immediate from the definition of the singular value decomposition, and an important tool in the computation of the singular values.

Proposition 1.1.9 ([10]). *The singular values of a square matrix are invariant under unitary transformation.*

Our work heavily relies on the analyticity of the singular values of a matrix-valued

functions depending on one parameter analytically. The classical results in this direction are presented next.

Theorem 1.1.10 (Rellich [25]). *An analytical Hermitian matrix-valued function* $A(t) : \mathbb{R} \to \mathbb{C}^{n\times n}$ *has a decomposition of the form*

$$A(t) = Q(t)\Lambda(t)Q(t)^*$$

where $Q(t) : \mathbb{R} \to \mathbb{C}^{n\times n}$ *is a unitary analytical matrix-valued function and* $\Lambda(t) : \mathbb{R} \to \mathbb{C}^{n\times n}$ *is a diagonal analytical matrix-valued function.*

An applications of the theorem above to $\begin{bmatrix} 0 & A(t) \\ A(t)^* & 0 \end{bmatrix}$, where $A(t) : \mathbb{R} \to \mathbb{C}^{m\times n}$ depends on its parameter analytically, yields the following result.

Theorem 1.1.11 ([31]). *Consider an analytical matrix-valued function* $A(t) : \mathbb{R} \to \mathbb{C}^{m\times n}$. *There exists a decompostion*

$$A(t) = U(t)\Sigma(t)V(t)^* \tag{1.1.10}$$

where $U(t), V(t) : \mathbb{R} \to \mathbb{C}^{n\times n}$ *are unitary analytical matrix-valued functions, and* $\Sigma(t) : \mathbb{R} \to \mathbb{C}^{m\times n}$ *is a diagonal analytical matrix-valued function.*

Referring to the last theorem, we denote the diagonal entries of $\Sigma(t)$ by $\sigma_j(t)$ for $j = 1, \ldots, \min(m, n)$ and call these analytical singular value functions of $A(t)$. The following expressions for their derivatives are derived in [14]:

$$\frac{d\sigma_i(t)}{dt} = \Re\left(u_j(t)\frac{dA(t)}{dt}v_j(t)\right).$$

Here $u_j(t), v_j(t)$ denote the jth columns of $U(t)$ and $V(t)$ as in (1.1.10) satisfying

$$A(t)v_j(t) = \sigma_j(t)u_j(t) \text{ and } u_j^*(t)A(t) = \sigma_j(t)v_j^*(t)$$

for $j = 1, \ldots, n$.

1.1.4 Pseudospectra

The ε-pseudospectrum of a matrix A is the subset of the complex plane consisting of the eigenvalues of all matrices that are at a distance of ε or closer to A. This set is related to the sensitivity of the eigenvalues of A. One measure for the sensitivity of an eigenvalue is its (absolute) condition number whose definition is given below.

Definition 1.1.12 ([34]). *Let λ be a simple eigenvalue of $A \in \mathbb{C}^{n\times n}$. The relative condition κ of this eigenvalue is defined by*

$$\kappa := \lim_{\delta\to 0^+} \sup_{\|\delta A\|_2\leq\delta} \frac{|\lambda(A+\delta A)-\lambda|}{\|\delta A\|_2}$$

where $\lambda(A+\delta A)$ denotes the eigenvalue of $A+\delta A$ corresponding to the eigenvalue λ of A (i.e., $\lambda(A+\delta A)=\lambda(1)$, where $\lambda(t)$ is the continuous function corresponding to an eigenvalue of $A+t\delta A$ such that $\lambda(0)=\lambda$).

The condition number defined above solely depends on the angle between the unit left and unit right eigenvectors corresponding to the simple eigenvalue. This is formally stated below.

Theorem 1.1.13 ([34]). *Let λ be a simple eigenvalue of $A \in \mathbb{C}^{n\times n}$, and x, y be unit right and unit left eigenvectors, respectively, corresponding to λ. We have*

$$\kappa = \frac{1}{y^*x}$$

Unlike a condition number which measures only the worst case sensitivity in a particular direction, the ϵ-pseudospectrum reveals the sensitivity in all directions. But it comes with the disadvantage of being computationally expensive. Its popularity since 1990s has been driven by its connection with the transient behavior of the autonomous systems $x'(t)=Ax(t)$ and $x_{k+1}=Ax_k$, as well as its usefulness to ensure stability in a robust sense. The comprehensive literature about the subject is available in [32]. A formal definition of this set is given next.

Definition 1.1.14 ([9]). *Let $A \in \mathbb{C}^{n\times n}$. For $\varepsilon > 0$ the ε-pseudospectrum of A is the set*

$$\Lambda_\varepsilon(A) := \{z \in \Lambda(B) \ : \ B \in \mathbb{C}^{n\times n} \quad \text{such that} \quad \|A - B\|_2 \leq \varepsilon\}$$

This set can be characterized in terms of the singular values due to the following observation.

Lemma 1.1.15 ([35, 32]). *Let $A \in \mathbb{C}^{n\times n}$ be a given matrix, $z \in \mathbb{C}$ be a given complex number, and let $\varepsilon = \sigma_{min}(A - zI)$. Furthermore, let us denote a consistent pair of unit left and right singular vectors associated with $\sigma_{min}(A-zI)$ by u and v. The perturbation $\delta A := -\varepsilon uv^*$ satisfies*

$$(A + \delta A - zI)v = 0, \qquad u^*(A + \delta A - zI) = 0. \tag{1.1.11}$$

Thus, z is an eigenvalue of $A + \delta A$ with the corresponding left and right eigenvectors u and v, respectively.

An implication of the theorem above is that if $\sigma_{\min}(A - zI) \leq \varepsilon$, then $z \in \Lambda_\varepsilon(A)$. The converse also holds due to the Eckart-Young theorem, that is $z \in \Lambda_\varepsilon(A)$ means $(A + \delta A - zI)$ is singular for some δA such that $\|\delta A\|_2 \leq \varepsilon$ thus we have $\sigma_{min}(A - zI) \leq \|\delta A\|_2 \leq \varepsilon$ by the Eckart Young theorem. This leads us to the following result.

Theorem 1.1.16 ([22]). *Let $A \in \mathbb{C}^{n\times n}$ and $\varepsilon > 0$. We have*

$$\Lambda_\varepsilon(A) = \{z \in \mathbb{C} \ : \ \sigma_{min}(A - zI) \leq \varepsilon\}, \tag{1.1.12}$$

or equivalently

$$\Lambda_\varepsilon(A) = \{z \in \mathbb{C} \ : \ \|(A - zI)^{-1}\| \geq \varepsilon^{-1}\}.$$

The second characterization in the theorem above is in terms of $\|(A-zI)^{-1}\|_2$, which is commonly referred as the residual norm. It clearly blows up as $z \in \mathbb{C}$ approaches an

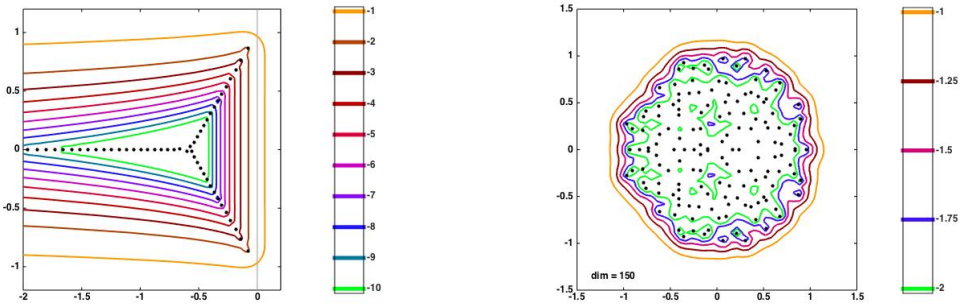


Figure 1.1: The ϵ-pseudospectrum for various ε for the 'airy' matrix on the left, and for a 'random' matrix on the right.

eigenvalue of a matrix A, so choosing smaller values of ε limits the set to points closer to these points of singularity. We denote the boundary of $\Lambda_\varepsilon(A)$ by $\partial\Lambda_\varepsilon(A)$. Thus

$$\partial\Lambda_\varepsilon(A) = \{z \in \mathbb{C} \ : \ \sigma_{min}(A - zI) = \varepsilon\}.$$

The ε-pseudospectrum of two particular matrices are illustrated in Figure 1.1 for $\varepsilon = 10^j, j = -10, -9, ... - 1$. This figure is generated by the Matlab toolbox Eigtool [37]. The solid dots correspond to the eigenvalues of the matrices. The color bars on the right-hand side represent the values of ε in logarithmic scale. On the left-hand side, the imaginary axis is marked with a gray line. Perturbations on the order of 10^{-1} causes the associated continuous time autonomous system to be unstable, even though the original system is stable. This left-hand plot corresponds to the pseudospectra of the **airy** matrix with dimension $n = 200$, for which the 2-norm of the smallest perturbation that makes the system unstable is $\varepsilon = 10^{-1.3}$. On the left-hand figure the ε pseudospectrum is connected for each value of ε, however this is not the general case as can be observed on the right-hand figure. This right-hand figure represents the pseudospectra of a **random** matrix of size 150.

1.2 History and motivation

According to [30], the ε-pseudospectrum is first mentioned by Landau in [17]. Kostin and Razzakov has provided a hand-drawn plot of a pseudospectrum in [12]. A computer-generated plot of a pseudospectrum has first appeared in [7]. Progresses in computer technology has eventually made plots of pseudospectra for large scale matrices possible. In [28], Nick Trefethen has given the illustrations of the pseudopectra of thirteen non-normal matrices. Various researchers has contributed to the topic of pseudospectra since then.

It is well known that eigenvalues are fundamental in natural phenomena such as resonance and stability. For instance, eigenvalues play a large role in whether an automobile's break system is too noisy or not, in whether a building collapses or stands in an earthquake [30]. But the eigenvalues of a matrix A by themselves often do not address issues such as what happens to the autonomous systems $x'(t) = Ax(t)$ or $x^{(k+1)} = Ax^{(k)}$ initially, excluding the special family of normal matrices. The theorem below demonstrates the well-behaved nature of normal matrices.

