Estimating Norms of Matrix Functions using Numerical Ranges

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Abstract

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Given a square matrix A, we consider sets S in the complex plane for which there exists a constant K such that

$$||p(A)|| \leq K \sup_{z \in S} |p(z)| \text{ for all polynomials } p, \tag{1}$$

where $|| \cdot ||$ is the operator norm induced by the 2-norm for vectors.

There are many choices for such a constant K and a set S. For example, when $K = 1$ and $S = \{z \in \mathbb{C} : |z| \leq ||A||\}$, the result (1) is known as von Neumann's inequality. If A is a normal matrix, then the inequality (1) holds with $K = 1$ and $S = \sigma(A)$, the set of eigenvalues of A.

In 2004, M. Crouzeix made the interesting conjecture that the inequality (1) holds for any square matrix $A \in \mathbb{C}^{n,n}$, where K is 2 and S is the numerical range of A defined by

$$W(A) = \{\mathbf{x}^* A \mathbf{x} : \mathbf{x} \in \mathbb{C}^n, ||\mathbf{x}|| = 1\}.$$

The conjecture is proved when the dimension n is 2, but it has not been proved or disproved yet for general matrices of size larger than 2. In this thesis, we show that the conjecture

holds for the matrices of the form

$$\begin{pmatrix} \lambda & \alpha_1 & & & \\ & \ddots & \ddots & & \\ & & & \lambda & \alpha_{n-1} \\ \alpha_n & & & & \lambda \end{pmatrix}, \tag{2}$$

where λ and α_js are complex numbers.

Additionally, we will define three constants for a given square matrix and show their relation. Then, we will show how they could be used for Crouzeix's conjecture. Moreover, we will compute the constants explicitly for the matrices of the form in (2).

Finally, we show an application of Crouzeix's conjecture to the generalized minimal residual method (GMRES). There are many results about the convergence rate of the GMRES algorithm when the numerical range of the coefficient matrix does not contain the origin, but we suggest a GMRES error bound which can be used even when the numerical range contains the origin.

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Chapter 1

INTRODUCTION

Notation: We will use the following notation throughout the thesis:

- $||\cdot||$ denotes the Euclidean norm for vectors and the spectral norm for matrices, where the latter is defined by

$$||A|| = \max\{||A\mathbf{x}|| : \mathbf{x} \in \mathbb{C}^n, ||\mathbf{x}|| = 1\} \text{ for } A \in \mathbb{C}^{n,n}.$$

- $||f||_S$ is the L^∞- norm of the function f on a subset S of the complex plane.

In many cases, we wish to estimate $||f(A)||$, where A is a matrix and f is a complex-valued function defined on a subset of the complex plane. For example, the stability of the difference scheme $\mathbf{y}_k = A\mathbf{y}_{k-1}$ is determined by $||A^k||$; the stability of the system of differential equations $\mathbf{y}'(t) = A\mathbf{y}(t)$ is determined by $||e^{tA}||$; the kth relative residual norm of the generalized minimal residual method for solving the linear system $A\mathbf{x} = \mathbf{b}$ is bounded by

$$\min\{||p(A)|| : p \text{ is a polynomial of degree at most } k \text{ with } p(0) = 1\}.$$

If A is a normal matrix (a matrix unitarily similar to a diagonal matrix), then it can be easily shown that $||f(A)||$ is the maximum absolute value of f over the spectrum $\sigma(A)$ (the set of all the eigenvalues of A); that is, $||f(A)|| = ||f||_{\sigma(A)}$. If A is nonnormal, however, then the spectrum of A is not enough to estimate $||f(A)||$. For example, if A is the Jordan block of size n with diagonal entry 0,

$$A = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix},$$

then $||A^k|| = 1$ for $1 \leq k < n$, but $\sigma(A) = \{0\}$.

In this thesis, we will show several ways to identify a subset S in the complex plane such that $||f(A)||$ can be bounded by using $||f||_S$, where the set S is independent of the functions f. For example, such a set S could be a disk of radius $||A||$ or the numerical range of A which will be discussed later. A brief outline of this thesis is as follows: Chapter 1 reviews some basic concepts of matrix functions and numerical ranges. Then, we show some known results to estimate the norms of matrix functions. In Chapter 2, we state a conjecture which estimates $||f(A)||$ using the numerical range of A and we prove it for a class of matrices. In Chapter 3, we define some constants related to a matrix and discuss their relations. Finally, in Chapter 4, we give an application of the conjecture stated in Chapter 2.

Remark 1. In this thesis, we focus on finite dimensional matrices, but many concepts go over to (bounded) linear operators on a Hilbert space (or on a Banach space). For example, $f(A)$ will be defined in the following section for a given analytic function f and a square matrix A, but the definition can be generalized to operators. Likewise, the concept of numerical ranges also can be generalized to any linear operator on a Banach space.

1.1 Matrix functions

Let A be an n by n complex valued matrix and f be an analytic function on a domain containing the spectrum of A. The assumption that f is analytic around the spectrum of A is not necessary to define $f(A)$, but it is enough to consider such functions for the arguments in this thesis. There are a few ways of defining matrix functions. We give two definitions here (see [22, 21]). Let $p(z) = a_m z^m + a_{m-1} z^{m-1} + \cdots + a_1 z + a_0$ be an ordinary polynomial in $z \in \mathbb{C}$ with complex-valued coefficients $a_0, \ldots, a_m$. Then, for any matrix $A \in \mathbb{C}^{n,n}$, we can naturally define $p(A)$ by

$$p(A) = a_m A^m + a_{m-1} A^{m-1} + \cdots + a_1 A + a_0 I,$$

where I is the n by n identity matrix. If A is diagonalizable, say $A = Q\Lambda Q^{-1}$ where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix with diagonal entries $\lambda_1, \ldots \lambda_n$, then we can derive the property

$$p(A) = Qp(\Lambda)Q^{-1},$$

where $p(\Lambda) = \mathrm{diag}(p(\lambda_1), \ldots, p(\lambda_n))$. If A is not diagonalizable, then we can express $p(A)$ using Jordan canonical form $A = VJV^{-1}$, where $J = \mathrm{diag}(J_{n_1}(\lambda_1), \ldots, J_{n_p}(\lambda_p))$ with

$$J_{n_k}(\lambda_k) = \begin{pmatrix} \lambda_k & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_k & 1 \\ & & & \lambda_k \end{pmatrix} \in \mathbb{C}^{n_k \times n_k},$$

as follows:

$$p(A) = Vp(J)V^{-1},$$

where

$$p(J) = \mathrm{diag}(p(J_{n_1}(\lambda_1)), \ldots, p(J_{n_p}(\lambda_p))).$$

Writing $J_r(\lambda) = \lambda I + N$ where I is the r by r identity matrix and N is the Jordan block of size r with diagonal entry 0 (note $N^i = O$ for $i \geq r$), the following shows how to construct the matrix $p(J_r(\lambda))$:

$$\begin{aligned} p(J_r(\lambda)) &= \sum_{j=0}^{m} a_j(\lambda I + N)^j = \sum_{j=0}^{m}\sum_{i=0}^{j} \frac{j!}{i!(j-i)!} a_j \lambda^{j-i} N^i \\ &= \sum_{i=0}^{m} \frac{1}{i!} \left\{ \sum_{j=i}^{m} \frac{j!}{(j-i)!} a_j \lambda^{j-i} \right\} N^i \\ &= \sum_{i=0}^{m} \frac{1}{i!} p^{(i)}(\lambda) N^i. \end{aligned}$$

Its component expression is

$$p(J_r(\lambda)) = \begin{pmatrix} p(\lambda) & p'(\lambda) & \frac{1}{2!}p''(\lambda) & \cdots & & \frac{1}{(r-1)!}p^{(r-1)}(\lambda) \\ 0 & p(\lambda) & p'(\lambda) & \ddots & & \vdots \\ 0 & 0 & p(\lambda) & \ddots & \ddots & \vdots \\ \vdots & \vdots & 0 & \ddots & \ddots & \frac{1}{2!}p''(\lambda) \\ \vdots & \vdots & \vdots & & \ddots & p'(\lambda) \\ 0 & 0 & 0 & \cdots & \cdots & p(\lambda) \end{pmatrix}.$$

Now we generalize $p(A)$ to $f(A)$ for any function f analytic around the spectrum of A.

Definition 2. ($f(A)$ via Jordan canonical form) Assume that A has the following Jordan canonical form:

$$A = V \begin{pmatrix} J_1 & & & \\ & J_2 & & \\ & & \ddots & \\ & & & J_p \end{pmatrix} V^{-1}, \text{ where } J_k = \begin{pmatrix} \lambda_k & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_k & 1 \\ & & & \lambda_k \end{pmatrix} \in \mathbb{C}^{n_k \times n_k}.$$

Then, $f(A)$ is defined by

$$f(A) = V \begin{pmatrix} f(J_1) & & & \\ & f(J_2) & & \\ & & \ddots & \\ & & & f(J_p) \end{pmatrix} V^{-1}, \text{ where } f(J_k) = \begin{pmatrix} f(\lambda_k) & f'(\lambda_k) & & \frac{f^{(n_k-1)}(\lambda_k)}{(n_k-1)!} \\ & f(\lambda_k) & \ddots & \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{pmatrix}.$$

The matrix function $f(A)$ is called the *primary matrix function* associated with the function $f(z)$ (Chapter 6, [21]). Here we note the following facts:

- The definition of $f(A)$ is independent of the ordering of blocks in the Jordan canonical form;

- If A has an eigendecomposition $A = Q\text{diag}(\lambda_1, \ldots, \lambda_n)Q^{-1}$, then

$$f(A) = Q\text{diag}(f(\lambda_1), \ldots, f(\lambda_n))Q^{-1}.$$

Example 3. *Consider the matrix* $A = \begin{bmatrix} -2 & 2 & -2 & 4 \\ -1 & 2 & -1 & 1 \\ 0 & 0 & 1 & 0 \\ -2 & 1 & -1 & 4 \end{bmatrix}$ *(see [31, p.56]), which has the Jordan canonical form* $A = PJP^{-1}$*, where* $P = \begin{bmatrix} -1 & -2 & 2 & -4 \\ 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ -1 & -1 & 1 & -2 \end{bmatrix}$ *and* $J = \begin{bmatrix} 2 & & & \\ & 1 & 1 & \\ & & 1 & \\ & & & 1 \end{bmatrix}$.

By Definition 2, we have

- $e^A = P \begin{bmatrix} e^2 & & & \\ & e & e & \\ & & e & \\ & & & e \end{bmatrix} P^{-1}$;

- $\sin(A) = P \begin{bmatrix} \sin(2) & & & \\ & \sin(1) & \cos(1) & \\ & & \sin(1) & \\ & & & \sin(1) \end{bmatrix} P^{-1}$;

- $\log(A) = P \begin{bmatrix} \log(2) & & & \\ & 0 & 1 & \\ & & 0 & \\ & & & 0 \end{bmatrix} P^{-1}$,

where log is the principle branch of logarithm.

The second way of defining $f(A)$ is to use the Cauchy integral formula [15] which states that if f is analytic inside and on a simple closed curve Γ and z_0 is any point inside of Γ, then

$$f(z_0) = \frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z - z_0} dz.$$

Definition 4. ($f(A)$ via Cauchy integral) If Γ is a simple closed curve or union of simple closed curves inside the domain of f enclosing the spectrum of $A \in \mathbb{C}^{n,n}$, then $f(A)$ is defined by

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

where I is the n by n identity matrix.

Note that the inverse matrix of $zI - A$ in the integrand is defined on Γ since Γ is disjoint from the spectrum of A. The Cauchy integral formula for matrices is hard to evaluate especially for $n > 2$, but it can be used to give a bound for $||f(A)||$ (which will be shown later). Moreover, the definition above can be generalized to bounded linear operators on a Banach space. Using the Cauchy integral formula, we can show the following result:

Theorem 5. *[17, Theorem 11.2.3] If f has a power series expansion*

$$f(z) = \sum_{k=0}^{\infty} c_k z^k$$

on an open disk containing the eigenvalues of A, then

$$f(A) = \sum_{k=0}^{\infty} c_k A^k.$$

By the theorem above, we have the following power series expansions for $e^A, \sin(A)$, and $\cos(A)$:

$$\begin{aligned} e^A &= \sum_{k=0}^{\infty} \frac{1}{k!} A^k \\ \sin(A) &= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} A^{2k+1} \\ \cos(A) &= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} A^{2k} \end{aligned}$$

When A is diagonalizable, it is easy to show that the two definitions for $f(A)$ - via Jordan canonical decomposition and Cauchy integral formula - are equivalent. Theorem 6.2.28 in [21] shows their equivalence for general matrices. We show the following properties of $f(A)$ without proof:

Theorem 6. *Let $A \in \mathbb{C}^{n,n}$ and let f, g be analytic functions in a domain containing the spectrum of A. Then,*

(a) $f(XAX^{-1}) = Xf(A)X^{-1}$ for any invertible matrix $X \in \mathbb{C}^{n,n}$.