Theorem 1.2.1 (Spectral theorem for normal matrices [10])**.** *Let $A \in \mathbb{C}^{n\times n}$ have the eigenvalues $\lambda_1, ..., \lambda_n$. The following statements are equivalent:*

(a) A is normal;

(b) A is unitarily diagonalizable;

(c) $\sum_{i=1}^{n}\sum_{j=1}^{n} |a_{ij}|^2 = \sum_{j=1}^{n} |\lambda_j|^2$;

(d) There is an orthonormal set consisting of n eigenvectors of A.

We give the definition of the spectral radius of a discrete-time dynamical system in Section 1.1.2 verbally. We redefine spectral radius in the usual form, Denoting the eigenvalues of the matrix A by $\lambda_1, ..., \lambda_n$, its spectral radius $\rho(A)$ is defined by

$$\rho(A) = \max\{|\lambda_j| \mid j = 1, \ldots, n\}$$

The spectral radius of A is closely related to the convergence of the power sequence $\{A^k\}$, equivalently the asymptotic stability of the dynamical system $x^{(k+1)} = Ax^{(k)}$. The following theorems are remarkable in this direction.

Theorem 1.2.2 ([26]). *Let $A \in \mathbb{C}^{n\times n}$. We have $\rho(A) < 1$ if and only if*

$$\lim_{k\to\infty} A^k = 0.$$

Theorem 1.2.3 (Gelfand's Formula, 1941 [26]). *For any matrix norm $\|.\|$, we have*

$$\rho(A) = \lim_{k\to\infty} \|A^k\|^{\frac{1}{k}}.$$

An extension of Theorem 1.2.2 is that if $\rho(A) > 1$, $\|A^k\|$ is not bounded as $k \to \infty$. For a normal matrix, more can be said beyond these asymptotic stability results, in particular what happens to $\|A^k\|$ initially for small k. For instance, by the orthogonality of the eigenvectors of a matrix A that is normal, it can be deduced that $\|A^k\| \leq \rho(A)^k$. Unfortunately, such results concerning the transient behavior does not extend to non-normal matrices. This remarkable difference between normal and nonnormal matrices is also apparent from pseudospectra. If A is normal $\Lambda_\varepsilon(A)$ is just the ε perturbation of the spectrum $\Lambda(A)$, it can indeed be shown that as in [9]

$$\Lambda_\varepsilon(A) \;=\; \Lambda(A) + \varepsilon.$$

This is no more true, if A is far from being normal. In the nonnormal case, when we perturb the nonnormal matrix by an amount of nor ε, the eigenvalues may exhibit changes much larger than ε.

The ε-pseudospectral abscissa and pseudospectral radius are defined by

$$\alpha_\varepsilon(A) := \max\{\Re(z) \;:\; z \in \Lambda_\varepsilon(A)\} \quad \text{and} \quad \rho_\varepsilon(A) := \max\{|z| \;:\; z \in \Lambda_\varepsilon(A)\},$$

respectively, and are indicators of the transient behaviors of the autonomous systems

$x'(t) = Ax(t)$ and $x^{(k+1)} = Ax^{(k)}$, respectively. In other words, the norms $\|x(t)\|$ and $\|x^{(k)}\|$ can be bounded for small t and k by means of the quantities $\alpha_\varepsilon(A)$ and $\rho_\varepsilon(A)$, respectively, thanks to the Kreiss matrix theorem (see for instance Chapter 18 of [32]). Beyond the transient behavior interpretation, these quantities also measure robust stability. For instance $\rho_\varepsilon(A) < 1$ ensures that not only the system $x^{(k+1)} = Ax^{(k)}$ itself is stable, but it remains stable under all perturbations of A of 2-norm bounded by ε.

1.2.1 Literature

The algorithms for the computation of these pseudospectral measures are inspired by the Byers' algorithm [6] for the distance to instability from a given square matrix, and its quadratically convergent variant by Boyd and Balakrishnan [2] as well as Bruinsma and Steinbuch [3]. These are all level-set approaches tailored around the idea of determining the level sets of the singular value function by solving eigenvalue problems of size twice the size of the original matrix. Burke-Lewis-Owerton has provided the first globally convergent algorithm for the computation of the ε-pseudospectral abscissa of a matrix [5]. This is based on determining the intersection points of the ε-pseudospectrum with given horizontal lines and vertical lines repeatedly, hence called the "criss-cross" algorithm. This algorithm is later extended for the computation of the ε-pseudospectral radius by Mengi and Overton ([19]). It performs radial and circular searches instead of vertical and horizontal searches.

The algorithms [5, 19] are not meant for matrices beyond medium scale. In [9] an algorithm is presented for the computation of the pseduspectral abscissa and radius of large-scale matrices. The suggested approach is a fixed-point iteration based on determining the rightmost eigenvalues of certain rank one perturbations of the large scale matrix repeatedly. More recently an approach for the computation of the pseudospectral abscissa of a large scale nonlinear eigenvalue problem is suggested in [18]. This approach benefits from global overestimators and underestimators introduced in [20, 33] for eigenvalue functions. Additionally, it reduces the sizes of the matrix-valued functions by restricting their domain to small subspaces, gradually expanding these subspaces, and

occasionally restarting subspaces from scratch. The subspace idea in [18] is inherited from [13].

1.3 Outline

The algorithm proposed in this thesis work is modified from the framework in [18] for the computation of the pseudospectral radius of a large scale matrix. We present it in the following order. In Section 2.1, we start with a technique that is based on global overestimators and that solves the following constrained problem locally.

$$\max_{w\in\mathbb{R}^2} \quad c^T w \quad \text{subject to} \quad \lambda(w) := \lambda_{min}(A(w)) \leq 0$$

Above, $c = (1, 0)$ and $A(w) := A - w_1 e^{iw_2} I$. The approach replaces the eigenvalue function $\lambda_{min}(A(w))$ with a quadratic function $q(\omega)$ that bounds $\lambda_{min}(A(w))$ from above globally, and solves the resulting convex and smooth optimization problem. It uses the optimal solution of this convex problem to refine the quadratic function $q(\omega)$, and repeats the procedure. The use of global overestimators or underestimators dates back to Piyavskii [24] and Shubert [27] for the optimization of Lipschitz continuous functions. More efficient and sophisticated variants are later proposed by Breiman and Cutler [1]. This suggested approach converges to a locally outermost point z_* only, i.e., a point z_* which has a neighborhood $\mathcal{N}$ such that z_* has the largest modulus among all points in$\Lambda_\varepsilon \cap \mathcal{N}$.

We perform angular searches to check whether the converged z_* is indeed a globally outermost point. Letting $r_* := |z_*|$, we solve the unconstrained optimization problem

$$\min_{\theta\in[0,2\pi)} \sigma_{min}(A - r_* e^{i\theta})$$

by constructing global underestimators for the singular value function $\sigma(\theta) = \sigma_{min}(A - r_* e^{i\theta})$ repeatedly and minimizing the underestimator function instead of the singular value function. The global minimizer of this problem is then used to refine the under-

estimator. The ideas here are borrowed from [20]. If the globally smallest value of this optimization problem is ε, then z_* corresponds to a point in the ε-pseudospectral radius that is globally outermost. Thus its modulus yields the ε-pseudospectral radius. Otherwise, the global minimizer z_{**} of the unconstrained minimization problem is a point strictly inside the ε-pseudospectral radius. We repeat the algorithm in the previous paragraph yielding a locally rightmost point starting from z_{**}. The details of the angular search are described in Section 2.2.

To deal with large scale matrices we also incorporate a subspace idea into our approach. Instead of computing a locally outermost point of the ε-pseudospectrum of the $n \times n$ matrix A, we compute a locally outermost point of ε-pseudospectrum of AW where W is a $n \times k$ rectangular matrix with orthonormal columns such that $n \gg k$. In other words, we restrict the domain of the linear map $v \to Av$ to $\mathrm{Col}(W)$. This results in substantial efficiency in singular value computation, hence in the computation of the outermost point in the ε-pseudospectrum. The subspace $\mathrm{Col}(W)$ is gradually expanded benefitting from the locally outermost point in the ε-pseudospectrum of AW. Some details of this subspace approach are spelled out in Section 2.3. When the subspace dimension reaches a prescribed amount, we restart keeping only the recently added directions and erasing old directions. This restart strategy is described, and the overall algorithm is presented in Section 2.4.

Finally, in Chapter 3, we provide numerical experiment results on dense and large sparse matrices taken from EigTool [37]. The results of the algorithm discussed here are compared with the results of the algorithm due to Guglielmi and Overton [9], as well as the algorithm due to Mengi and Overton [19].

Chapter 2

COMPUTATION OF THE PSEUDOSPECTRAL RADIUS

The ε-pseudospectral radius of a matrix A is defined as the modulus of the outermost point in its ε-pseudospectrum for a given value of ε. This quantity is motivated by its relevance to the transient behavior of $x_k = Ax_{k-1}$. In particular, it is possible to deduce tight lower and upper bounds for $\sup_{k\in\mathbb{Z}^+} \|x_k\|_2$ using this quantity.

2.1 Local convergence by radial search

The ε-pseudospectral radius of the matrix A can be posed as the optimization problem

$$\begin{aligned} &\text{maximize} && |z| \\ &\text{subject to} && \sigma_{min}(\widetilde{F}(z)) \leq \varepsilon \end{aligned}$$

where $\widetilde{F}(z) := zI - A$. Using the fact that the singular values of a matrix A is the positive square roots of the eigenvalues of A^*A, this problem is equivalent to

$$\begin{aligned} &\text{maximize} && |z| \\ &\text{subject to} && \lambda_{min}(\widetilde{F}(z)^*\widetilde{F}(z) - \varepsilon^2 I) \leq 0 \end{aligned} \tag{2.1.1}$$

The problem above is nonconvex and, due to the eigenvalue constraint, it is also nonsmooth. We use polar coordinates, so we represent the optimization problems in terms

of $w = (r, \theta) \in \mathbb{R}^2$ such that $z = re^{i\theta}$. Then the problem turned

$$\begin{aligned} &\text{maximize} && c^T w \\ &\text{subject to} && \lambda(w) := \lambda_{min}(F(w)^* F(w) - \varepsilon^2 I) \leq 0 \end{aligned} \tag{2.1.2}$$

where $F(w := (r, \theta)) = re^{i\theta} I - A$ and $c = [1 \;\; 0]^T$. To overcome the nonconvexity and nonsmoothness of the eigenvalue function, we use global overestimators. Algorithmic use of global overestimators or underestimators dates back to Piyavskii-Shubert, but more recently Breiman and Cutler have proposed an efficient approach [1]. The overestimator functions are constructed based on the following classical results [14, 25].