(b) If $A = diag(A_1, \ldots, A_r)$ is block diagonal, then $f(A) = diag(f(A_1), \ldots, f(A_r))$.

(c) The eigenvalues of $f(A)$ are $f(\lambda_i)$, where the λ_i are the eigenvalues of A.

(d) $f(A^T) = f(A)^T$.

(e) $f(A)$ commutes with A and if X commutes with A then X commutes with $f(A)$.

(f) If $h(z) = f(z) + g(z)$, then $h(A) = f(A) + g(A)$. Similarly, if $h(z) = f(z)g(z)$, then $h(A) = f(A)g(A)$.

(g) $f(I \otimes A) = I \otimes f(A)$ and $f(A \otimes I) = f(A) \otimes I$, where I is an identity matrix and $\otimes$ is the Kronecker product.

Note that we have the following identities by (f) in Theorem 6:

$$\begin{aligned} \sin^2(A) + \cos^2(A) &= I \\ \cos(A) + i\sin(A) &= e^{iA} \\ I + A + A^2 + \cdots &= (I - A)^{-1} \text{ (for } A \text{ with } \rho(A) < 1) \end{aligned}$$

1.2 Numerical ranges

The numerical range or field of values of a matrix $A \in \mathbb{C}^{n,n}$ is a set in the complex plane defined by

$$W(A) = \{\mathbf{x}^* A \mathbf{x} : \mathbf{x} \in \mathbb{C}^n, ||\mathbf{x}|| = 1\},$$

where $\mathbf{x}^*$ is the conjugate transpose of the column vector $\mathbf{x}$. More generally, if T is a bounded linear operator on a Hilbert space $\mathcal{H}$, then $W(T)$ consists of the complex values $\langle T\mathbf{x}, \mathbf{x}\rangle$ with unit vectors $\mathbf{x} \in \mathcal{H}$. If λ is an eigenvalue of $A \in \mathbb{C}^{n,n}$ with a unit eigenvector $\mathbf{x}$, then $\lambda = \mathbf{x}^* A\mathbf{x} \in W(A)$. Therefore, all the eigenvalues of A are contained in $W(A)$. The numerical range gives more information about A than the spectrum $\sigma(A)$ does alone. For example, there are many matrices A such that $\sigma(A)$ is the singleton $\{\lambda\}$, but if $W(A) = \{\lambda\}$ then $A = \lambda I$; if A is Hermitian ($A = A^*$), then $\sigma(A) \subset \mathbb{R}$, but the converse does not hold. Meanwhile, A is Hermitian *if and only if* $W(A) \subset \mathbb{R}$. The following are general properties of the numerical range.

Theorem 7. *Let $A \in \mathbb{C}^{n,n}$. Then,*

(a) $W(\alpha A + \beta I) = \alpha W(A) + \beta$ for any $\alpha, \beta \in \mathbb{C}$.

(b) $W(U^* AU) = W(A)$ for any unitary matrix $U \in \mathbb{C}^{n,n}$.

(c) $W(A)$ is a compact convex subset of $\mathbb{C}$ (Toeplitz-Hausdorff theorem).

(d) $\sigma(A) \subset W(A) \subset \{z \in \mathbb{C} : |z| \leq ||A||\}$.

(e) If A is a normal matrix, then $W(A)$ is a convex polygon whose vertices are eigenvalues of A.

(f) If A is Hermitian, then $W(A) = [\lambda_{\min}(A), \lambda_{\max}(A)]$, where $\lambda_{\min}$ and $\lambda_{\max}$ denote the minimum and maximum eigenvalue of A, respectively.

(g) If A is a 2 by 2 matrix with eigenvalues λ_1 and λ_2, then $W(A)$ is an elliptical disk with foci λ_1, λ_2 and minor axis with length $(tr(A^*A) - |\lambda_1|^2 - |\lambda_2|^2)^{1/2}$, where $tr(\cdot)$ denotes the trace of a matrix.

For a bounded linear operator T on a complex Hilbert space, $W(T)$ is a bounded convex subset of $\mathbb{C}$, but it is not closed in general. For example, if T is the unilateral shift, defined on l^2 by

$$T(x_1, x_2, \ldots) = (0, x_1, x_2, \ldots),$$

then the numerical range of T is the open unit disk centered at the origin.

By the Toeplitz-Hausdorff theorem, it is enough to know its boundary to determine the numerical range of $A \in \mathbb{C}^{n,n}$. Here we show a computational algorithm suggested by Johnson [23]. Given $A \in \mathbb{C}^{n,n}$, we can write $A = A_H + A_K$, where $A_H = (A + A^*)/2$ is the Hermitian part of A and $A_K = (A - A^*)/2$ is the skew-Hermitian part of A. Since $\mathrm{Re}(\mathbf{x}^* A\mathbf{x})$, the real part of $\mathbf{x}^* A\mathbf{x}$, is $\mathbf{x}^* A_H \mathbf{x}$,

$$\min\{\mathrm{Re}(z) : z \in W(A)\} = \min_{||\mathbf{x}||=1} \mathbf{x}^* A_H \mathbf{x} = \lambda_{\min}(A_H),$$
$$\max\{\mathrm{Re}(z) : z \in W(A)\} = \max_{||\mathbf{x}||=1} \mathbf{x}^* A_H \mathbf{x} = \lambda_{\max}(A_H).$$

Therefore the numerical range of A lies within the two vertical lines $x = \lambda_{\min}(A_H)$ and $x = \lambda_{\max}(A_H)$, and its boundary is tangent to the lines at the points $\mathbf{x}^* A\mathbf{x}$ where $\mathbf{x}$ is a unit eigenvector of A_H corresponding to $\lambda_{\min}(A_H)$ or $\lambda_{\max}(A_H)$. Since $W(e^{i\theta}A) = e^{i\theta}W(A)$, applying the same argument above to $e^{i\theta}A$ for each $\theta \in [0, \pi]$ determines the intersections between the boundary of $W(A)$ and two parallel lines (whose slopes are $\tan(\pi/2 - \theta)$) within which $W(A)$ lies. Figure 1.1 shows such an example when $\theta = 0, \pi/4, \pi/2$. The following summarizes the algorithm to find the boundary of $W(A)$: for each $\theta \in [0, \pi]$,

1. Let $A_\theta = (e^{i\theta}A + e^{-i\theta}A^*)/2$.

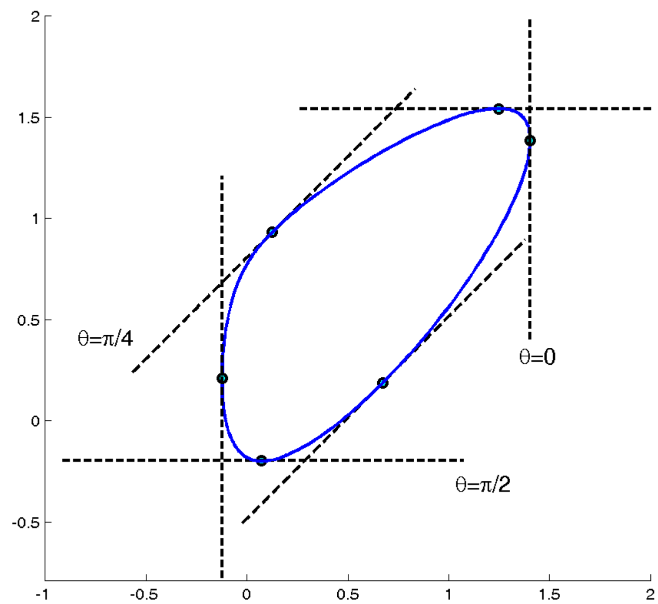
2. Find unit eigenvectors $\mathbf{x}$ of A_θ corresponding to $\lambda_{\min}(A_\theta)$ and $\lambda_{\max}(A_\theta)$.

3. Then, $\mathbf{x}^* A\mathbf{x}$ is a point on the boundary of $W(A)$.

Figure 1.2 shows the numerical ranges for various test matrices - grcar, circulant, perturbed Jordan block, and hanowa matrices, using MATLAB function 'gallery'. Each test matrix is described below:

- `gallery('grcar',n)` generates an n by n Toeplitz matrix with -1s on the subdiagonal,

Figure 1.1: Construction of the boundary of a numerical range.



1s on the diagonal, and 3 superdiagonals of 1s. For example, when $n = 5$, it is

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 1 \\ 0 & -1 & 1 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}.$$

The Grcar matrix was introduced in [18], and it is a popular example of a matrix whose spectrum is in the right half-plane but whose numerical range is not.

- `gallery('circul',n)` generates the circulant matrix whose first row is $(1, 2, \ldots, n)$ and each row is obtained from the previous one by cyclically permuting the entries one step forward. For example, when $n = 4$, it is

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 1 & 2 & 3 \\ 3 & 4 & 1 & 2 \\ 2 & 3 & 4 & 1 \end{pmatrix}.$$

The eigenvectors of the circulant matrix of size n are given by $u_k = (1, \omega_k, {\omega_k}^2, \ldots, {\omega_k}^{n-1})^T$, where $\omega_k = e^{2\pi ik/n}$ for $k = 1, \ldots, n$, and the corresponding eigenvalues are given by

$$\begin{aligned} \lambda_k &= (1, 2, \ldots, n)u_k \\ &= \sum_{j=1}^{n} j{\omega_k}^{j-1}. \end{aligned}$$

Using the identities

$$\sum_{j=1}^{n} j \cos\left(\frac{2\pi k(j-1)}{n}\right) = \begin{cases} \frac{-n}{2}, & \text{if } k \neq n \\ \frac{n(n+1)}{2}, & \text{if } k = n \end{cases},$$

we can show that the real values of λ_k are $-n/2$ for $k = 1, \ldots, n-1$ and $n(n+1)/2$ for $k = n$.