Lemma 2.1.1. *Let $A(w) := F(w)^* F(w) - \varepsilon^2 I$ where $F(\omega)$ is as in (2.1.2), and $\Phi : \mathbb{R} \to \mathbb{C}^{n \times n}$ be defined by $\Phi(\alpha) := A(\hat{w} + \alpha p)$ for given $\hat{w}, p \in \mathcal{D}$. Then the following hold:*

(i) *There is an ordering $\phi_1(\alpha), .., \phi_n(\alpha)$ of the eigenvalues of $\Phi(\alpha)$ so that each eigenvalue $\phi_j(\alpha)$ for $j = 1, ..., n$ is analytic on $\mathbb{R}$;*

(ii) *Suppose that $\phi(\alpha) := \lambda(\Phi(\alpha))$ is simple for all α on an open interval I in $\mathbb{R}$. Then $\phi(\alpha)$ is analytic on I;*

(iii) *The left-hand $\phi'_-(\alpha)$ and the right-hand $\phi'_+(\alpha)$ derivatives of $\phi(\alpha) := \lambda_{min}(\Phi(\alpha))$ exist everywhere. Furthermore, $\phi'_-(\alpha) \geq \phi'_+(\alpha)$ at all $\alpha \in \mathbb{R}$;*

(iv) *The eigenvalue function $\lambda_{min}(A(w))$ is twice continuously differentiable at all $w \in \mathbb{R}^2$ where it is simple. Furthermore, at all such w, we have*

$$\begin{aligned} \frac{\partial \lambda_{min}(A(w))}{\partial r} &= \frac{\partial \lambda_{min}(F(w)^* F(w) - \varepsilon^2 I)}{\partial r} \\ &= x_n^*(w) \frac{\partial A(w)}{\partial r} x_{n(w)} \\ \frac{\partial^2 \lambda_{min}(A(w))}{\partial r \, \partial \theta} &= x_n^*(w) \frac{\partial^2 \lambda_{min}(A(w))}{\partial r \, \partial \theta} x_n(w) + \\ &\quad 2\Re \left[\sum_{m=1}^{n-1} \frac{1}{\lambda_{min}(A(w)) - \lambda_m(w)} \left(x_n^*(w) \frac{\partial A(w)}{\partial r} x_n(w) \right) \left(x_n^*(w) \frac{\partial A(w)}{\partial \theta} x_m(w) \right) \right] \end{aligned}$$

where $x_j(w)$ denotes a unit eigenvector of $A(w)$ corresponding to its jth largest

eigenvalue.

Theorem 2.1.2 below exploits Lemma 2.1.1, and Taylor's theorem to construct quadratic support functions for the eigenvalue function $\lambda_{min}(A(w))$.

Theorem 2.1.2. *Suppose $w_k = (r_k, \theta_k) \in \mathbb{R}^2$ is such that $\sigma_{min}[F(w_k)]$ is simple. Let γ be a scalar satisfying*

$$\lambda_{max}\{\nabla^2 \lambda_{min}(A(w))\} \leq \gamma. \tag{2.1.3}$$

We have

$$\lambda(w) \leq q_k(w) := \lambda_k + \nabla\lambda_k^T(w - w_k) + \frac{\gamma}{2}\|(w - w_k)\|^2 \tag{2.1.4}$$

where $\lambda_k := \lambda(w_k)$ and $\nabla\lambda_k := \nabla\lambda(w_k)$.

Proof. See the proof of Theorem 2.2 in [20]. □

By replacing the eigenvalue constraint in our optimization problem with the support function in (2.1.4), we obtain the following convex and smooth optimization problem.

$$\begin{array}{lll} \text{maximize} & c^T w & \\ \text{subject to} & q_k(\omega) = \lambda_k + \nabla\lambda_k^T(w - w_k) + \frac{\gamma}{2}\|w - w_k)\|^2 & \leq \quad 0 \end{array} \tag{2.1.5}$$

Let $w_0 = r_0 e^{i\theta_0}$ be an eigenvalue of A with the largest modulus. Clearly, $\lambda_{min}(A(w_0)) = 0 \leq \varepsilon$, so the initial point w_0 is feasible with respect to (2.1.1). The algorithm generates a sequence of feasible points $\{w_k = (r_k, \theta_k)\}$ in $\mathbb{R}^2$ such that w_{k+1} is defined as the unique maximizer of (2.1.5). The maximizer w_{k+1} must be feasible with respect to the original problem (2.1.1), because

$$\mathcal{F}_k := \{w \in \mathbb{R}^2 \mid q_k(w) \leq 0\} \subseteq \mathcal{F} := \{w \in \mathbb{R}^2 \mid \lambda_{min}(A(w)) \leq 0\}.$$

By applying the Karush-Kuhn-Tucker conditions, the maximizer w_{k+1} of (2.1.5) must satisfy

$$c = \mu\nabla q_k(w_{k+1}) \text{ and } q_k(w_{k+1}) = 0. \tag{2.1.6}$$

for some scalar $\mu \in \mathbb{R}^+$, where

$$\nabla q_k(w) = \nabla\lambda_k + \gamma(w - w_k)$$
$$\nabla\lambda_k = \begin{bmatrix} \Re\left(v_k^* \frac{\partial F(w_k)}{\partial r} F(w_k) v_k + v_k^* F(w_k)^* \frac{\partial F(w_k)}{\partial r} v_k\right) \\ \Im\left(v_k^* \frac{\partial F(w_k)}{\partial \theta} F(w_k) v_k + v_k^* F(w_k)^* \frac{\partial F(w_k)}{\partial \theta} v_k\right) \end{bmatrix}$$

By explicitly solving (2.1.6), we deduce the update rule

$$w_{k+1} = w_k + \frac{1}{\gamma}\left[\frac{1}{\mu_+}c - \nabla\lambda_k\right], \ \ where \ \ \mu_+ = \frac{1}{\sqrt{\|\nabla\lambda_k\|^2 - 2\gamma\lambda_k}}. \tag{2.1.7}$$

Next we discuss how an upper bound γ for the second derivatives of the eigenvalue function satisfying (2.1.3) can be obtained analytically. By Theorem 6.1 in [20], we have

$$\lambda_{max}\{\nabla^2\lambda_{\min}(A(w))\} \leq \lambda_{max}\{\nabla^2 A(w)\}, \tag{2.1.8}$$

where

$$\nabla^2 A(w) := \begin{bmatrix} \frac{\partial^2 A(w)}{\partial^2 r^2} & \frac{\partial^2 A(w)}{\partial r\,\partial\theta} \\ \frac{\partial^2 A(w)}{\partial\theta\,\partial r} & \frac{\partial^2 A(w)}{\partial^2\theta^2} \end{bmatrix}.$$

Explicit calculations yield

$$\nabla^2 A(w) = \begin{bmatrix} 2I & i(e^{-i\theta}A^* - e^{i\theta}A) \\ i(e^{-i\theta}A - e^{i\theta}A^*) & r(e^{i\theta}A^* + e^{-i\theta}A) \end{bmatrix} \tag{2.1.9}$$

Moreover the ε-pseudospectral radius of A is bounded above by $\|A\|_2 + \varepsilon$, so in (2.1.9) above $r \leq \|A\|_2 + \varepsilon$. Now an application of Gersgorin's Theorem ([10],Theorem 6.1.1) to the eigenvalues of $\nabla^2 A(w)$ combined with (2.1.8) gives rise to

$$\lambda_{max}[\nabla^2\lambda_{min}(A(w))] \ \leq \ \gamma := \max(2 + 2\|A\|, 2\varepsilon\|A\| + 2\|A\|^2 + 2\|A\|). \tag{2.1.10}$$

In practice, we let the γ value be prescribed by the user. Table 2.1 lists numerical results

for four different choices of γ. We first compute $\rho_\epsilon(A)$ the ϵ-psedospectral radius of A by means of the algorithm in [19]. These values are given in the second column of the table. The columns of Error_1, Error_2, Error_3 and Error_4 list the relative errors

$$\frac{|r_k - \rho_\varepsilon|}{\|A\|}. \tag{2.1.11}$$

at termination for four different choices of γ after a fixed number of iterations. For the columns of Error_1, Error_2, Error_3 and Error_4, we set γ to $\max(2+2\|A\|, 2\varepsilon\|A\|+2\|A\|^2+2\|A\|)$, $\min(2+2\|A\|, 2\varepsilon\|A\|+2\|A\|^2+2\|A\|)$, $\sqrt{\|A\|}$ and $\varepsilon\sqrt{\|A\|}$, respectively. The test matrices are created by Eigtool [37]. In Table 2.1 the smaller relative errors are observed for smaller values of γ. We also perform numerical experiments for smaller matrices with the same choices of γ values. The results are listed in Table 2.2. Here we usually retrieve the ε-pseudospectral radius with about the same relative error for four different choices of γ. However, on some examples the choice of $\varepsilon\sqrt{\|A\|}$ still yields more accurate values.

Next we discuss the convergence of the feasible sequence $\{w_k\}$ defined by the recurrence (2.1.7) to a point w_* that satisfies the first order optimality conditions

$$c = \mu\nabla\lambda_{min}(A(w_*)) \;\; \exists\mu > 0, \;\text{ and }\; \lambda_{min}(A(w_*)) = 0.$$

Lemma 2.1.3 ([20]). *The sequence $\{c^T w_k\}$ is monotone increasing and convergent.*

The monotonicity of the sequence $\{c^T w_k\}$ follows from

$$w_{k+1} = \arg\max_{q_k(w)\le 0} c^T w$$

and the fact that $q_k(w_k) = 0$ meaning w_k is feasible with respect to this problem. This leads us to conclude that $c^T w_{k+1} \ge c^T w_k$. Additionally, denoting the global minimizer of the original problem (2.1.1) by w_{**}, we have $c^T w_{**} \ge c^T w_k$ for all k. Hence, by the monotone convergence theorem, the sequence $\{c^T w_k\}$ is convergent.

Theorem 2.1.4 (Convergence [18]). *Suppose that $\lambda_{min}(A(w_k))$ is simple for each k.*

(i) *If* $\nabla\lambda_{min}(A(w_k)) \neq 0$ *for all* k *sufficiently large, then* $\lambda_{min}(A(w_k)) \to 0$ *as* $k \to \infty$.

(ii) *If there exists a real scalar* $L > 0$ *such that* $\|\lambda_{min}(A(w_k))\|_2 > L$ *for all* k *sufficiently large, then*

$$\frac{(1,0).\nabla\lambda_{min}(A(w_k))}{\|\nabla\lambda_{min}(A(w_k))\|} \to 1 \ \ as \ \ k \to \infty.$$

The first part of the theorem shows that ω_k is approaching the boundary of $\Lambda_\varepsilon(A)$ in the limit as $k \to \infty$. The second part means that $\nabla\lambda_{min}(A(w_k))$ points in the direction of $(1, 0)$ as $k \to \infty$. The proofs of part (i) and (ii) are similar to the proofs of Lemma 3.5 and Theorem 3.6 in [20]. **Algorithm 1** summarizes this locally convergent approach.

2.2 Global convergence by angular search

For a general constrained maximization problem, if the objective function is continuous and concave, and the feasible region is a convex and closed set, then a local maximizer is also a global maximizer. We call such problems convex programs. Unfortunately, the problem (2.1.1) concerning the computation of $\rho_\varepsilon(A)$ for a given matrix A is not a convex program excluding very special A. Furthermore, the sequence generated $\{w_k\}$ in $\mathbb{R}^2$ in the previous section typically converges to a point w_* is on the boundary of $\Lambda_\varepsilon(A)$ with a vertical tangent line in the polar coordinates. Equivalently, $w_* = (r_*, \theta_*)$ is a point on the boundary of $\Lambda_\varepsilon(A)$, and this boundary is tangent at w_* to the circle centered at the origin of radius r_* in the Cartesian coordinates. These conclusions follow from Theorem 2.1.4. This convergence property holds under the assumption $\nabla\lambda_{min}(A(w_k)) \neq 0$, and the simplicity of $\sigma_{min}(F(r_k, \theta_k))$ for each k, where $w_k = (r_k, \theta_k)$ and $F(r, \theta) := re^{i\theta}I - A$.

The converged point w_* may or may not have the largest moduli among the points in $\Lambda_\varepsilon(A)$. We check whether $w_* = (r_*, \theta_*)$ is indeed a point with greatest moduli by solving the unconstrained minimization problem

$$\text{minimize}_{\theta\in[0,2\pi)} \ \sigma_{min}(F(r_*, \theta))$$

globally. This global minimization is achieved by means of the algorithm in [33]. The algorithm generates a sequence $\{\theta_k\}$ of real numbers, and constructs a piecewise quadratic function $Q_k(\theta) := \max_{\ell=0,\ldots,k} q_\ell(\theta)$ such that

$$Q_k(\theta_\ell) = \sigma_{min}(F(r_*, \theta_\ell)) \; \ell = 0, \ldots, k \quad \text{and} \quad Q_k(\theta) \leq \sigma_{min}(F(r_*, \theta)) \; \forall \theta.$$

It solves the problem

$$\text{minimizer}_{\theta \in [0, 2\pi)} \; Q_k(\theta),$$

and lets θ_{k+1} be a global minimizer of this problem. The piecewise quadratic function is then refined as

$$Q_{k+1}(\theta) := \max \left\{ Q_k(\theta), \; \sigma_{k+1} + \sigma'_{k+1}(\theta - \theta_{k+1}) + \frac{\gamma}{2}(\theta - \theta_{k+1})^2 \right\}$$

where $\sigma_{k+1} := \sigma_{min}(F(r_*, \theta_{k+1}))$, $\sigma'_{k+1} := \partial \sigma_{min}(F(r_*, \theta_{k+1}))/\partial\theta$ and γ is a global lower bound on $\partial^2 \sigma_{min}(F(r_*, \theta))/\partial\theta^2$ over $\theta \in [0, 2\pi)$. Here we also benefit from the expression

$$\frac{\partial \sigma_{min}(F(r_*, \theta_{k+1}))}{\partial \theta} = \Re \left(u^* \frac{\partial F(r_*, \theta_{k+1})}{\partial \theta} v \right),$$

where u, v represent a consistent pair of unit left and right singular vectors associated with $\sigma_{min}(F(r_*, \theta))$.

Algorithm 2 below describes how the local search of the previous section can be combined with this angular search idea. Note that it is essential to start from $w_0 = (r_0, \theta_0)$ such that $r_0 e^{i\theta_0}$ is the eigenvalue of A with the largest modulus. In this case if the angular search determines that the smallest value of $\sigma_{min}(F(r_*, \theta))$ over θ is ε, then it can be concluded that w_* is a point in $\Lambda_\varepsilon(A)$ that is furthest away from the origin. Otherwise, there is a point θ_{**} such that $\sigma_{min}(F(r_*, \theta_{**})) < \varepsilon$. This point lies strictly inside $\Lambda_\varepsilon(A)$, so we repeat the local search starting from (r_*, θ_{**}).

2.3 Pseudospectra of matrices restricted to subspaces

Large matrices are computationally difficult. We encounter large scale matrices in eigenvalue computations and when solving linear systems of equations. Projections onto suitable small subspaces, which allows us to approximate large matrices by small matrices, is an effective approach to handle large scale matrices. One subspace that is commonly employed is the Krylov subspace defined, for a given $A \in \mathbb{C}^{n\times n}$ and $x \in \mathbb{C}^n$, by

$$\mathcal{K}_n = \text{span}\{x, Ax, ..., A^n x\}$$

Here, we adopt the subspace idea for the computation of the pseudospectral abscissa proposed in [13]. The main idea is to restrict the domain of the map $v \mapsto (A - zI)v$ to small subspaces, to gradually expand these subspaces, and to occasionally restart them.

Let S be an isometry with more rows than columns and satisfying $S^*S = I$, let us also denote the column space of S by $\mathcal{S}$. A linear map whose domain is restricted to $\mathcal{S}$ is defined below along with the definition of its ε-pseudospectrum, and ε-pseudospectral radius.

$$F_S(z) := F(z)S = (A - zI)S \tag{2.3.1}$$

$$\Lambda_\varepsilon(F_S) := \{z \in \mathbb{C} \ : \ \sigma_{min}(F(z)S) \leq \varepsilon\} \tag{2.3.2}$$

$$\rho_\varepsilon(F_S) := \max\{|z| \ : \ z \in \Lambda_\varepsilon(F_S)\}. \tag{2.3.3}$$

Lemma 2.3.1 (Monotonicity [18])**.** *Two isometries S_1, S_2 such that $Col(S_1) \subseteq Col(S_2)$ satisfy the following:*

(1) $\Lambda_\varepsilon(F_{S_1}) \subseteq \Lambda_\varepsilon(F_{S_2})$*;*

(2) $\rho_\varepsilon(F_{S_1}) \leq \rho_\varepsilon(F_{S_2})$.

Proof. (1) Let us use the notation $\mathcal{S}_j := \text{Col}(S_j)$ for $j = 1, 2$. By the variational charac-

terization of the minimum singular value,

$$\sigma_{min}(F_{S_1}(z)) = \min_{v\in\mathcal{S}_1,\|v\|_2=1} \|F(z)v\|_2 \;\geq\; \min_{v\in\mathcal{S}_2,\|v\|_2=1} \|F(z)v\|_2 = \sigma_{min}(F_{S_2}(z)),$$

where the inequality is due to $\mathcal{S}_1 \subseteq \mathcal{S}_2$. Now, if $z \in \Lambda_\varepsilon(F_{S_1})$, then $\sigma_{min}(F_{S_1}(z)) \leq \varepsilon$. Consequently, $\sigma_{min}(F_{S_2}(z)) \leq \varepsilon$, so $z \in \Lambda_\varepsilon(F_{S_2})$. (2) This is immediate from (1). □

Theorem 2.3.2 ([18]). *Let $z \in \Lambda_\varepsilon(F)$ and let v be a unit right singular vector associated with $\sigma_{min}[F(z)]$. Then $z \in \Lambda_\varepsilon(F_v)$.*

Proof. By the singular value characterization of $\Lambda_\epsilon(F)$, we must have

$$\sigma_{min}(F(z)) = \|F(z)v\|_2 = \sigma_{min}(F(z)v).$$

Hence, if $z \in \Lambda_\varepsilon(F)$, then $\sigma_{min}(F(z)v) = \sigma_{min}(F(z)) \leq \varepsilon$. This shows $z \in \Lambda_\varepsilon(F_v)$. □

Corollary 2.3.3 (Low Dimensionality [18]). *Let z_* be a globally rightmost point of $\Lambda_\varepsilon(F)$ and v_* be a unit right singular vector associated with $\sigma_{min}(F(z_*))$. We have $\rho_\varepsilon(F) = \rho_\varepsilon(F_{v_*})$.*

Proof. By Theorem 2.3.2, we have $z_* \in \Lambda_\varepsilon(F_{v_*})$. This implies that $\rho_\varepsilon(F) = |z_*| \leq \rho_\varepsilon(F_{v_*})$. We also have $\rho_\varepsilon(F) \geq \rho_\varepsilon(F_{v_*})$ by monotonicity (Lemma 2.3.1), hence the desired equality. □

For the next result $\mathcal{V}(z)$ denotes the set of right singular vectors corresponding to $\sigma_{min}(F(z))$.