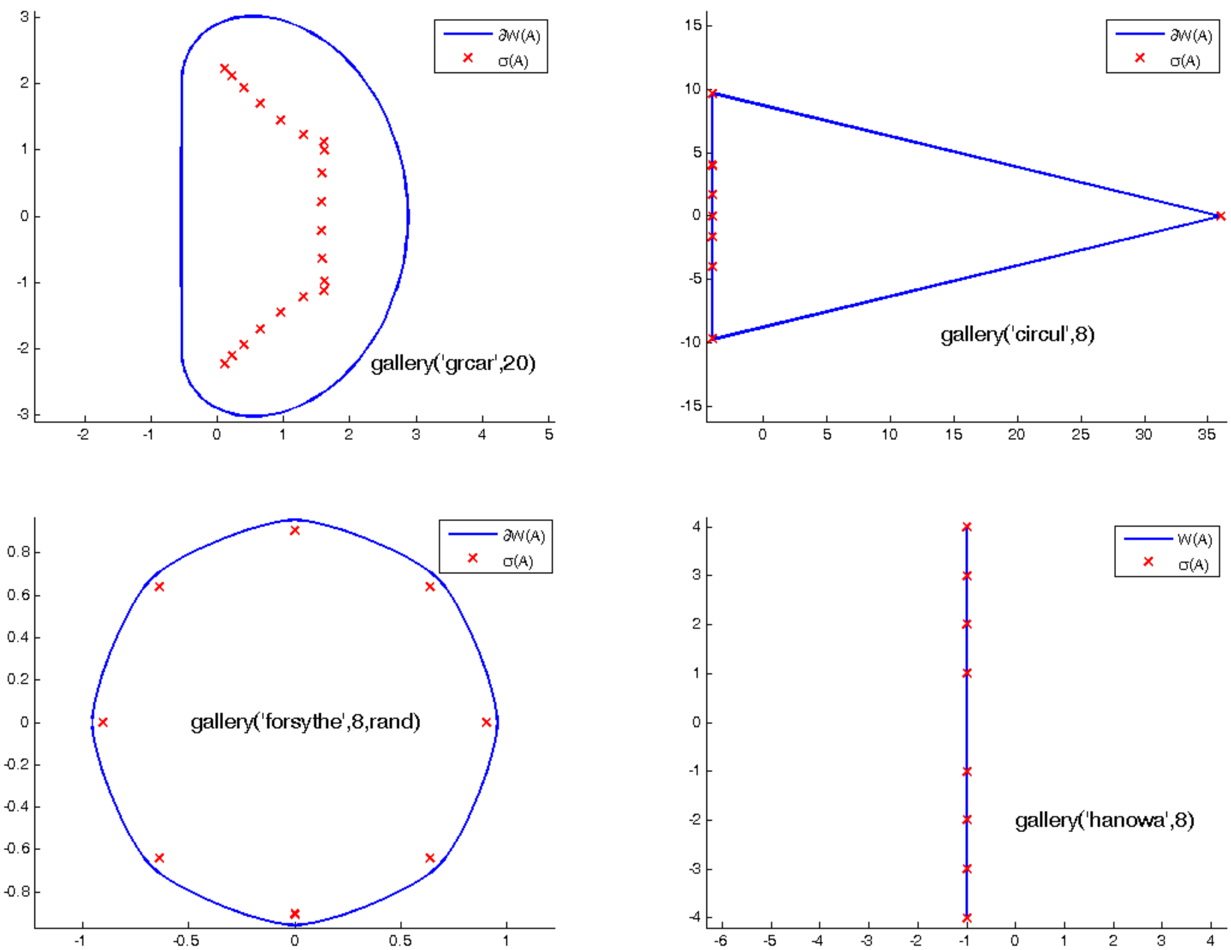
- `gallery('forsythe',n,`ν`)` generates the n by n perturbed Jordan block

$$\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ \nu & & & 0 \end{pmatrix}.$$

The $n \times n$ Forsythe matrix is the companion matrix of the polynomial $p(z) = z^n - \nu$.

- `gallery('hanowa',n)` generates an n by n (normal) matrix whose eigenvalues lie on

Figure 1.2: Examples of $W(A)$; the red **x**s denote eigenvalues.



a vertical line. For example, when $n = 4$, we have the following matrix

$$\begin{pmatrix} -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & -2 \\ 1 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 \end{pmatrix}.$$

As we define the spectral radius $\rho(A)$ of a matrix A as the largest absolute value in the spectrum of A, we define the numerical radius $r(A)$ as the largest absolute value in the numerical range of A; that is,

$$r(A) = \max_{z \in W(A)} |z| = \max_{||\mathbf{x}||=1} |\mathbf{x}^* A \mathbf{x}|.$$

The following are well-known results about the numerical radius.

Theorem 8. *For $A, B \in \mathbb{C}^{n,n}$,*

(a) $r(A) = 0$ *if and only if* $A = O$*,*

(b) $r(\alpha A) = |\alpha| r(A)$ *for any* $\alpha \in \mathbb{C}$*,*

(c) $r(A + B) \leq r(A) + r(B)$*,*

(d) $r(A) \leq r(|A|)$*, where* $|A| \in \mathbb{C}^{n,n}$ *such that* $|A|_{ij} = |A_{ij}|$*,*

(e) $r(A^k) \leq r(A)^k$ *for* $k = 1, 2, \ldots$ *(the power inequality for the numerical radius),*

(f) $r(A_1 \oplus \cdots \oplus A_m) = \max_{1 \leq j \leq m} r(A_j)$*,*

(g) $\rho(A) \leq r(A) \leq ||A|| \leq 2r(A)$*,*

(h) $r(U^* A U) = r(A)$ *for any unitary matrix* U*.*

From (g), we have $||A||/2 \leq r(A)$. Since $||A^k|| \leq 2r(A^k) \leq 2r(A)^k$ for any positive integer k, we have the following stronger result between $||A||$ and $r(A)$:

$$\sup_{k \in \mathbb{N}} \left(\frac{||A^k||}{2} \right)^{1/k} \leq r(A),$$

which will be discussed again in Chapter 3.

A matrix $A \in \mathbb{C}^{n,n}$ is called a contraction if $||A|| \leq 1$, and it is called a numerical contraction if $r(A) \leq 1$. In [2], T. Ando has proved the following property of numerical contractions.

Theorem 9. *For $A \in \mathbb{C}^{n,n}$, the following are equivalent:*

(a) A is a numerical contraction.

(b) $A = (I+M)^{1/2}C(I-M)^{1/2}$ for a Hermitian contraction M and a contraction C. Moreover, there exist such matrices C and M such that C is isometric on the range of $I-M$.

(c) $A = 2(I-C^*C)^{1/2}C$ for a contraction C.

Using Theorem 9, H. Watanabe proved the following interesting result (see [39], where the result is shown to be true for any bounded linear operator on a Hilbert space):

Corollary 10. *If $A \in \mathbb{C}^{n,n}$ is a numerical contraction, then $Ax = x$ implies $A^*x = x$.*

Proof. First, the following argument shows that the result holds when A is a contraction:

$$\begin{aligned} ||A^*x - x||^2 &= ||A^*x||^2 + ||x||^2 - 2\mathrm{Re}(A^*x, x) \\ &\leq 2||x||^2 - 2\mathrm{Re}(x, Ax) \quad (\text{since } ||A^*|| = ||A|| \leq 1) \\ &= 0 \quad (\text{since } Ax = x). \end{aligned}$$

If A is a numerical contraction, then by Theorem 9 there exist a Hermitian contraction M and a contraction C such that

$$A = (I+M)^{1/2}C(I-M)^{1/2}$$

and that C is isometric on the range of $I-M$. Assume $Ax = x$ for a nonzero vector x.

Since

$$\begin{aligned} ||x||^2 &= x^*Ax = x^*(I+M)^{1/2}C(I-M)^{1/2}x \\ &\le ||(I+M)^{1/2}x|| \cdot ||C(I-M)^{1/2}x|| \\ &\le ||(I+M)^{1/2}x|| \cdot ||(I-M)^{1/2}x|| \quad \text{(since } ||C|| \le 1) \\ &\le \frac{1}{2}\left(||(I+M)^{1/2}x||^2 + ||(I-M)^{1/2}x||^2\right) \\ &= ||x||^2, \end{aligned}$$

we have

$$C(I-M)^{1/2}x = \delta(I+M)^{1/2}x, \tag{1.1}$$

for some $\delta > 0$ and $x^*(I+M)x = x^*(I-M)x$ which implies

$$x^*Mx = 0. \tag{1.2}$$

Since C is isometric on the range of $I-M$, we have from (1.1) and (1.2),

$$\begin{aligned} ||x||^2 = x^*(I-M)x &= x^*(I-M)^{1/2}C^*C(I-M)^{1/2}x \\ &= \delta x^*(I-M)^{1/2}C^*(I+M)^{1/2}x \\ &= \delta x^*A^*x \\ &= \delta||x||^2. \end{aligned}$$

Therefore, $\delta = 1$ and $x = Ax = (I+M)x$ by (1.1), which implies $Mx = 0$ and thus $Cx = x$ from (1.1). Since C is a contraction, we have $C^*x = x$. Now, the result $A^*x = x$ is proved by the following argument:

$$\begin{aligned} A^*x &= (I-M)^{1/2}C^*(I+M)^{1/2}x \\ &= (I-M)^{1/2}C^*x \quad \text{(since } Mx = 0) \\ &= (I-M)^{1/2}x \\ &= x \quad \text{(since } Mx = 0). \end{aligned}$$

□

Remark 11. The factorization in (b) in Theorem 9 can be expressed as $A = 2\cos(B)C\sin(B)$ for a Hermitian matrix B such that $\frac{1}{2}(I + M) = \cos^2(B)$.

1.3 Estimating $||f(A)||$ using sets in the complex plane

Let A be an n by n matrix (or a bounded linear operator on a Hilbert space). For a fixed constant $K > 0$, a closed subset Ω of $\mathbb{C}$ is called a K-*spectral set* for A if it contains the spectrum of A and $||f(A)|| \leq K||f||_\Omega$ for all rational functions f with poles outside Ω. In particular, in case that $K = 1$, Ω is called a *spectral set* for A.

In the beginning of the introduction, we have seen that if A is a normal matrix, then $||f(A)|| = ||f||_{\sigma(A)}$. A simple proof of the result is as follows: if A is normal, there exist a unitary matrix U and a diagonal matrix $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$ such that $A = UDU^*$. Thus,

$$||f(A)|| = ||Uf(D)U^*|| = ||f(D)|| = \max_{1\leq j\leq n} |f(\lambda_j)| = ||f||_{\sigma(A)}.$$

What if A is not normal? In this section, we state various K-spectral sets of matrices.

Theorem 12. *(Von Neumann's inequality, [29]) If $A \in \mathbb{C}^{n,n}$ is a contraction, then for any polynomial p we have*

$$||p(A)|| \leq ||p||_{\mathbb{D}}, \tag{1.3}$$

where $\mathbb{D}$ denotes the unit disk centered at 0.

Von Neumann's inequality is widely used in the theory of contractions. The original inequality of von Neumann considers linear contractions on a Hilbert space. A simple proof of the theorem is based on the following arguments (see [11]):

1. The inequality (1.3) holds for any Möbius transformation p of the form $p(z) = (z - \lambda)(1 - \overline{\lambda}z)^{-1}$, where $\lambda \in \mathbb{C}$ and $|\lambda| < 1$.

2. Therefore, it holds for finite Blaschke products which have the form

$$\zeta \prod_{j=1}^{N} (z-\lambda_j)(1-\overline{\lambda}_j z)^{-1},$$

where ζ and λ_js are complex numbers with $|\zeta| = 1$ and $|\lambda_j| < 1$.

3. The proof now results from the following theorem in [14]: If f is analytic on the unit disk $\mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$ satisfying $\sup_{z\in\mathbb{D}} |f(z)| \leq 1$, then f is uniformly approximated on $\overline{\mathbb{D}}$ by convex combinations of finite Blaschke products (a convex combination of the functions $g_1, \ldots, g_m$ is a function of the form $\sum_{j=1}^{m} \alpha_j g_j$, where $\alpha_j \geq 0$ for all j and $\sum_{j=1}^{m} \alpha_j = 1$).

Another proof of Theorem 12 comes directly from the following celebrated theorem:

Theorem 13. *(Sz.-Nagy dilation theorem) Every contraction T on a Hilbert space $\mathcal{H}$ has a unitary dilation U to a Hilbert space $\mathcal{K}$ containing $\mathcal{H}$, with*

$$T^n = P_{\mathcal{H}} U^n P_{\mathcal{H}},\ n \geq 0,$$

where $P_{\mathcal{H}}$ is the orthogonal projection $\mathcal{K} \to \mathcal{H}$.

By the dilation theorem, we have

$$||p(T)|| = ||P_{\mathcal{H}} p(U) P_{\mathcal{H}}|| \leq ||p(U)|| \leq ||p||_{\mathbb{D}}$$

for every polynomial p.

The inequality (1.3) can be extended to analytic functions defined on the unit disk. Moreover, replacing A by $A/||A||$ in (1.3), we have

$$||p(A)|| \leq ||p||_{D(||A||,0)}$$

for any matrix $A \in \mathbb{C}^{n,n}$, where $D(r,0)$ is the disk of radius r centered at the origin. Similarly, Von Neumann's inequality for a closed half plane $\prod$ with $W(A) \subset \prod$ is expressed as follows:

$$||p(A)|| \leq ||p||_{\prod}.$$

In [1] Ando extended Theorem 12 by showing that if $A, B \in \mathbb{C}^{n,n}$ are commuting contractions, then

$$||p(A,B)|| \leq ||p||_{\mathbb{D}\times\mathbb{D}}$$

for every polynomial p in two variables. In [38] Varopoulos showed that the generalization to a triple of commuting contractions fails.

The following theorem shows that any disk containing the numerical range of a matrix A is a 2-spectral set for the matrix:

Theorem 14. *(Theorem 3.4 in [6]) For any $A \in \mathbb{C}^{n,n}$ and any polynomial p,*

$$||p(A)|| \leq 2\,||p||_D,$$

where D is any disk containing the numerical range of A.