Corollary 2.3.4 ([18]). *Let z_* be a globally rightmost point of $\Lambda_\varepsilon(F)$. Then $\rho_\varepsilon(F) = \rho_\varepsilon(F_S)$ if and only if $\mathcal{V}(z_*) \cap Col(S) \neq \emptyset$.*

Proof. First let us suppose $\mathcal{V}(z_*) \cap Col(S) \neq \emptyset$. In this case, there exists a unit right singular vector $v_* \in Col(S)$ associated with $F(z_*)$. By Lemma 2.3.1, we deduce

$$\rho_\varepsilon(F_{v_*}) \leq \rho_\varepsilon(F_S) \leq \rho_\varepsilon(F).$$

But Corollary 2.3.3 implies $\rho_\varepsilon(F_{v_*}) = \rho_\varepsilon(F)$, which yields $\rho_\varepsilon(F_S) = \rho_\varepsilon(F)$.

As for the converse, suppose $\rho_\varepsilon(F) = \rho_\varepsilon(F_S)$. Let z_S be an outermost point of $\Lambda_\varepsilon(F_S)$. By monotonicity $z_S \in \Lambda_\varepsilon(F)$ and $|z_S| = \rho_\varepsilon(F_S) = \rho_\varepsilon(F)$, so z_S is also an outermost point of $\Lambda_\varepsilon(F)$. Denoting a right singular vector associated with $\sigma_{min}(F_S(z_S))$ by v_*, we observe

$$\|F(z_S)Sv_*\|_2 = \sigma_{min}(F_S(z_S)) = \sigma_{min}(F(z_S)).$$

This means that Sv_* is a right singular vector associated with $\sigma_{min}(F(z_S))$, hence $\mathcal{V}(z_S) \cap Col(S) \neq \emptyset$ completing the proof. □

The last corollary shows that there exist small subspaces $\mathcal{S}$ such that $\rho_\varepsilon(F) = \rho_\varepsilon(F_S)$ where S is an isometry satisfying $\mathcal{S} = Col(S)$. This motivates the computation of $\rho_\epsilon(F_S)$ instead of $\rho_\epsilon(F)$ for an $n \times p$ isometry S with $p \ll n$ for efficiency reasons. A reasonable choice for the subspace is the span of right singular vectors corresponding to $\sigma_{min}(F(z))$ for various z close to an outermost point in $\Lambda_\varepsilon(F)$. This leads us to the following framework to adaptively expand the subspaces.

Subspace Selection:

(1) $\mathcal{S}_k := \text{span}\{v_0, ..., v_k\}$ where v_j is a right singular vector corresponding to $\sigma_{min}[F(z_j)]$ for $j = 1, ..., k$.

(2) z_{k+1} is an outermost point of $\Lambda_\varepsilon(F_{S_k})$ for $k \in \mathbb{N}$ for an isometry S_k such that $\mathcal{S}_k = Col(S_k)$.

We use this subspace idea only together with the local search. In particular, the angular searches are still performed on the full matrix A to ensure convergence to a globally outermost point. A description of the proposed subspace approach together with the local search is given in **Algorithm 3**. In this description, we use the notation $\sigma_{min}(w := (r, \theta)) = \sigma_{min}(A - re^{i\theta})$, and $\partial\sigma_{min}(w)$ represents the generalized gradient of $\sigma_{min}(w)$ defined by

$$\partial\sigma_{min}(w) := \text{co}\left\{\lim_{k\to\infty} \nabla\sigma_{min}(\widetilde{w}_k) \;\mid\; \widetilde{w}_k \to w_*,\;\; \widetilde{w}_k \notin \Omega\right\}.$$

Above, co(H) denotes the convex hull of a set H, and Ω is the subset of $\mathbb{R}^2$ of measure zero on which $\sigma_{min}(w)$ is not differentiable. The conditions

$$\sigma_{min}(w_{k+1}) = \varepsilon \quad \text{and} \quad c.(1,0) \in \partial\sigma_{min}(w_{k+1}) \; \exists c \in \mathbb{R}^+$$

on line 6 of **Algorithm 3** in terms of this generalized gradient constitute the first order optimality conditions to have w_{k+1} on the boundary of $\Lambda_\varepsilon(A)$ and tangential to a circle centered at the origin.

Table 2.3 illustrates applications of **Algorithm 3** to the matrices **'landau(100)'** and **'airy(300)'** starting from the eigenvalues of these matrices with the largest moduli. In both of the examples, our numerical implementation terminates with seven dimensional subspaces, because the relative errors are close to the machine precision. An angular search confirm convergence to an outermost point globally in both cases. We observe superlinear convergence on the left-hand side for the Landau matrix. This is the typical rate of convergence behavior we observe in various examples.

2.4 Restarts and the overall algorithm

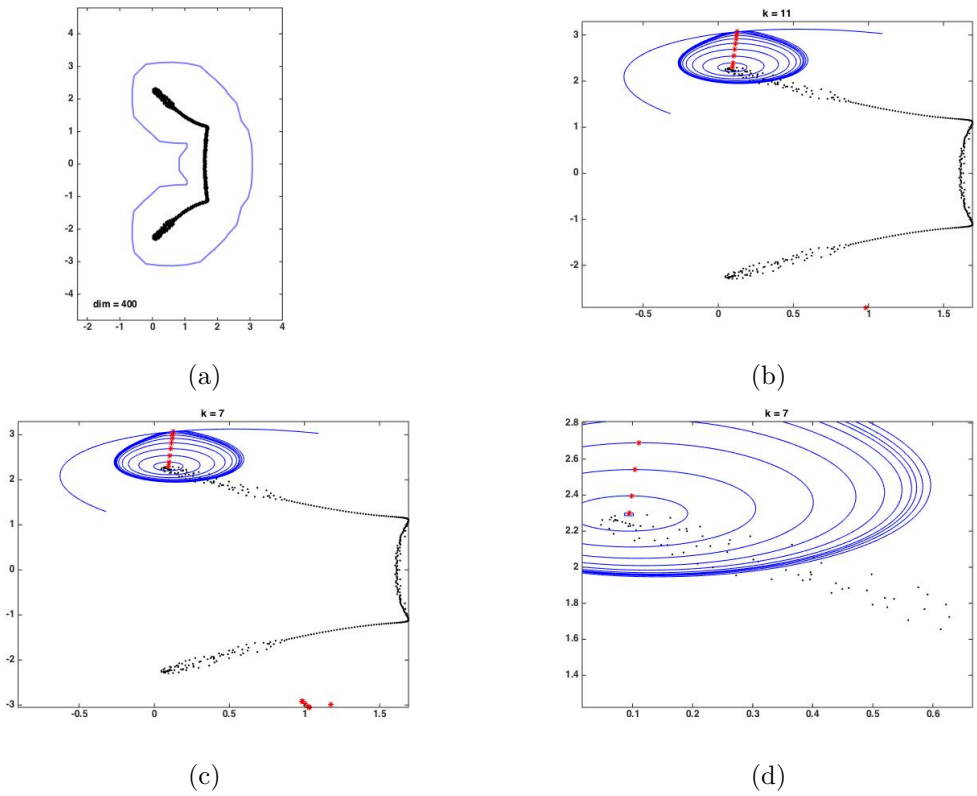
The subspace idea becomes rather inefficient when the subspace dimension gets closer to the size of the matrix A. Consequently, we incorporate a restart strategy that helps us to get rid of the right singular vectors of $\sigma_{min}[F(z_k)]$ at points z_k that are far away from outermost points of $\Lambda_\varepsilon(A)$. We disregard the earlier vectors and favor only the lastly added few vectors. The restarted subspace is for instance can be given by $\text{span}\{v_{k-j}, ..., v_k\}$. In practice, we only keep the right singular vector that is added latest, so we restart with the one dimensional subspace $\mathcal{S}_k = \text{span}\{v_k\}$. The angular search idea in Section 2.2 facilitates this restart strategy further. If the local search results in a point $z_* = r_* e^{i\theta}$ that is not outermost globally, the angular search detects this and provides also a point $z_{**} = r_* e^{i\theta_*}$ that lies strictly inside $\Lambda_\varepsilon(A)$. Then the algorithm restarts with the one dimensional subspace spanned by the right singular vector corresponding to $\sigma_{min}[F(z_{**})]$.

Algorithm 4 summarizes the overall approach. The algorithm starts from an eigenvalue z_0 with the largest modulus. It finds the outermost point z_{k+1} in $\Lambda_\varepsilon(F_{S_k})$ locally by an application of the algorithm in Section 2.1 repeatedly. If this point is also on the boundary of $\Lambda_\varepsilon(A)$, and is tangent to a circle centered at the origin, an angular search is performed. An angular search either confirms that the converged point is globally outermost, or otherwise restarts a local search with a one dimensional subspace. If the point z_{k+1} converged by the local search is not on the boundary of $\Lambda_\varepsilon(A)$, or is not tangent to a circle centered at the origin, then the subspace dimension is checked. If the subspace dimension has not reached the prescribed dimension k_{max}, it expands the subspace with the addition of the right singular vector corresponding to $\sigma_{min}(F(z_k))$. Otherwise, the local search is again restarted with a one dimensional subspace as discussed in the previous paragraph.

Table 2.4 illustrates the progress of **Algorithm 4** on the 400×400 **Grcar** matrix. This example is taken from eigtool [37]. Angular search occurs three times in this example. But the subspace dimension never exceeds 11. Eventually, before the final angular search, we observe superlinear convergence.

Figure 2.1 is a visualization of the Grcar example of Table 2.4. The figure on the upper left-hand side is the ε-pseudospectrum of this matrix for $\varepsilon = 10^{-2}$. The upper right figure displays the iterates of the subspace framework before the first angular search by marking them with red asterisks, whereas the bottom left figure displays the iterates before the final angular search similarly. The bottom right figure is a zoom of the bottom left figure. In this figure, it is possible to observe that the $\Lambda_\varepsilon(F_{S_k})$ grows monotonically as k increases.