Proof. A simple argument shows that for a subset Ω of $\mathbb{C}$ containing $W(A)$ and complex values $\alpha \neq 0, \beta \in \mathbb{C}$,

$$||p(A)|| \leq 2\,||p||_{\Omega}, \forall p \iff ||p(\tilde{A})|| \leq 2\,||p||_{\tilde{\Omega}}, \forall p$$

where $\tilde{A} = \alpha A + \beta I$ and $\tilde{\Omega} = \alpha\Omega + \beta$. Thus, we may assume that $W(A) \subset \mathbb{D}$, or equivalently that $r(A) \leq 1$. Then from the remark after Theorem 9 we can express A as $2\cos(B)C\sin(B)$ for a Hermitian matrix B. For the continuous function $g(x) = \max(1, 2|\cos(x)|)$, we define the matrices $H = g(B)$ and $T = H^{-1}AH$ using the continuous functional calculus for self-adjoint operators. Since it is clear that $||\sin(B)H|| \leq 1$ and $2||H^{-1}\cos(B)|| \leq 1$, T is a contraction. Moreover, since $||H|| \leq 2$ and $||H^{-1}|| \leq 1$,

$$||p(A)|| \leq ||H|| \cdot ||p(T)|| \cdot ||H^{-1}|| \leq 2\,||p(T)|| \leq 2\,||p||_{\mathbb{D}},$$

where the last inequality follows from Theorem 12. $\square$

In particular, Theorem 14 implies that if $W(A)$ is a disk, then

$$||p(A)|| \leq 2\,||p||_{W(A)} \tag{1.4}$$

for every polynomial p. For example, the result is true for Jordan blocks. Crouzeix made a conjecture that (1.4) holds for any matrix $A \in \mathbb{C}^{n,n}$ (whose numerical range may not be a disk), which will be discussed in the next chapter. The restriction that $W(A)$ is a disk in (1.4) can be eliminated (but with a rather large constant factor):

Theorem 15. *For any $A \in \mathbb{C}^{n,n}$ and any polynomial p,*

$$||p(A)|| \leq 11.08\,||p||_{W(A)}. \tag{1.5}$$

The following is a rough sketch of the proof in [7]:

(a) The relation (1.5) holds *if and only if* $||p(A)|| \leq 11.08\,||p||_{\Omega}$ for any bounded convex domain of $\mathbb{C}$ such that $W(A) \subset \Omega$. In the paper, the boundary of Ω is assumed to be smooth and has a strictly positive curvature at each point.

(b) Using the Cauchy integral formula, we can represent $p(A)$ as a finite sum of integrals on $\partial\Omega$.

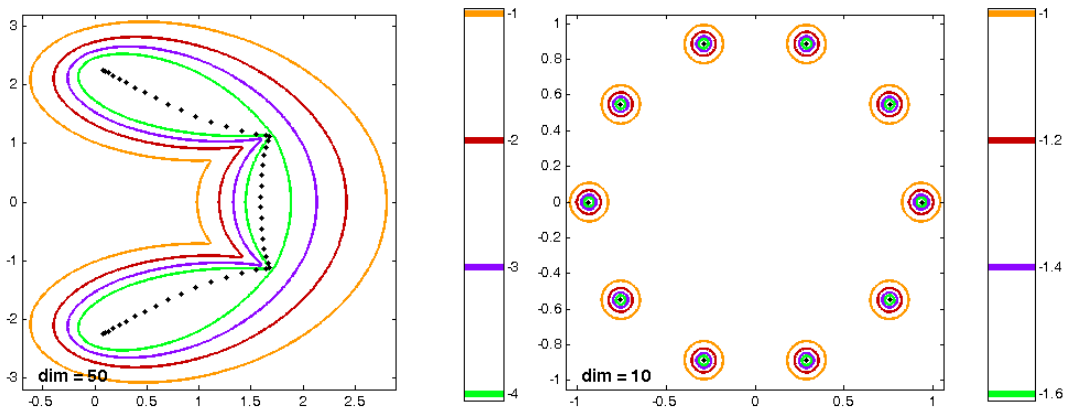
(c) Estimate each integral in the sum by considering (rather complicated) geometric properties of $\partial\Omega$.

Crouzeix wrote a concluding remark in [7] as follows:

> The constant 11.08 is not optimal. There is no doubt that refinements are possible which would decrease this bound. We are convinced that our estimate is very pessimistic, but to improve it drastically, it is clear that we have to find a completely different method.

In the next chapter, we will discuss the inequality (1.4) further and prove it for a class of matrices using a bijective conformal mapping from $W(A)$ to the unit disk.

Figure 1.3: Pseudospectra of a Grcar matrix and a Forsythe matrix



We close this section by introducing another K-spectral set. For each $\epsilon > 0$, the ϵ-pseudospectrum of $A \in \mathbb{C}^{n,n}$ (see [36]) is defined by

$$\sigma_\epsilon(A) = \{z \in \mathbb{C} : ||(zI - A)^{-1}|| > \epsilon^{-1}\}.$$

An equivalent definition of the ϵ-pseudospectrum is

$$\sigma_\epsilon(A) = \{z \in \sigma(A + E) : ||E|| < \epsilon\}.$$

If A is normal, then

$$\sigma_\epsilon(A) = \sigma(A) + \Delta_\epsilon,$$

where $\Delta_\epsilon = \{z \in \mathbb{C} : |z| < \epsilon\}$ for each $\epsilon > 0$ ([36, Theorem 2.2]). In general, $\sigma_\epsilon(A)$ is nonempty, open, and bounded, with at most n connected components, each containing one or more eigenvalues of A ([36, Theorem 2.4]). Figure 1.3 shows the pseudospectra of the Grcar matrix of size 50 for $\epsilon = 10^{-1}$, 10^{-2}, 10^{-3}, 10^{-4} and a Forsythe matrix of size 10 for $\epsilon = 10^{-1}$, $10^{-1.2}$, $10^{-1.4}$, and $10^{-1.6}$. The figures are generated by the MATLAB toolbox EigTool developed by T. G. Wright [40, 41].

If L_ϵ denotes the length of the boundary $\partial\sigma_\epsilon = \{z \in \mathbb{C} : ||(zI - A)^{-1}|| = \epsilon^{-1}\}$ of $\sigma_\epsilon(A)$, then by the Cauchy integral formula

$$\begin{aligned} ||f(A)|| &= ||\frac{1}{2\pi i}\int_{\partial\sigma_\epsilon}(zI-A)^{-1}f(z)dz|| \\ &\leq \frac{L_\epsilon}{2\pi\epsilon}||f||_{\partial\sigma_\epsilon} \end{aligned}$$

for any function f analytic on $\sigma_\epsilon(A)$.

Chapter 2

CROUZEIX'S CONJECTURE

2.1 Introduction

In [6, 7], M. Crouzeix made the following conjecture.

Conjecture 16. *For any* $A \in \mathbb{C}^{n,n}$ *and any polynomial* p*,*

$$||p(A)|| \leq 2\,||p||_{W(A)}. \tag{2.1}$$

We can take p in (2.1) to be any analytic function on $W(A)$ by Mergelyan's theorem ([15, Chap. XIII]) which states that if K is a compact subset of $\mathbb{C}$ such that $\mathbb{C}\backslash K$ is connected, then any continuous function $f : K \to \mathbb{C}$ which is analytic on the interior of K can be approximated uniformly on K by polynomials. The constant 2 can be attained by the polynomial $p(z) = z$ and the matrix $A = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}$, in which case $W(A)$ is the unit disk centered at the origin.

If A is diagonalizable, say $A = VDV^{-1}$, then we may simply consider the relation

$$||p(A)|| \leq \kappa(V)\,||p||_{\sigma(A)}, \tag{2.2}$$

where $\kappa(V) = ||V|| \cdot ||V^{-1}||$ is the condition number of V. The inequality is easy to prove:

$$||p(A)|| = ||Vp(D)V^{-1}|| \leq \kappa(V)\,||p(D)|| = \kappa(V)\,||p||_{\sigma(A)}.$$

If A is highly nonnormal, *i.e.*, if $\kappa(V) \gg 1$ (see [13] for measures of nonnormality of matrices), then the bound $\kappa(V)\,||p||_{\sigma(A)}$ may be very large and so not useful to estimate $||p(A)||$. Table 2.1 shows such examples where A is a Grcar matrix and $p(z) = z$ for each size $n = 10, 20, 30, 40, 50$; in this case, $||p(A)||$ is the spectral norm $||A||$, $||p||_{W(A)}$ is the

Table 2.1: $2\,r(A)$ v.s. $\kappa(V)\,\rho(A)$ for a Grcar matrix A

n	$\|\|A\|\|$	$2\ r(A)$	$\kappa(V)$	$\rho(A)$	$\kappa(V)\cdot\rho(A)$
10	3.1066	5.6856	13.2664	2.1384	28.3965
20	3.1992	6.2327	685.9348	2.2279	1.5282e+003
30	3.2215	6.3630	4.2196e+004	2.2475	9.4834e+004
40	3.2298	6.4128	2.8389e+006	2.2547	6.4009e+006
50	3.2337	6.4370	2.0077e+008	2.2582	4.5338e+008

numerical radius $r(A)$, and $||p||_{\sigma(A)}$ is the spectral radius $\rho(A)$.

Inequality (2.1) holds for the following classes of matrices:

- A is similar to a diagonal matrix via a similarity transformation with condition number at most 2 (see the inequality (2.2));

- $W(A)$ is a disk (see (1.4));

- A is of the form

$$\begin{pmatrix} \lambda & \alpha_1 & & \\ & \ddots & \ddots & \\ & & \lambda & \alpha_{n-1} \\ \alpha_n & & & \lambda \end{pmatrix},$$

  where λ and α_js are complex values [4]; in particular, since any 2 by 2 matrix is unitarily similar to a matrix of the form $\begin{pmatrix} \lambda & \alpha_1 \\ \alpha_2 & \lambda \end{pmatrix}$, (2.1) holds for 2 by 2 matrices (see also [6] for another proof).

In [8], an attempt to prove Crouzeix's conjecture in the case of 3×3 nilpotent matrices is described, but the conjecture is not proved or disproved for the whole matrices of size 3.

2.2 Crouzeix's conjecture for a class of matrices

In [20], we showed that Crouzeix's conjecture holds for the perturbed Jordan blocks of the form

$$\begin{pmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \lambda & 1 \\ \nu & & & \lambda \end{pmatrix},$$

where λ, ν are complex numbers. In [4], we extended the result to the form $J_\alpha + \lambda I$, $\lambda \in \mathbb{C}$, $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{C}^n$, where I is the n by n identity matrix and

$$J_\alpha = \begin{pmatrix} 0 & \alpha_1 & & \\ & \ddots & \ddots & \\ & & 0 & \alpha_{n-1} \\ \alpha_n & & & 0 \end{pmatrix}. \tag{2.3}$$

This section describes the work in [4]. Note that if $\alpha_j = |\alpha_j| e^{i\theta_j}$ and $\mu = e^{i(\theta_1+\cdots+\theta_n)/n}$, then $J_\alpha = \mu D J_{|\alpha|} D^{-1}$, where $|\alpha| = (|\alpha_1|, \ldots, |\alpha_n|)$ and $D = \mathrm{diag}(z_1, \ldots, z_n)$ with $z_j = \mu^{j-1} e^{-i(\theta_1+\cdots+\theta_{j-1})}$. Since D is unitary, we may assume without loss of generality that $\lambda = 0$ and $\alpha_j \geq 0$ for each $j = 1, \ldots, n$ by the following lemma.

Lemma 17. *(Lemma 1 in [4]) Let $A, B \in \mathbb{C}^{n,n}$. If either $A = \mu B + \lambda I$, where $\mu \neq 0, \lambda \in \mathbb{C}$, or A is unitarily similar to B, then (2.1) holds for A if and only if it holds for B.*

Proof. If $A = \mu B + \lambda I$, for a given polynomial p we define the polynomial q by $q(z) = p(\mu z + \lambda)$. Then the result follows from the relations $W(A) = \mu W(B) + \lambda$ and $||p(A)|| = ||q(B)||$. Meanwhile, if A is unitarily similar to B, then the result comes from the facts that $W(A) = W(B)$ and $||p(A)|| = ||p(B)||$. □

Moreover, since the inequality (2.1) holds when $W(A)$ is a disk, we may assume that each α_j is positive by the following lemma.

Lemma 18. *(Lemma 2 in [4]) If $\alpha_j = 0$ for some j, then $W(J_\alpha)$ is a disk.*

Proof. Since $W(J_\alpha) = W(J_\beta)$ for any circulant permutation β of α, we may assume $\alpha_n = 0$. Let z be an arbitrary element of $W(J_\alpha)$. Then, $z = \mathbf{x}^* J_\alpha \mathbf{x}$ for a unit vector $\mathbf{x}$. A direct computation shows that $e^{i\theta} z = \mathbf{y}^* J_\alpha \mathbf{y}$ for any real θ, where $\mathbf{y}$ is a unit vector defined by $\mathbf{y} = \mathrm{diag}(1, e^{i\theta}, \ldots, e^{(n-1)i\theta})\mathbf{x}$. Since θ and $\mathbf{x}$ are arbitrary, we conclude that $W(J_\alpha)$ is a disk centered at the origin. □

Thus it is enough to prove (2.1) for the matrix J_α in the form (2.3), assuming that the α_js are positive. Since (2.1) is already proven when $n = 2$, we will also assume that the matrix size is at least 3. From now on, we will follow the convention that $\alpha_{n+j} = \alpha_j$ for any $j \geq 1$.

Lemma 19. *(Lemma 3 in [4]) The following are some properties of J_α.*

(a) $||J_\alpha^k|| = \max\{\alpha_1 \cdots \alpha_k, \alpha_2 \cdots \alpha_{k+1}, \ldots, \alpha_n \alpha_1 \cdots \alpha_{k-1}\}$ *for any $k = 1, \ldots, n$.*

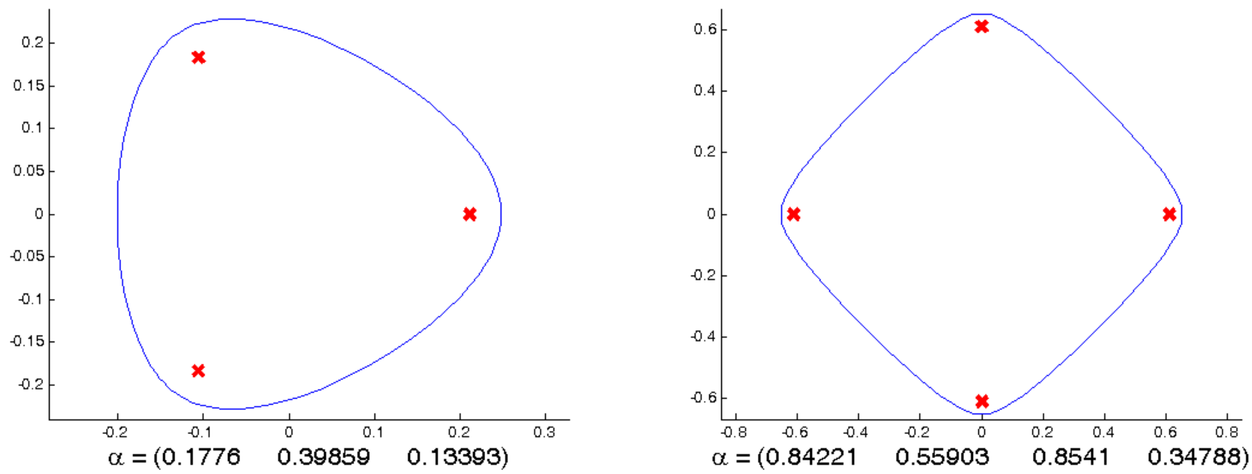
(b) J_α has the n distinct eigenvalues $(\alpha_1 \cdots \alpha_n)^{1/n} e^{2\pi i k/n}$, $k = 1, \ldots, n$. In particular, the positive eigenvalue $(\alpha_1 \cdots \alpha_n)^{1/n}$ which is $||J_\alpha^n||^{1/n}$ is the spectral radius of J_α.

(c) $W(J_\alpha)$ consists of n identical sectors around the origin. Moreover, each sector consists of two symmetric pieces along the line bisecting the sector.

Proof. (a) and (b) are easy to show. For (c), let $z = \mathbf{x}^* J_\alpha \mathbf{x}$ be an arbitrary element of $W(J_\alpha)$ for a unit vector $\mathbf{x}$ and let $\omega_k = e^{2\pi i k/n}$ for $k = 1, \ldots, n$. Then, a simple computation shows that $\omega_k z = \mathbf{y}^* J_\alpha \mathbf{y}$, where $\mathbf{y} = \mathrm{diag}(1, \omega_k, \ldots, \omega_k^{n-1})\mathbf{x}$. Since $\mathbf{y}$ is a unit vector, we have proved that $\omega_k z \in W(J_\alpha)$ for $k = 1, \ldots, n$ whenever $z \in W(J_\alpha)$, which implies that $W(J_\alpha)$ consists of n identical sectors. Moreover, since α_js are positive, if $z = \mathbf{x}^* J_\alpha \mathbf{x}$ is any element in $W(J_\alpha)$, then $\overline{z} = \overline{\mathbf{x}}^* J_\alpha \overline{\mathbf{x}}$ is also an element of $W(J_\alpha)$. Thus, we conclude that each sector $\{z \in W(J_\alpha) : 2(k-1)\pi/n \leq \arg(z) \leq 2k\pi/n\}$ consists of two symmetric subsectors along the line $\arg(z) = (2k-1)\pi/n$. □

Figure 2.1 shows examples of $W(J_\alpha)$ for α generated randomly with $n = 3, 4$, where the eigenvalues are marked with $\mathbf{x}$s. Before we prove Crouzeix's conjecture for J_α, we will show a sufficient condition for the conjecture for general matrices ([20, 4]) and see some concepts related to the conjecture.

Figure 2.1: Examples of $W(J_\alpha)$



Theorem 20. *Let $A \in \mathbb{C}^{n,n}$ and g be a bijective conformal mapping from $W(A)$ to the unit disk $\mathbb{D}$ centered at the origin. If*

$$\min_{\kappa(X)\leq 2} ||Xg(A)X^{-1}|| \leq 1, \tag{2.4}$$

where $\kappa(X) = ||X|| \cdot ||X^{-1}||$ is the condition number of X, then Crouzeix's conjecture holds for A.

Proof. Assume that there exists a matrix X such that $\kappa(X)$ is at most 2 and $C = Xg(A)X^{-1}$ is a contraction. Then, for any polynomial p,

$$\begin{aligned} ||p(A)|| &= ||(p \circ g^{-1})(g(A))|| \\ &= ||X^{-1}(p \circ g^{-1})(C)X|| \\ &\leq 2\,||(p \circ g^{-1})(C)|| \\ &\leq 2\,||p \circ g^{-1}||_{\mathbb{D}} \\ &= 2\,||p||_{W(A)}, \end{aligned}$$

where the second inequality comes from von Neumann's inequality . □

Remark 21. Theorem 20 gives us a numerical method to verify Crouzeix's conjecture; we can compute $g(A)$ (approximately) using, say, a Schwarz–Christoffel mapping from a polygonal approximation of $W(A)$ to $\mathbb{D}$ (see, e.g., [10]), then solve a constrained optimization problem to minimize $||Xg(A)X^{-1}||$ subject to $\kappa(X) \leq 2$.

Here we define a constant related to the left hand side of (2.4).

Definition 22. For $A \in \mathbb{C}^{n,n}$, we define $\tau(A)$ by

$$\tau(A) = \min_{\kappa(X)\leq 2} ||XAX^{-1}||. \tag{2.5}$$

Note that in terms of $\tau(\cdot)$, Theorem 20 says that

$$\text{if } \tau(g(A)) \leq 1, \text{ then Crouzeix's conjecture holds for } A, \tag{2.6}$$

where g is a bijective conformal mapping from $W(A)$ to the unit disk.

Recall that we have shown the following relation (just after Theorem 8):

$$\sup_{k\in\mathbb{N}} \left(\frac{||A^k||}{2}\right)^{1/k} \leq r(A),$$

where $r(A)$ is the numerical radius of A. Here we define another constant for matrices:

Definition 23. For $A \in \mathbb{C}^{n,n}$, we define $s(A)$ by

$$s(A) = \sup_{k\in\mathbb{N}} \left(\frac{||A^k||}{2}\right)^{1/k}. \tag{2.7}$$

Under a certain condition, we can express $s(A)$ as the maximum of a finite set.

Lemma 24. *Assume that* $||A^m||^{1/m} = \rho(A)$ *for some* $m \in \mathbb{N}$. *Then,*

$$s(A) = \max\left\{\frac{||A||}{2}, \left(\frac{||A^2||}{2}\right)^{1/2}, \ldots, \left(\frac{||A^{m-1}||}{2}\right)^{1/(m-1)}, ||A^m||^{1/m}\right\}. \tag{2.8}$$

Proof. Since

$$s(A) \geq \lim_{k\to\infty} \left(\frac{||A^k||}{2}\right)^{1/k} = \rho(A) = ||A^m||^{1/m},$$

$s(A)$ is greater than or equal to the right hand side in (2.8). Moreover, since for any $k \in \mathbb{N}$

$$\begin{aligned} \left(\frac{||A^{m+k}||}{2}\right)^{1/(m+k)} &\leq \left(\frac{||A^k||}{2}\right)^{1/(m+k)} ||A^m||^{1/(m+k)} \\ &= \left(\frac{||A^k||}{2}\right)^{1/k \cdot k/(m+k)} ||A^m||^{1/m \cdot m/(m+k)} \\ &\leq \max\left\{\left(\frac{||A^k||}{2}\right)^{1/k}, ||A^m||^{1/m}\right\}, \end{aligned}$$

we have the result (2.8). □

Now we show some relations among the constants $s(A)$, $\tau(A)$, and $r(A)$.

Lemma 25. *For $A \in \mathbb{C}^{n,n}$, we have the relation*

$$\rho(A) \leq s(A) \leq \tau(A) \leq r(A).$$

Proof. The relation $\rho(A) \leq s(A)$ follows from the Gelfand's formula

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

To prove $s(A) \leq \tau(A)$, let X be any matrix with $\kappa(X) \leq 2$ and let $B = XAX^{-1}$. Then, for any $k \in \mathbb{N}$

$$||A^k|| = ||X^{-1}B^kX|| \leq 2\,||B^k|| \leq 2\,||B||^k,$$

which implies that

$$\left(\frac{||A^k||}{2}\right)^{1/k} \leq ||B|| = ||XAX^{-1}||.$$

By taking the supremum for $k \in \mathbb{N}$ in the left hand side and the infimum for X with $\kappa(X) \leq 2$ in the right hand side, the relation $s(A) \leq \tau(A)$ is proved.