Finally, we investigate the dependence of the convergence of Algorithm 4 on the starting point. For global convergence, it is essential to start from the eigenvalue with the largest modulus. This is illustrated in Table 2.5 and 2.6, which depict the results of **Algorithm 4** when it is initiated from the largest modulus and the smallest modulus eigenvalues of the input matrix. The algorithm produces different results depending on the choice of the initial point.



(a) (b)

(c) (d)

Figure 2.1: The upper left figure illustrates the ε-pseudospectrum of the 400×400 **Grcar** matrix for $\varepsilon = 10^{-2}$. When **Algorithm 4** is applied to this example, three angular searches deemed to be necessary. The upper right figure is the progress of the algorithm before the first angular search, which is performed when the subspace dimensions reaches to 11. After the angular search, the algorithm starts with a one dimensional subspace. The bottom left figures depict the progress of the algorithm before the second and the third angular search, respectively. In this case, the subspace dimension reaches to 7 before the angular search. The bottom right figure is a zoom of the bottom left figure.

Call	ρ_ε	Error_1	Error_2	Error_3	Error_4
airy(100)	$1.4215e+003$	$2.8e-006$	$1.6e-007$	$1.6e-013$	$1.6e-013$
basor(100)	$6.1350e+000$	$6.5e-008$	$6.5e-008$	$6.5e-008$	$6.5e-008$
boeing('O')	$1.1495e+003$	$9.3e-006$	$9.3e-006$	$7.5e-007$	$1.0e-016$
boeing('S')	$1.1501e+003$	$8.9e-006$	$8.9e-006$	$7.5e-007$	$4.3e-017$
chebspec(100)	$8.6935e+002$	$1.7e-006$	$3.2e-007$	$2.5e-016$	$2.7e-016$
convdiff(100)	$1.5860e+005$	$6.3e-013$	$6.2e-013$	$6.9e-021$	$6.9e-021$
davies(100)	$5.8501e+004$	$1.7e-011$	$1.7e-011$	$9.8e-019$	$9.8e-019$
demmel(10)	$5.5544e+001$	$9.3e-004$	$9.3e-004$	$1.1e-008$	$1.0e-009$
frank(100)	$5.3195e+002$	$6.6e-002$	$2.0e-004$	$1.3e-006$	$4.3e-008$
gallery3(100)*	$4.7965e+000$	$1.7e-005$	$4.7e-006$	$4.7e-006$	$4.7e-006$
gallery5(100)	$3.3693e+001$	$3.3e-004$	$3.2e-004$	$2.5e-014$	$6.9e-015$
gaussseidel(100,'C')	$1.0090e+000$	$8.9e-016$	$8.9e-016$	$8.9e-016$	$8.9e-016$
gaussseidel(100,'D')	$8.4370e-001$	$6.1e-015$	$6.1e-015$	$6.1e-015$	$6.1e-015$
gaussseidel(100,'U')	$9.9430e-001$	$8.8e-012$	$8.8e-012$	$8.8e-012$	$8.8e-012$
godunov(100)	$2.8276e+002$	$6.3e-002$	$9.0e-004$	$3.1e-013$	$3.1e-013$
grcar(100)	$2.8522e+000$	$1.7e-001$	$1.7e-001$	$3.6e-004$	$6.1e-008$
hatano(100)	$2.8651e+000$	$6.3e-010$	$6.3e-010$	$6.3e-010$	$6.3e-010$
kahan(100)	$1.1380e+000$	$1.5e-005$	$9.7e-016$	$9.7e-016$	$9.7e-016$
landau(100)	$9.9760e-001$	$1.2e-016$	$1.2e-016$	$1.2e-016$	$1.2e-016$
orrsommerfeld(100)	$2.9600e+000$	$3.6e-008$	$3.5e-008$	$3.0e-008$	$2.5e-016$
random(100)	$1.0494e+000$	$1.6e-007$	$1.7e-013$	$1.6e-013$	$1.6e-013$
randomtri(100)	$3.2500e-001$	$5.4e-005$	$7.1e-005$	$7.6e-005$	$1.2e-015$
riffle(100)	$5.1000e-001$	$7.8e-005$	$7.6e-005$	$3.7e-005$	$6.9e-016$
transient(100)	$1.2332e+000$	$3.9e-007$	$3.9e-007$	$3.9e-007$	$3.9e-007$
twisted(100)	$2.7777e+000$	$2.4e-012$	$2.4e-012$	$2.4e-012$	$2.4e-012$

Table 2.1: Results of **Algorithm 4** on various 100×100 matrices taken from EigTool for $\varepsilon = 10^{-2}$. The first column shows the ε-pseudospectral radius computed by the routine in EigTool, which is an implementation of the algorithm introduced in [19]. The other columns demonstrate the relative errors after a fixed number of iterations for four different choices of γ values.

Call	ρ_ε	Error_1	Error_2	Error_3	Error_4
airy(10)	$2.8224e+000$	$2.6e-007$	$2.6e-007$	$2.6e-007$	$2.6e-007$
basor(10)	$5.9305e+000$	$3.6e-007$	$3.6e-007$	$3.6e-007$	$3.6e-007$
boeing('O')*	$2.8370e+003$	$1.1e-004$	$1.1e-004$	$6.1e-018$	$7.5e-015$
boeing('S')*	$2.8647e+003$	$1.1e-004$	$1.1e-004$	$2.5e-017$	$1.3e-015$
chebspec(10)	$3.9204e+001$	$5.4e-010$	$2.9e-010$	$2.9e-010$	$2.9e-010$
companion(10)	$2.3860e+002$	$5.4e-016$	$4.3e-016$	$6.1e-016$	$3.6e-016$
convdiff(10)	$3.6733e+009$	$2.9e-010$	$2.9.2e-010$	$2.9e-010$	$2.9e-010$
davies(10)	$1.2538e+002$	$2.1e-011$	$2.1e-011$	$2.1e-011$	$2.1e-011$
frank(10)	$3.47298e+001$	0	0	0	0
gallery3(10)	$1.7874e+001$	$1.5e-016$	$8.3e-017$	$2.0e-016$	$9.6e-017$
gallery5(10)*	$1.8073e+002$	$7.1e-003$	$8.6e-015$	$2.2e-015$	$2.0e-015$
gaussseidel(10,'C')	$1.2436e+000$	0	0	0	0
gaussseidel(10,'D')	$8.09e-001$	$1.4e-012$	$1.4e-012$	$1.4e-012$	$1.4e-012$
gaussseidel(10,'U')	$1.2242e+00$	$8.9e-016$	0	0	0
godunov(10)*	$5.0242e+002$	$2.4e-004$	$7.5e-015$	$8.8e-015$	$7.5e-015$
grcar(10)	$2.7654e+000$	$1.7e-008$	$1.7e-008$	$1.7e-008$	$1.7e-008$
hatano(10)	$2.8524e+000$	$2.4e-015$	$2.4e-015$	$2.4e-015$	$2.4e-015$
kahan(10)*	$1.4580e+000$	$1.1e-005$	$1.1e-015$	$1.1e-015$	$1.1e-015$
landau(10)	$4.4232e+000$	$2.7e-008$	$2.7e-008$	$2.7e-008$	$2.7e-008$
orrsommerfeld(10)	$1.3141e+000$	$3.0e-007$	$3.0e-007$	$3.0e-007$	$3.0e-007$
random(10)	$1.5001e+000$	0	0	0	0
randomtri(10)	$8.6210e-001$	$3.4e-012$	$3.4e-012$	$3.4e-012$	$3.4e-012$
riffle(10)	$1.0466e+000$	$1.4e-015$	$1.4e-015$	$1.4e-015$	$1.4e-015$
transient(10)	$1.4321e+000$	$4.9e-015$	$4.9e-015$	$4.9e-015$	$4.9e-015$
twisted(10)	$2.6022e+000$	$8.8e-016$	$8.8e-016$	$8.8e-016$	$8.8e-016$

Table 2.2: Results of **Algorithm 4** on various 10×10 matrices matrices for four different choices of γ values. Here ε is chosen as $10^{-0.5}$.

Algorithm 1 Local Algorithm

Require: A square matrix A and a positive real scalar ε

1: Let $z_0 = r_0 e^{i\theta_0}$ be any point in $\Lambda_\varepsilon(F)$ and consider $w_0 = (r_0, \theta_0)$ with $k \leftarrow 0$
2: Calculate $\sigma_0 := \sigma_{min}[F(w_0)]$ and an associated unit right singular vector v_0.
3: Calculate $\lambda_0, \nabla\lambda_0$ using σ_0, v_0, w_0.
4: **while** $(\lambda_k \neq 0)$ or $(\nabla\lambda_k \neq c.(1,0)\ \ \forall c \in \mathbb{R}^+)$ **do**
5: Apply the recurrence (2.1.7) to find w_{k+1} given $w_k, \lambda_k, \nabla\lambda_k$.
6: Calculate $\sigma_{k+1} := \sigma_{min}[F(w_{k+1})]$and an associated unit right singular vector v_{k+1}.
7: Calculate $\lambda_{k+1}, \nabla\lambda_{k+1}$ using $\sigma_{k+1}, v_{k+1}, w_{k+1}$.
8: Increment k.
9: **end while**
10: **Output:**w_k

Algorithm 2 Globally Convergent Algorithm

Require: A square matrix A and a positive real scalar ε

$w_0 \leftarrow (r_0, \theta_0)$, where $r_0 e^{i\theta_0}$ is the eigenvalue of F that is furthest away from the origin.
Convergence $\leftarrow$ False.
while $\neg$ *Convergence* **do**
  Local Search: Apply Algorithm 1 starting from w_0 yielding a point $w_* = (r_*, \theta_*)$ such that $w_* \in \partial\Lambda_\varepsilon(F)$ with a vertical tangent line.
  Angular Search: $w_* \leftarrow \arg\min_{\theta\in[0,2\pi)} \sigma_{min}(F(r_*, \theta))$ and $\sigma_* \leftarrow \sigma_{min}(F(r_*, \theta_*))$.
  if $\sigma_* = \varepsilon$ **then**
    Convergence $\leftarrow$ *True.*
  else
    $w_0 \leftarrow (r_*, \theta_*)$.
  end if
end while
Output: w_*.