Finally, to prove $\tau(A) \leq r(A)$, we can use the theorem proved by Okubo and Ando in [30] stating that if $r(A) \leq 1$, there exists a matrix X such that $\kappa(X)$ is at most 2 and XAX^{-1} is a contraction. We can restate the theorem in terms of $\tau(\cdot)$ as follows: if $r(A) \leq 1$, then $\tau(A) \leq 1$; or equivalently, $\tau(A) \leq r(A)$. □

Now we return to the case of J_α. First, we will prove that $s(J_\alpha) = \tau(J_\alpha)$. By Lemma 19, $\rho(J_\alpha) = (\alpha_1 \cdots \alpha_n)^{1/n}$ which is $||J_\alpha^n||^{1/n}$. Thus, applying Lemma 24 to J_α, we can express $s(J_\alpha)$ simply by

$$s(J_\alpha) = \max \left\{ \frac{||J_\alpha||}{2}, \left(\frac{||J_\alpha^2||}{2}\right)^{1/2}, \ldots, \left(\frac{||J_\alpha^{n-1}||}{2}\right)^{1/(n-1)}, ||J_\alpha^n||^{1/n} \right\}. \tag{2.9}$$

Lemma 26. *$s(J_\alpha) = \tau(J_\alpha)$.*

Proof. Since $s(J_\alpha) \leq \tau(J_\alpha)$ from Lemma 25, we will show $\tau(J_\alpha) \leq s(J_\alpha)$, *i.e.*, there exists a matrix X such that $\kappa(X) \leq 2$ and $||XJ_\alpha X^{-1}|| \leq s(J_\alpha)$. We denote $s(J_\alpha)$ by s for convenience of notation and define a matrix X by $\mathrm{diag}(x_1, \ldots, x_n)$, where

$$\begin{aligned} x_1 &= \max\{1, \frac{\alpha_n}{s}, \frac{\alpha_n\alpha_{n-1}}{s^2}, \ldots, \frac{\alpha_n\alpha_{n-1}\cdots\alpha_2}{s^{n-1}}\}, \\ x_2 &= \max\{1, \frac{\alpha_1}{s}, \frac{\alpha_1\alpha_n}{s^2}, \ldots, \frac{\alpha_1\alpha_n\cdots\alpha_3}{s^{n-1}}\}, \\ &\vdots \\ x_n &= \max\{1, \frac{\alpha_{n-1}}{s}, \frac{\alpha_{n-1}\alpha_{n-2}}{s^2}, \ldots, \frac{\alpha_{n-1}\alpha_{n-2}\cdots\alpha_1}{s^{n-1}}\}. \end{aligned}$$

Then, since $||X|| = \max_{1\leq j\leq n} x_j$ and $||X^{-1}|| = 1/\min_{1\leq j\leq n} x_j$, the condition $\kappa(X) \leq 2$ would be satisfied if $1 \leq x_j \leq 2$ for each j. We know from Lemma 19 that

$$||J_\alpha^k|| = \max\{\alpha_j\alpha_{j+1}\cdots\alpha_{k+j-1} : 1 \leq j \leq n\}$$

for any $k = 1, 2 \ldots, n$. It is clear by the definition of $s = s(J_\alpha)$ that $\left(||J_\alpha^k||/2\right)^{1/k} \leq s$ for $1 \leq k < n$, which implies $x_j \leq 2$. Moreover, since the condition $x_j \geq 1$ is clear from the definition of x_j, we have $1 \leq x_j \leq 2$ for each $j = 1, \ldots, n$. Now it remains to prove $||XJ_\alpha X^{-1}|| \leq s$. It is easy to check that $XJ_\alpha X^{-1} = J_\beta$, where

$$\beta = (\frac{x_1}{x_2}\alpha_1, \frac{x_2}{x_3}\alpha_2, \ldots, \frac{x_{n-1}}{x_n}\alpha_{n-1}, \frac{x_n}{x_1}\alpha_n).$$

Since $||J_\beta|| = \max_{1\leq j\leq n} \beta_j$, the inequality $||XJ_\alpha X^{-1}|| \leq s$ is equivalent to show that $\beta_j \leq s$

for each j, *i.e.*, $x_j\alpha_j \le sx_{j+1}$. When $j=1$,

$$\begin{aligned} x_1\alpha_1 &= \max\{\alpha_1, \frac{\alpha_1\alpha_n}{s}, \frac{\alpha_1\alpha_n\alpha_{n-1}}{s^2}, \dots, \frac{\alpha_1\alpha_n\alpha_{n-1}\cdots\alpha_3}{s^{n-2}}, \frac{\alpha_1\cdots\alpha_n}{s^{n-1}}\} \\ sx_2 &= \max\{s, \alpha_1, \frac{\alpha_1\alpha_n}{s}, \dots, \frac{\alpha_1\alpha_n\cdots\alpha_3}{s^{n-2}}\}. \end{aligned}$$

Therefore,

$$x_1\alpha_1 \le sx_2 \iff \frac{\alpha_1\cdots\alpha_n}{s^{n-1}} \le s \iff \alpha_1\cdots\alpha_n \le s^n$$

and the last inequality holds since $s \ge ||J_\alpha^n||^{1/n} = (\alpha_1\cdots\alpha_n)^{1/n}$ by the definition of s. The same argument shows $x_j\alpha_j \le sx_{j+1}$ for other js. □

The proof in the lemma above shows that there exist a nonsingular matrix X with $\kappa(X) \le 2$ and a contraction C such that

$$J_\alpha = s(J_\alpha)X^{-1}CX. \tag{2.10}$$

From the result, we have the following interesting corollary:

Corollary 27. *For any polynomial p, we have*

$$||p(J_\alpha)|| \le 2||p||_{D(s(J_\alpha),0)}. \tag{2.11}$$

Moreover, if $||p(J_\alpha)|| \le 2||p||_{D(r,0)}$ for every polynomial p, then $r \ge s(J_\alpha)$.

Proof. The inequality (2.11) is clear from (2.10) and von Neumann's inequality. Assume that for a positive constant r

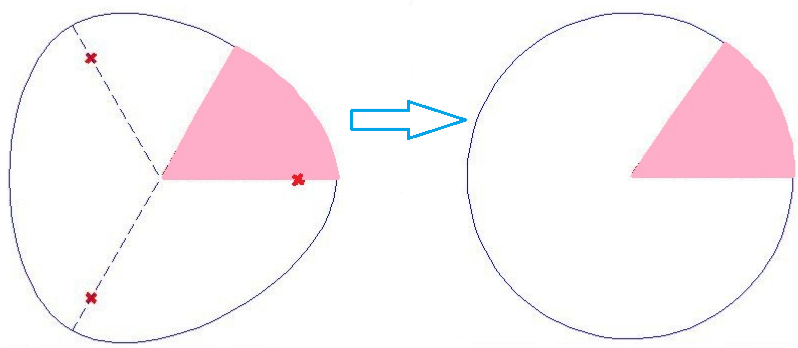
$$||p(J_\alpha)|| \le 2||p||_{D(r,0)}, \ \forall\, p$$

Then, in particular, it holds for the polynomials $p(z) = z^k$ for each $k \in \mathbb{N}$, which implies

$$\left(\frac{||J_\alpha^k||}{2}\right)^{1/k} \le r.$$

Since k is arbitrary, we conclude that $s(J_\alpha) \le r$. □

Figure 2.2: A conformal mapping from $W(J_\alpha)$ to the unit disk



The second statement of the corollary above can be generalized to any square matrix; that is, if

$$||p(A)|| \leq 2||p||_{D(r,0)},\ \forall\, p, \tag{2.12}$$

then $r \geq s(A)$. Since it is clear that

$$||p(A)|| \leq 2||p||_{D(\tau(A),0)},\ \forall\, p,$$

the smallest positive value r satisfying the relation (2.12) is between $s(A)$ and $\tau(A)$.

The sector $\{z \in W(J_\alpha) : 0 \leq \arg(z) \leq \pi/n\}$ in $W(J_\alpha)$ can be conformally mapped to a corresponding sector of the unit disk (see Figure 2.2) and the mapping is reflected n times to obtain a bijective conformal map φ from the entire region $W(J_\alpha)$ onto the unit disk by the Schwarz reflection principle [15, p.282] such that $\varphi(\lambda) = c\lambda$ for any eigenvalue λ of J_α, where c is a positive constant. Since $s(J_\alpha) = \tau(J_\alpha)$ by Lemma 26 and $\varphi(J_\alpha) = cJ_\alpha$ (which follows from $\varphi(\lambda) = c\lambda$ for any $\lambda \in \sigma(J_\alpha)$), if $c \cdot s(J_\alpha) \leq 1$, then Crouzeix's conjecture holds for J_α by (2.6). Moreover, the converse is also true; that is, if Crouzeix's conjecture holds for J_α, then we have $c \cdot s(J_\alpha) \leq 1$. The following theorem summarizes our argument. From now on, we will denote $s(J_\alpha)$ by s for convenience of notation.

Theorem 28. *(Corollary 5 in [4]) Crouzeix's conjecture holds for J_α if and only if $cs \leq 1$.*

Proof. Assume that Crouzeix's conjecture holds for J_α. That is,

$$||f(J_\alpha)|| \leq 2\,||f||_{W(J_\alpha)}$$

for any function f analytic on $W(J_\alpha)$. In particular, if $f = \varphi^k$, $k \in \mathbb{N}$, where φ is the conformal mapping described above, then we have $||c^k J_\alpha^k|| \leq 2$ for any $k \in \mathbb{N}$. Thus we have

$$c \cdot \left(\frac{||J_\alpha^k||}{2}\right)^{1/k} \leq 1$$

for any k, which implies $cs \leq 1$. □

Before we prove the inequality $cs \leq 1$ which guarantees Crouzeix's conjecture for J_α, we show some properties of the constant s.

Lemma 29. *(Lemma 6 in [4]) For $s = s(J_\alpha)$ defined in (2.9),*

(a) $\rho(J_\alpha) \leq s$ and $s \in W(J_\alpha)$;

(b) If $s = \left(\frac{||J_\alpha^k||}{2}\right)^{1/k}$ for some $k = 1, \ldots, n-2$, then $W(J_\alpha)$ contains the disk of radius s centered at the origin .

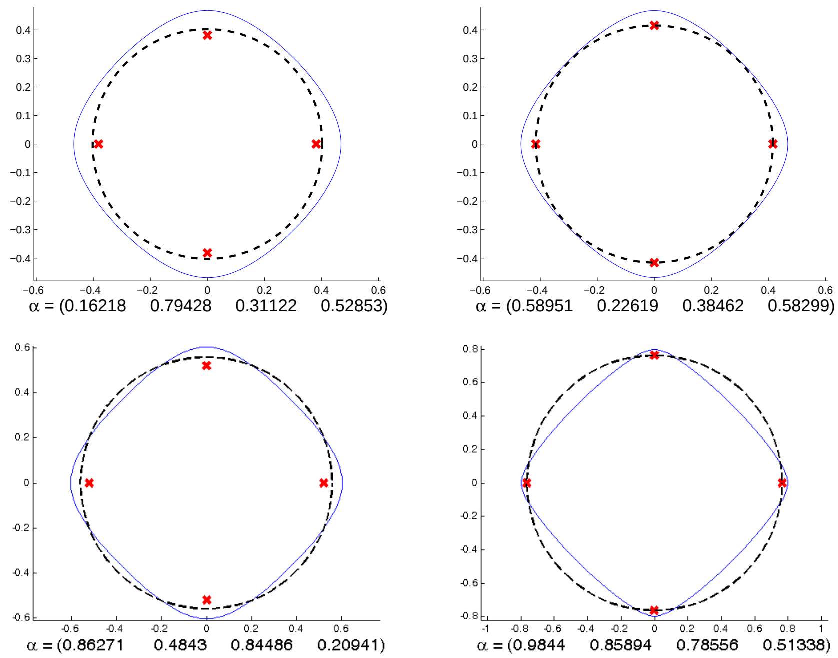
Proof. By definition of s, $||J_\alpha^n||^{1/n} \leq s$. Thus, the inequality $\rho(J_\alpha) \leq s$ follows from the fact $\rho(J_\alpha) = ||J_\alpha^n||^{1/n}$ (Lemma 19). If $s = ||J_\alpha^n||^{1/n}$, then s is the positive eigenvalue of J_α and thus $s \in W(J_\alpha)$. Meanwhile, if $s = \left(\frac{||J_\alpha^k||}{2}\right)^{1/k}$ for some $k < n$, then we may assume $s = \left(\frac{\alpha_1 \cdots \alpha_k}{2}\right)^{1/k}$, since $W(J_\alpha) = W(J_\beta)$ and $||J_\alpha^k|| = ||J_\beta^k||$ for any cyclic permutation β of α. Consider the case $k < n-1$. For a given $\theta \in \mathbb{R}$, the vector $q_\theta \in \mathbb{C}^n$ defined by

$$q_\theta = \frac{1}{\sqrt{k}}\left(\frac{1}{\sqrt{2}}, e^{i\theta}, \ldots, e^{i(k-1)\theta}, \frac{1}{\sqrt{2}}e^{ik\theta}, 0, \ldots, 0\right)^T,$$

is a unit vector and

$$q_\theta^* J_\alpha q_\theta = e^{i\theta}\frac{1}{k}\left(\frac{\alpha_1}{\sqrt{2}} + \alpha_2 + \cdots + \alpha_{k-1} + \frac{\alpha_k}{\sqrt{2}}\right) \in W(J_\alpha).$$

Figure 2.3: $W(J_\alpha)$ and the the disk of radius s centered at the origin (when $n = 4$).



Since $W(J_\alpha)$ is a convex set containing the origin and we have

$$\frac{1}{k}\left(\frac{\alpha_1}{\sqrt{2}} + \alpha_2 + \cdots + \alpha_{k-1} + \frac{\alpha_k}{\sqrt{2}}\right) \geq \left(\frac{\alpha_1 \cdots \alpha_k}{2}\right)^{1/k} = s,$$

the point $se^{i\theta}$ is in $W(J_\alpha)$. Since it is true for any $\theta \in \mathbb{R}$, the disk of radius s centered at the origin is contained in $W(J_\alpha)$. In the case $k = n - 1$, if we define the unit vector q by $q = \frac{1}{\sqrt{n-1}}(\frac{1}{\sqrt{2}}, 1, \ldots, 1, \frac{1}{\sqrt{2}})^T$, then

$$\begin{aligned} q^* J_\alpha q &= \frac{1}{n-1}\left(\frac{\alpha_1}{\sqrt{2}} + \alpha_2 + \cdots + \alpha_{n-2} + \frac{\alpha_{n-1}}{\sqrt{2}} + \frac{\alpha_n}{2}\right) \\ &\geq \left(\frac{\alpha_1 \cdots \alpha_{n-1}}{2}\right)^{1/(n-1)} + \frac{\alpha_n}{2(n-1)} \\ &> s. \end{aligned}$$

Therefore, $s \in W(J_\alpha)$. □

Figure 2.3 shows examples for which the second property in the lemma above may not hold when $s = \left(||J_\alpha^{n-1}||/2\right)^{1/(n-1)}$ or $s = ||J_\alpha^n||^{1/n}$ (where $n = 4$). The constant s is $\left(||J_\alpha^3||/2\right)^{1/3}$ in the left figures and $||J_\alpha^4||^{1/4}$ in the right figures. Meanwhile, the disk of radius s is contained in $W(J_\alpha)$ in the top figures but not in the bottom figures.

Theorem 30. *(Theorem 7 in [4]) Crouzeix's conjecture holds for J_α.*

Proof. We will show $cs \leq 1$. If $s = ||J_\alpha^n||^{1/n}$, then it is the positive eigenvalue of J_α and thus $cs = \varphi(s) \leq 1$. If $s = \left(||J_\alpha^k||/2\right)^{1/k}$ for $1 \leq k \leq n-2$, then the inequality $cs \leq 1$ follows from Lemma 29 and the Schwarz lemma [15, p.260]; that is, applying the Schwarz lemma to the map $\varphi|_{D(s,0)}$, we have $|\varphi(z)| \leq |z|/s$ for any z with $|z| \leq s$. In particular, if z is an eigenvalue of J_α, then $|z| \leq s$ is satisfied and $\varphi(z) = cz$. Therefore, $|\varphi(z)| \leq |z|/s$ implies $cs \leq 1$ since z is nonzero. Finally, consider the case $s = \left(||J_\alpha^{n-1}||/2\right)^{1/(n-1)}$. In the ensuing lemmas, we will show that there exist an open set U and a bijective conformal map ψ in U such that

$$\rho(J_\alpha) \subset U \subset W(J_\alpha),$$
$$\psi(0) = 0,\ \psi(\lambda) = s^{-1}\lambda \text{ for some } \lambda \in \rho(J_\alpha),$$
$$V = \psi(U) \text{ contains the unit disk.}$$

Then, the analytic function $g : V \to \mathbb{D}$ defined by $g = \varphi \circ \psi^{-1}$ satisfies that $g(0) = 0$ and $g(s^{-1}\lambda) = c\lambda$. Since V contains the unit disk, the Schwarz lemma implies that $|g(z)| \leq |z|$ for any $z \in V$. In particular, by plugging in $s^{-1}\lambda$ for z, we have the inequality $cs \leq 1$. □

Now we will find such an open set U and a map ψ described in the proof of Theorem 30, assuming that $s = \left(||J_\alpha^{n-1}||/2\right)^{1/(n-1)}$; that is,

$$\begin{aligned}
&\psi : U \to V \text{ is a bijective conformal mapping such that}\\
&\psi(0) = 0,\ \psi(\lambda) = s^{-1}\lambda \text{ for a } \lambda \in \sigma(J_\alpha),\\
&\text{where } U \text{ is an open subset of } W(J_\alpha) \text{ containing } \sigma(J_\alpha) \text{ and}\\
&V = \psi(U) \text{ contains the unit disk centered at the origin.}
\end{aligned} \tag{2.13}$$

For simplicity of computation, we may assume the following about s:

- Since $||J_{\alpha/s}^k||^{1/k} = s^{-1}||J_\alpha^k||^{1/k}$ for any k, we may assume that $s = 1$.

- If $\beta = (\alpha_{k+1}, \alpha_{k+2}, \ldots, \alpha_n, \alpha_1, \ldots, \alpha_k)$ is a cyclic permutation of α, then $J_\beta = P^k J_\alpha (P^T)^k$, where P is the unitary permutation matrix $\begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ 1 & & & 0 \end{bmatrix}$. Therefore by Lemma 17 we may assume that $s = (\alpha_1 \cdots \alpha_{n-1}/2)^{1/(n-1)}$.

Lemma 31. *(Lemma 8 in [4]) The vectors α satisfying the conditions*

$$s = (\alpha_1 \cdots \alpha_{n-1}/2)^{1/(n-1)} = 1$$

are exactly the ones satisfying the following:

$$\begin{aligned} &\alpha_1 \cdots \alpha_{n-1} = 2, \\ &1 \leq \alpha_j \cdots \alpha_{n-1} \leq 2 \text{ for any } j = 2, \ldots, n-1, \\ &\alpha_n \leq \frac{1}{2}. \end{aligned} \tag{2.14}$$

In particular, α_n is independent of $\alpha_1, \ldots, \alpha_{n-1}$.

Proof. Assume $s = (\alpha_1 \cdots \alpha_{n-1}/2)^{1/(n-1)} = 1$. Then, $\alpha_1 \cdots \alpha_{n-1} = 2$ is clear and the inequality $\alpha_n \leq 1/2$ follows from the relation

$$1 \geq ||J_\alpha^n||^{1/n} = (\alpha_1 \cdots \alpha_n)^{1/n} = (2\alpha_n)^{1/n}.$$

Moreover, since $\left(||J_\alpha^k||/2\right)^{1/k} \leq 1$, we have $\alpha_1 \cdots \alpha_j \leq 2$ and $\alpha_j \cdots \alpha_{n-1} \leq 2$ for any $j < n$. The inequality $1 \leq \alpha_j \cdots \alpha_{n-1}$ follows from the relation $\alpha_j \cdots \alpha_{n-1} = 2/(\alpha_1 \cdots \alpha_{j-1}) \geq 1$.

Conversely, assume that α satisfies (2.14). Since $\alpha_1 \cdots \alpha_{n-1} = 2$ and $\alpha_n \leq 1/2$, we have $||J_\alpha^n||^{1/n} \leq 1$ and $(\alpha_1 \cdots \alpha_{n-1}/2)^{1/(n-1)} = 1$. Therefore, it is enough to show that $||J_\alpha^k/2||^{1/k} \leq 1$ for any $k = 1, \ldots, n-1$, which is equivalent to prove that $\alpha_j \alpha_{j+1} \cdots \alpha_{k-1} \alpha_k \leq 2$ for any j and k:

(a) $1 \leq j \leq n-2$: since $1 \leq \alpha_{j+1} \cdots \alpha_{n-1} \leq 2$, we have

$$\alpha_1 \cdots \alpha_j = \frac{2}{\alpha_{j+1} \cdots \alpha_{n-1}} \in [1, 2].$$

(b) $2 \leq j \leq k \leq n-2$: since $1 \leq \alpha_1 \cdots \alpha_{j-1} \leq 2$ and $1 \leq \alpha_{k+1} \cdots \alpha_{n-1} \leq 2$, we have

$$\alpha_j \cdots \alpha_k = \frac{2}{(\alpha_1 \cdots \alpha_{j-1})(\alpha_{k+1} \cdots \alpha_{n-1})} \in [\frac{1}{2}, 2].$$

(c) $j \leq n$: it is clear that $\alpha_j \cdots \alpha_n \leq 2\alpha_n \leq 1$.

(d) $k < j \leq n-1$: it is clear that $\alpha_j \cdots \alpha_n \alpha_1 \cdots \alpha_k \leq 2\alpha_n \alpha_1 \cdots \alpha_k \leq 4\alpha_n \leq 2$.

□

From now on, we assume that α satisfies the conditions in (2.14). As the lemma above says, the $n-1$ components $\alpha_1, \ldots, \alpha_{n-1}$ are independent on α_n. The following gives a way to construct the first $n-1$ components of α using $n-2$ independent variables.

Corollary 32. *If $\alpha_1, \ldots, \alpha_{n-1}$ satisfy (2.14), then they can be expressed as*

$$\alpha_1 = \frac{2}{\beta_1}, \; \alpha_2 = \frac{\beta_1}{\beta_2}, \; \ldots, \alpha_{n-2} = \frac{\beta_{n-3}}{\beta_{n-2}}, \; \alpha_{n-1} = \beta_{n-2}, \tag{2.15}$$

where $1 \leq \beta_j \leq 2$ for $j = 1, \ldots, n-2$. Conversely, $\alpha_1, \ldots, \alpha_{n-1}$ in (2.15) satisfy (2.14).

Proof. Assume that $\alpha_1, \ldots, \alpha_{n-1}$ satisfy (2.14). Define β_j by $\beta_j = \alpha_{j+1} \cdots \alpha_{n-1}$ for $j = 1, \ldots, n-2$. Since $2 = \alpha_1 \cdots \alpha_{n-1} = \alpha_1 \beta_1$, we have $\alpha_1 = 2/\beta_1$. For $1 < j < n-1$,

$$\alpha_j = \frac{\alpha_j \cdots \alpha_{n-1}}{\alpha_{j+1} \cdots \alpha_{n-1}} = \frac{\beta_{j-1}}{\beta_j}.$$

Finally, $\alpha_{n-1} = \beta_{n-2}$ is clear. Conversely, assume that $\alpha_1, \ldots, \alpha_{n-1}$ are constructed as in

(2.15) for the independent variables $\beta_1, \ldots \beta_{n-2} \in [1, 2]$. Then,

$$\begin{aligned}\alpha_1 \cdots \alpha_{n-1} &= \frac{2}{\beta_1} \cdot \frac{\beta_1}{\beta_2} \cdots \frac{\beta_{n-3}}{\beta_{n-2}} \cdot \beta_{n-2} = 2,\\ \alpha_j \cdots \alpha_{n-1} &= \frac{\beta_{j-1}}{\beta_j} \cdot \frac{\beta_j}{\beta_{j+1}} \cdots \frac{\beta_{n-3}}{\beta_{n-2}} \cdot \beta_{n-2} = \beta_{j-1} \in [1, 2].\end{aligned}$$

□

The relation (2.15) can also be expressed using matrices: if α satisfies (2.14) with $\alpha_n = 0$, then $J_\alpha = X_\beta J_\gamma X_\beta^{-1}$, where $X_\beta = \mathrm{diag}(\sqrt{2}, \beta_1, \ldots, \beta_{n-2}, \sqrt{2})$ and $\gamma = (\sqrt{2}, 1, \ldots, 1, \sqrt{2}, 0)$. In particular, γ itself satisfies (2.14) (we have $\alpha = \gamma$ when $\beta_j = \sqrt{2}$ for any j). It is easy to check that $W(J_\gamma)$ is the unit disk and $q^T J_\gamma q = 1$ where q is the unit vector defined by

$$q = \frac{1}{\sqrt{n-1}}(\frac{1}{\sqrt{2}}, 1, \ldots, 1, \frac{1}{\sqrt{2}})^T. \tag{2.16}$$

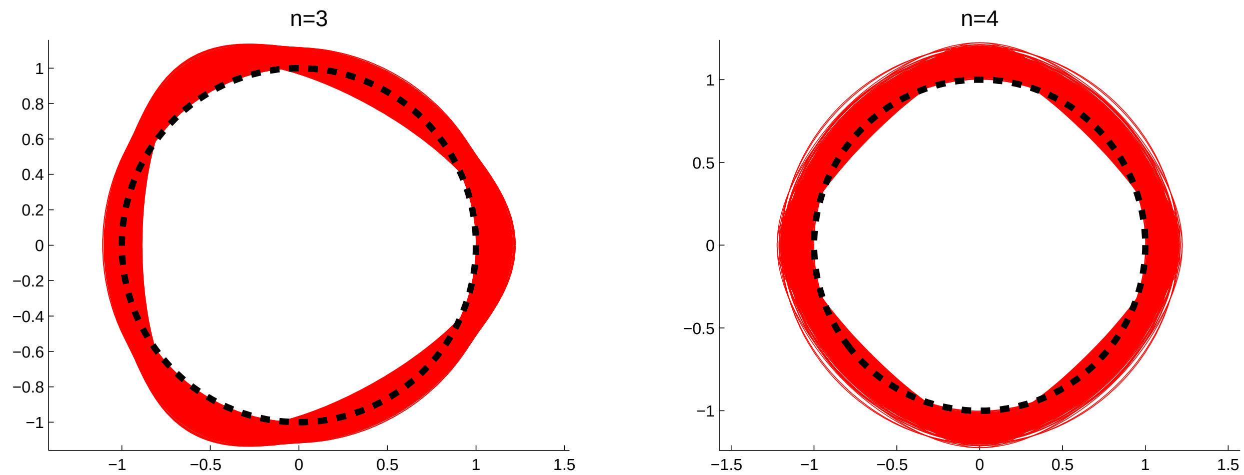
Roughly speaking, the vector γ which is obtained by choosing each β_j as $\sqrt{2}$ is a kind of average among αs satisfying (2.14) with $\alpha_n = 0$. Figure 2.4 shows the numerical ranges of J_γ and J_α for various α satisfying (2.14) (with $0 < \alpha_n \leq 1/2$). In the figures, the red lines denote the boundary of $W(J_\alpha)$ for 1000 αs generated randomly satisfying (2.14), and the boundary of $W(J_\gamma)$ which is the unit circle is the dotted black thick line. We can construct a set U in (2.13) using the unit vector q in (2.16).