Algorithm 3 Local Search with Subspace Restrictions

Require: A square matrix A and a positive real scalar ε

$z_0 \leftarrow$ an outermost eigenvalue of A, and $k \leftarrow 0$.
$S_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right singular vector associated with $\sigma_{min}[F(z_0)]$.
Convergence $\leftarrow$ False.
  while $\neq$ *Convergence* **do**
    Local Search: Apply Algorithm 1 to determine maximizer $w_{k+1} = (r_*, \theta_*)$ such that $z_{k+1} = r_* e^{i\theta_*} \in \partial\Lambda_\varepsilon(F_{S_k})$ is tangent to the circle centered at the origin of radius r_*.
    if $(\sigma_{min}(w_{k+1}) = \varepsilon)$ and $(c.(1,0) \in \partial\sigma_{min}(w_{k+1})\ \exists c \in \mathbb{R}^+)$ **then**
      Convergence $\leftarrow$ True.
    else
    $\mathcal{S}_{k+1} \leftarrow \text{span}(\mathcal{S}_k \cup \{v_{k+1}\})$, where v_{k+1} is a right singular vector associated with $\sigma_{min}[F(w_{k+1})]$.
      Increment k.
    end if
  end while
Output: w_{k+1}.

	landau(100) with $\varepsilon = 10^{-2}$			**airy(300)** with $\varepsilon = 10^{-4}$	
dimension	$\rho_\varepsilon(F_{\mathcal{S}_k})$	Rel. Error	dimension	$\rho_\varepsilon(F_{\mathcal{S}_k})$	Rel. Error
k = 1	1.008573182746177	$4.8e-005$	k =1	115102.27780548498503	$2.1e-011$
k = 2	1.008622026675976	$1.7e-007$	k = 2	115102.277803100136225	$1.9e-013$
k = 3	1.008621908490280	$6.9e-013$	k = 3	115102.277803077900899	0
k = 4	1.008621908489588	0	k = 4	115102.277803077900899	0
k = 5	1.008621908489588	0	k = 5	115102.277803077886347	0
k = 6	1.008621908489588	0	k = 6	115102.277803077886347	0
k = 7	1.008621908489588	0	k = 4	115102.277803077900899	0

Table 2.3: Iterations of Algorithm 3 are listed for the 100×100 **Landau** matrix and 300×300 **airy** matrix. Both of the matrices are taken from Eigtool. For the Landau matrix on the left, we observe superlinear convergence with respect to the subspace dimension. For the airy matrix on the right, the convergence occurs too quickly, so it is not possible to draw a rate of convergence conclusion.

Algorithm 4 Computation of ε-pseudospectral Radius of a Large-Scale Matrix

Require: A square matrix A, a positive real scalar ε, and a positive integer k_{max}
$z_0 \rightarrow$ an eigenvalue of A with the largest modulus, and $k \leftarrow 0$.
$\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right singular vector associated with $\sigma_{min}[F(z_0)]$.
Convergence $\rightarrow$ False.
while $\neg$*Convergence* **do**
  Local Search: Apply Algorith 1 to find $w_{k+1} = (r_*, \theta_*)$ such that $z_{k+1} = r_* e^{i\theta_*} \in \partial\Lambda_\varepsilon(F_{\mathcal{S}_k})$ with a vetical tangent line.
  if $(\sigma_{min}(w_{k+1}) = \varepsilon)$ and $(c.(1,0) \in \partial\sigma_{min}(w_{k+1}) \ \exists c \in \mathbb{R}^+)$ **then**
    Angular Search: $\theta_* \leftarrow \arg\min_{\theta\in[0,2\pi)} \sigma_{min}(r_*, \theta)$ and $\sigma_* \leftarrow \sigma_{min}(r_*, \theta_*)$.
    if $\sigma_{min}(r_*, \theta_*) = \varepsilon$ **then**
      Convergence $\leftarrow$ True.
    else
      $z_0 \leftarrow r_* e^{i\theta_*}$ and $k \leftarrow 0$.
      $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right singular vector associated with $\sigma_{min}[F(z_0)]$.
    end if
  else
    if $k = k_{max}$ **then**
      $z_0 \leftarrow z_{k+1}$ and $k \leftarrow 0$.
      $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right singular vector associated with $\sigma_{min}[F(z_0)]$.
    else
      $\mathcal{S}_{k+1} \leftarrow \text{span}(\mathcal{S}_k \cup \{v_{k+1}\})$, where v_{k+1} is a right singular related to $\sigma_{min}[F(z_{k+1})]$.
      Increment k.
    end if
  end if
  end while
Output: w_{k+1}.

Before First Angular Search		Before Second Angular Search		Before Third Angular Search	
dimension	Rel. Error	dimension	Rel. Error	dimension	Rel. Error
k = 1	$2.9e-001$	k =1	$4.3e-002$	k = 1	$1.0e-004$
k = 2	$2.6e-001$	k = 2	$2.7e-002$	k = 2	$3.2e-010$
k = 3	$2.1e-001$	k = 3	$1.1e-002$	k = 3	0
k = 4	$1.6e-001$	k= 4	$1.5e-003$	k = 4	0
k = 5	$1.2e-001$	k = 5	$8.0e-004$	k =5	0
k = 6	$9.3e-002$	k = 6	$7.1e-004$	k = 6	0
k = 7	$7.1e-002$	k = 7	$7.1e-004$	k = 7	0
k = 8	$5.6e-002$				
k = 9	$4.7e-002$				
k = 10	$4.6e-002$				
k = 11	$4.6e-002$				

Table 2.4: The progress of Algorithm 4 on the 400×400 **Grcar** matrix with $\varepsilon = 10^{-2}$ is illustrated. Three angular searches turn out to be necessary for global convergence. Subspace dimensions grow to 11, 7 and 7 before the applications of the angular searches.

Call	Largest Modulus	Smallest Modulus
convdiff(100)	$1.585983432465092e+005$	$5.141502626179558e+002$
riffle(100)	$6.684391491757834e-001$	$6.684391491757830e-001$
gallery5(100)	$3.369301264903174e+001$	$3.009873713611608e+001$

Table 2.5: The results returned by Algorithm 4 are listed for three matrices and for $\varepsilon = 10^{-4}$ when it is started from the eigenvalue with the largest modulus and from the eigenvalue with the smallest modulus.

Call	Largest Modulus	Smallest Modulus
convdiff(100)	$1.585983331052690e+005$	$5.961714828990463e+001$
riffle(100)	$5.099537791428121e-001$	$3.658741062905901e-001$
gallery5(100)	$4.650261694825272e+000$	$1.296145179556653e+00$

Table 2.6: The results are listed as in Table 2.5 but for $\varepsilon = 10^{-2}$.

Chapter 3

NUMERICAL RESULTS AND CONCLUDING REMARKS

In this chapter we present numerical results on some dense and sparse matrices taken from EigTool. Comparisons are performed with the algorithms introduced in [19] and [9], whose Matlab implementations are available on the web [1], [2]. The running times are measured in seconds, and using the **'tic toc'** commands in Matlab.

3.1 Dense and large sparse matrices

Running times of the algorithms in [19], [9] and Algorithm 4 are listed for various matrices and for $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-2}$ in Table 3.1 and Table 3.2, respectively. For Algorithm 4 and the Guglielmi-Overton algorithm, the relative errors defined as in (2.1.11) are also listed. When calculating these relative errros, $\rho_\varepsilon(A)$ is set equal to the values returned by the algorithm in [19], as this algorithm is extremely reliably and guaranteed to converge globally. We observe Algorithm 4 running faster than the Guglielmi-Overton algorithm on certain examples, and the opposite on other examples. Thus, superiority of one over the other is not clear. The results are also mixed for the relative errors

Table 3.3 and 3.4 for $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-2}$ provide additional results on some matrices with sensitive eigenvalues again taken from EigTool. In these examples, Algorithm 4 outperforms the algorithm in [9]. The latter even fails to return any result in

[1] `home.ku.edu.tr/~emengi/software/robuststability.html`
[2] `http://www.cs.nyu.edu/overton/software/psapsr/index.html`

Call	Radial-Circular [19]		G0 [9]		Algorithm 4	
	$\rho_\varepsilon(A)$	Time	R.Error	Time	R.Error	Time
airy(100)	$1.421530343095846e+03$	0.128686	$1.4e-015$	0.112700	$2.8e-015$	0.278038
airy(200)	$2.273729388837051e+04$	1.239163	$3.5e-015$	0.299156	$4.4e-015$	**0.24392**
airy(300)	$1.151022778030781e+05$	2.071003	$8.7e-016$	0.751727	$1.7e-015$	**0.59140**
grcar(100)	$2.852156096323250e+00$	0.563856	$7.1e-007$	2.917595	**6.1e-008**	7.700043
grcar(200)	$3.044111942833691e+00$	3.111310	$4.5e-005$	13.23464	**2.3e-007**	22.41166
grcar(300)	$3.112886972929427e+00$	10.35882	$2.2e-004$	32.33104	**2.1e-007**	54.86054
landau(100)	$9.987369366174040e-01$	0.205141	$1.7e-015$	0.070803	**1.4e-015**	0.199973
landau(200)	$9.986738414723663e-01$	0.497259	$5.6e-016$	0.290836	$3.1e-015$	0.482470
landau(300)	$9.997634683202712e-01$	1.708333	$9.9e-012$	0.644866	$9.9e-012$	1.225988

Table 3.1: A comparison of the running times of the three algorithms, [19] on the left, [9] in the middle, and Algorithm 4 on the right are provided. Running times are listed for all three algorithms. Relative errors are also listed but only for [9] and Algorithm 4 setting $\rho_\varepsilon(A)$ equal to the results returned by [19]. In all examples in this table $\varepsilon = 10^{-4}$.

Call	Radial-Circular [19]		G0 [9]		Algorithm 4	
	$\rho_\varepsilon(A)$	Time	R.Error	Time	R.Error	Time
airy(100)	$1.421540716466253e+03$	0.431686	$1.3e-015$	0.106321	$1.6e-013$	0.286386
airy(200)	$2.273731037526303e+04$	0.301536	$1.6e-014$	0.301536	$2.5e-011$	0.232880
airy(300)	$1.151022901107116e+05$	0.750562	$8.7e-016$	0.750562	0	0.602322
grcar(100)	$3.073508959045583e+00$	2.845931	$2.0e-004$	2.845931	$1.4e-007$	1.895643
grcar(200)	$3.176681601813824e+00$	13.05483	$3.3e-004$	2.23464	**2.3e-007**	7.148907
grcar(300)	$3.112886972929427e+00$	32.16144	$1.6e-004$	32.33104	$6.3e-008$	24.28514
landau(100)	$9.987369366174040e-01$	0.123417	$2.1e-011$	0.070803	$9.8e-010$	0.207350
landau(200)	$9.986738414723663e-01$	0.36554	$2.1e-011$	0.290836	$9.8e-010$	0.507489
landau(300)	$9.997634683202712e-01$	1.001046	$6.8e-011$	0.644866	$8.3e-010$	1.395247

Table 3.2: A comparison of the three algorithms as in Table 3.1, but for $\varepsilon = 10^{-2}$.

Call	Radial-Circular [19]		G0 [9]		Algorithm 4	
	$\rho_\varepsilon(A)$	Time	R.Error	Time	R.Error	Time
convdifffd(10)	$1.20777567716643e+02$	12.0824	eigs failed	-	$6.6e-011$	11.84696
dwave(2048)	$9.789022820577140e-01$	2023.06	eigs failed	-	$5.4e-002$	80.2456
olmstead(500)	$2.544018078191012e+03$	8.30617	eigs failed	-	$2.7e-010$	1.60091
supg(20)	$8.389519537007646e-02$	8.306173	eigs failed	-	$3.4e-006$	22.7190

Table 3.3: A comparison of the running times of the three algorithms on matrices with sensitive eigenvalues: [19] on the left, [9] in the middle, and Algorithm 4 on the right. The columns should be interpreted as in Table 3.1. Here $\varepsilon = 10^{-4}$.

some cases, because it calls the implicitly restarted Arnoldi package eigs, which cannot compute the desired singular value to desired accuracy.

Call	Radial-Circular [19]		G0 [9]		Algorithm 4	
	$\rho_\varepsilon(A)$	Time	R.Error	Time	R.Error	Time
convdifffd(10)	$1.290869591712596e+02$	11.4223	eigs failed	-	$6.6e-011$	11.84696
dwave(2048)	$9.888025406495821e-01$	1511.66	$1.8e-010$	84.26052	$7.1e-015$	299.408
olmstead(500)	$2.544108221698483e+03$	8.50491	$8.7e-016$	0.979768	0	1.60854
supg(20)	$1.027485979694405e-01$	8.93065	eigs failed	-	$3.0e-009$	20.0901

Table 3.4: A comparison of the three algorithms on sensitive matrices as in Table 3.3 but with $\varepsilon = 10^{-2}$.

3.2 Concluding remarks

In this thesis work, we have extended the algorithm in [18] for the computation of the pseudospectral radius of a matrix. Our approach benefits from the global overestimator and underestimator functions for eigenvalue functions in [20] and [33] to overcome the nonsmooth nature of the problem. Additionally, the subspace approach in [13] combined with a restart strategy is adopted to deal with large matrices. The algorithm based on radial circular searches in [19] is still the most reliable choice, however the framework here is applicable to large matrices unlike that algorithm, which is suitable for only small and medium scale matrices. The numerical experiments indicate that the proposed framework and the algorithm in [9] exhibit similar running time behavior, however the algorithm here appears to be more reliable on matrices with sensitive eigenvalues. The algorithm introduced should be improved in certain directions. In particular, it should be supplied with better stopping criteria, and it can be generalized for nonlinear eigenvalue problems.

Bibliography

[1] L. Breiman and A. Cutler. A deterministic algorithm for global optimization, Math. Program., 58 (1993), pp.179-199.

[2] S. Boyd and V. Balakrishnan. A regularity result for the singular values of a transfer matrix and a quadratically convergent algorithm for computing its L_∞-norm. *Systems and Control Letters*, 15:1-7, 1990.

[3] N. A. Bruinsma and M. Steinbuch. A fast algorithm to compute the H_∞-norm of a transfer function matrix. *Systems and Control Letter*, 14:287-293, 1990.

[4] A. Bunse-Gerstner, R. Byers, V. Mehrmann, and N. K. Nichols. Numerical computation of an analytic singular value decomposition of a matrix valued function. *Numer. Math.*,60:1-39, 1991.

[5] J. V. Burke, A. S. Lewis and M. L. Overton. Robust stability and a criss-cross algorithm for pseudospectra. *IMA J. Numer. Anal.*, 23:359-375, 2003.

[6] R. Byers. A bisection method for measuring the distance of a stable matrix to the unstable matrices. SIAM J. Sci. Stat. Comp., 9:875-881, 1988.

[7] J. W. Demmel. A counter example for two conjectures about stability. *IEEE Trans. Auto. Control*, AC-32340-343, 1987.

[8] S. Gerschgorin. On bounding the eigenvalues of a matrix (in german). *Izv. Akad. Nauk. SSSR Otd Mat. Estest.,* 1:749-754, 1931.

[9] N. Guglielmi and M. L. Overton. Fast algorithms for the approximation of the pseudospectral abscissa and pseudospectral radius of a matrix.*SIAM J. Matrix Anal. Appl.,* 32(4):1166-1192, 201.

[10] R. A. Horn and C. A. Johnson. *Matrix Analysis*. Cambridge University Press, Cambridge, UK, 1990.

[11] T. Kato. *A short introduction to Perturbation Theory for Linear Operators.* Springer-Verlag 1982.

[12] V. I. Kostin and S. I. Razzakov. On convergence of the power orthogonal method of spectrum computing, Trans. Inst. Math. Sib. Branch Acad. Sci., v. 6, pp. 55-84.

[13] D. Kressner and B. Vandereycken. Subspace methods for computing the pseudospectral abscissa and the stablity radius. *SIAM J. Matrix Anal. Appl.*, 35(1):292-313, 2014.

[14] P. Lancaster. On eigenvalues of matrices dependent on a parameter. *Numer. Math.*, 6:377-387, 1964.

[15] P. Lancaster and M. Tismenetsky. *The Theory of Matrices: With Applications.* Academic Press,1985.

[16] P. Lancaster ans P. Psarrakos. On the pseudospectra of a matrix polynomials. *SIAM J. Matrix Anal. Appl.,* 27(1):115-129, 2005.

[17] H. J. Landau. On Szeü's eigenvalue distribution theorem and non-Hermitian kernels, J. Analyse Math., 28 (1975), pp.335-357.

[18] K. Meerbergen, E. Mengi, W. Michiels and R. Van Beeumen. Computation of psudospectral abscissa for large scale nonlinear eigenvalue problems. *IMA J. Numer. Anal.,* Submitted.

[19] E. Mengi and M. L. Overton. Algorithms for the computation of the pseudospectral radius and the numerical radius of a matrix. *IMA J. Numer. Anal.* , 25(4):648-669, 2005.

[20] E. Mengi. A support function based algorithm for optimization with eigenvalue constraints. *SIAM J. Optim.,* 2014 Submitted.

[21] E. Mengi. *Numerical Methods*, Lecture Notes, 2014.

[22] W. Michiels and S. I. Niculescu. *Stability and Stabilization of Time-Delay Systems (Advances in Design & Control) (Advances in Design and Control).*Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2007.

[23] C. B. Moler. *Numerical Computing with MATLAB*: Revised Reprint, Society for Industrial and Applied Mathematics, 2010.

[24] S. A. Pijavskii. *An algoritm for finding the absolute extremum of a function*, USSR Computational Mathematics and Mathematical Physics (1972) 57-67.

[25] F. Rellich. *Perturbation Theory of Eigenvalue Problems.* Gordon and Breach, 1969.

[26] Y. Saad. *Numerical Methods for Large Scale Eigenvalue Problems*, Society for Industrial and Applied Mathematics, 2011.

[27] B. Shubert. *A sequential method seeking the global maximum of a function*, SIAM Journal of Numerical Analysis 9 (3) (1972) 379-388.

[28] L. N. Trefethen. Pseudospectra of matrices. In D. F. Griffiths and G. A. Watson, eds., Numerical Analysis 1991, Longman, 1992.

[29] L. N. Trefethen, S. C. Reddy, and T. A. Driscoll. *Hydrodynamic stability without eigenvalues*, Science, 261 (1993), pp.578-584.

[30] L. N. Trefethen. *Pseudospectra of linear operators* ICIAM '95: Proceedings of the Third Internatinal Congress on Industrial and Applied Mathematics, Akademie-Verlag, Berlin, 1996,401-434; also SIAM Review 39 (1997), 383-406.

[31] L. N. Trefethen and D. Bau. *Numerical Linear Algebra.* SIAM, 1997.

[32] L. N. Trefethen and M. Embree. *Spectra and Pseudospectra: The Bahavior of Nonnormal Matrices and Operators*, Princeton University Press, Princeton, NJ, 200.

[33] E. Mengi, E. A. Yildirim, and M. Kilic. Numerical optimization of eigenvalues of Hermitian matrix functions. *SIAM J. Matrix Anal. Appl.,* 35(2):699-724, 2014.

[34] J. H. Wilkinson. *The Algebraic Eigenvalue Problem.* Clarendon Press, 1965.

[35] J. H. Wilkinson. *Sensitivity of eigenvalues II*, Util. Math., 30 (1986), pp. 243-286.

[36] T. G. Wright and L. N. Trefethen. Pseudospectra of rectangular matrices. *IMA J. Numer. Anal.,* 22(4):501-519, 2002.

[37] T. G. Wright. Eigtool: a graphical tool for nonsymmetric eigenproblems. Oxford University Computing Laboratory. **https://github.com/eigtool/eigtool**.