Lemma 33. *(Lemma 9 in [4]) For the unit vector q in (2.16) and for each $\theta \in [0, 2\pi)$, define $w(\theta)$ by $w(\theta) = q_\theta^* J_\alpha q_\theta$, where $q_\theta = diag(1, e^{i\theta}, e^{2i\theta}, \ldots, e^{(n-1)i\theta})q$. Then the bounded open set U surrounded by the curve $\{w(\theta) : 0 \leq \theta < 2\pi\}$ is a subset of $W(J_\alpha)$ containing the spectrum of J_α.*

Proof. Note that $w(\theta)$ can be expressed by

$$w(\theta) = e^{i\theta}(a + e^{-in\theta}\frac{\alpha_n}{2(n-1)}),$$

Figure 2.4: $W(J_\gamma)$ and $W(X_\beta J_\gamma X_\beta^{-1})$



where the constant a is defined by

$$\begin{aligned} a &= q^* J_{\tilde{\alpha}} q \\ &= \frac{1}{n-1}\left(\frac{\alpha_1}{\sqrt{2}} + \alpha_2 \cdots + \alpha_{n-2} + \frac{\alpha_{n-1}}{\sqrt{2}}\right), \end{aligned} \tag{2.17}$$

where $\tilde{\alpha} = (\alpha_1, \ldots, \alpha_{n-1}, 0)$. We can easily check the following properties of $w(\theta)$:

(a) $|w(\theta)| > 0$ for all θ.

(b) $w(\theta + \frac{2\pi k}{n}) = w(\theta)$ for any integer k and $|w(\frac{2\pi}{n} - \theta)| = |w(\theta)|$ for $0 \le \theta \le \frac{\pi}{n}$.

(c) $\arg(w(\theta)) = \theta$ for $\theta = k\pi/n$, $k = 1, \ldots, 2n$.

(d) $w(\theta)$ is a one-to-one function on $[0, \frac{\pi}{n}]$.

Therefore the open set U bounded by the curve $w(\theta)$ is a star-shaped domain with respect to the origin. Since

$$w(\frac{2k\pi}{n}) = e^{2\pi ik/n}(a + \frac{\alpha_n}{2(n-1)}) \text{ and}$$
$$a \geq \left(\frac{\alpha_1}{\sqrt{2}} \cdot \alpha_2 \cdots \alpha_{n-2} \cdot \frac{\alpha_{n-1}}{\sqrt{2}}\right)^{1/(n-1)} = 1,$$

the domain U contains all the eigenvalues $e^{2\pi ik/n}(2\alpha_n)^{1/n}$ of J_α, $k = 1, \ldots, n$. Moreover, since q_θ is a unit vector for each θ, U is a subset of $W(J_\alpha)$. □

The next step is to find a bijective conformal mapping ψ in U such that

$$\begin{aligned} \psi(0) &= 0, \\ \psi(\lambda) &= \lambda \text{ for } \lambda \in \sigma(J_\alpha), \text{ and} \\ \psi(U) &\supset \mathbb{D}. \end{aligned}$$

Note that since $s = 1$ is assumed, the condition $\psi(\lambda) = s^{-1}\lambda$ in (2.13) is now $\psi(\lambda) = \lambda$. Since the minimal polynomial of J_α is $z^n - \alpha_1 \cdots \alpha_n = z^n - 2\alpha_n$, we seek such a function ψ of the form

$$\psi(z) = z(1 - \xi(z^n - 2\alpha_n))$$

for an analytic function $\xi = \xi(z)$. Fortunately, we can simply choose ξ as a constant:

Lemma 34. *(Lemma 10 in [4]) Let $\xi = \alpha_n/[2(n-1)a^{n+1}]$, where a is the constant in (2.17). Then, the polynomial $\psi(z) = z(1 - \xi(z^n - 2\alpha_n))$ of degree $n + 1$ maps U into a region which contains the unit disk, where U is the open set defined in Lemma 33.*

Proof. It is enough to show that $|\psi(w_\theta)| \geq 1$ for any θ, where $w_\theta = w(\theta)$ is defined in Lemma 33. Since

$$\begin{aligned} \psi(w_\theta) &= (1 + 2\xi\alpha_n)w_\theta - \xi w_\theta^{n+1} \\ &= (1 + 2\xi\alpha_n)(w_\theta - e^{i(n+1)\theta}\xi a^{n+1}) \\ &\quad +2\xi^2\alpha_n e^{i(n+1)\theta}a^{n+1} + \xi(e^{i(n+1)\theta}a^{n+1} - w_\theta^{n+1}), \end{aligned}$$

we have

$$\begin{aligned}
|\psi(w_\theta)| &\geq (1+2\xi\alpha_n)|w_\theta - e^{i(n+1)\theta}\xi a^{n+1}| - 2\xi^2\alpha_n a^{n+1} - \xi a^{n+1}|\left(\frac{w_\theta}{e^{i\theta}a}\right)^{n+1} - 1| \\
&= (1+2\xi\alpha_n)|a - 2i\sin(n\theta)\xi a^{n+1}| - 2\xi^2\alpha_n a^{n+1} - \xi a^{n+1}|(1+e^{-in\theta}a^n\xi)^{n+1} - 1| \\
&\geq a(1+2\xi\alpha_n) - 2\xi^2\alpha_n a^{n+1} - \xi a^{n+1}\sum_{k=1}^{n+1}\binom{n+1}{k}(\xi a^n)^k \\
&= a - \xi a^{n+1}\left(2\alpha_n(\xi - a^{-n}) + (1+\xi a^n)^{n+1} - 1\right) \\
&= a - \frac{\alpha_n}{2(n-1)}\left(2\alpha_n a^{-n}(\frac{\alpha_n}{2a(n-1)} - 1) + (1+\frac{\alpha_n}{2a(n-1)})^{n+1} - 1\right).
\end{aligned}$$

Let $x = a^{-1}$ and $t = \frac{\alpha_n}{2(n-1)}$. The right hand side above is not less than 1, if the following inequality holds for $0 \leq x \leq 1$ and $0 \leq t \leq \frac{1}{4(n-1)}$:

$$x^{-1} - t\left(4(n-1)(tx-1)tx^n + (tx+1)^{n+1} - 1\right) \geq 1.$$

If we define $f(x;t)$ by

$$f(x;t) = x + tx\left((tx+1)^{n+1} - 1 - 4(n-1)(1-tx)tx^n\right),$$

then the inequality above is equivalent to $f(x;t) \leq 1$. Differentiating f with respect to x, we have

$$\begin{aligned}
f_x(x;t) &= 1 - t\left(1 + 4t(n^2-1)x^n - 4t^2(n-1)(n+2)x^{n+1} - [1+(n+2)tx](tx+1)^n\right) \\
&\geq 1 - t\left(1 + 4t(n^2-1)x^n\right) \\
&\geq 1 - t\left(1 + 4t(n^2-1)\right).
\end{aligned}$$

Since the map $t \mapsto t\left(1 + 4t(n^2-1)\right)$ has the maximum value $\frac{n+2}{4(n-1)}$ which is less than 1, we have $f_x(x;t) \geq 0$ for any x and t. Therefore, $f(x;t)$ is an increasing function of x for each t and the inequality $f(x;t) \leq 1$ follows by showing $f(1;t) \leq 1$ which is equivalent to

$$(t+1)^{n+1} - 4(n-1)(1-t)t \leq 1 \tag{2.18}$$

for $0 \le t \le \frac{1}{4(n-1)}$. Letting $g(t)$ be the right hand side in the inequality above, we will show that $g(t)$ is a decreasing function for each $n \ge 3$. Since $g'(t) = (n+1)(t+1)^n + 4(n-1)(2t-1)$ is an increasing function, we have the following:

$$\begin{aligned} & g'(t) < 0 \text{ for all } 0 \le t \le \frac{1}{4(n-1)} \\ \iff \quad & g'(\frac{1}{4(n-1)}) < 0 \\ \iff \quad & (\frac{1}{4(n-1)} + 1)^n < \frac{4n-6}{n+1}. \end{aligned}$$

Since the map $n \mapsto (\frac{1}{4(n-1)} + 1)^n$ is an decreasing function whose value at $n = 3$ is about 1.4238 and the map $n \mapsto \frac{4n-6}{n+1}$ is an increasing function whose value at $n = 3$ is 1.5, $g'(t) < 0$ for all t and $g(t)$ has the maximum value 1 at $t = 0$. Therefore the inequality (2.18) is true. □

The final step is to show that the map ψ is injective in U:

Lemma 35. *(Lemma 11 in [4]) The polynomial ψ is one-to-one in U.*

Proof. Assume $\psi(z) = \psi(w)$ for $z \ne w \in U$. Then from the definition of ψ we have

$$\frac{z^{n+1} - w^{n+1}}{z - w} = 2(n-1)a^{n+1}\alpha_n^{-1} + 2\alpha_n.$$

Since the left hand side is at most $(n+1)\max_\theta |w_\theta|^n$, it is enough to show that

$$(a + \frac{\alpha_n}{2(n-1)})^n < 2 \cdot \frac{(n-1)a^{n+1}\alpha_n^{-1} + \alpha_n}{n+1} \tag{2.19}$$

for any $n \ge 3$. The left hand side is at most $1.43a^n$, since

$$(a + \frac{\alpha_n}{2(n-1)})^n = a^n(1 + \frac{\alpha_n}{2a(n-1)})^n \le a^n(1 + \frac{1}{4(n-1)})^n \le a^n(1 + \frac{1}{8})^3 \le 1.43a^n.$$

Meanwhile, the right hand side is at least $2a^n$, since

$$2 \cdot \frac{(n-1)a^{n+1}\alpha_n^{-1} + \alpha_n}{n+1} \ge \frac{2(n-1)a^{n+1}\alpha_n^{-1}}{n+1} \ge \frac{4(n-1)a^n}{n+1} \ge 2a^n.$$

Therefore (2.19) is true and the injectivity is proved. □

Throughout this section, we have shown that Crouzeix's conjecture holds for the matrices of the form

$$\begin{pmatrix} \lambda & \alpha_1 & & \\ & \lambda & \ddots & \\ & & \ddots & \alpha_{n-1} \\ \alpha_n & & & \lambda \end{pmatrix},$$

where λ and α_js are arbitrary complex numbers. Moreover, we defined the two constants $s(A)$ and $\tau(A)$ for a given matrix $A \in \mathbb{C}^{n,n}$. In the next chapter, we will discuss more about such constants.

2.3 *Constants related to a matrix*

Recall two definitions $s(A)$ and $\tau(A)$ for a matrix $A \in \mathbb{C}^{n,n}$:

$$\begin{aligned} s(A) &= \sup_{k\in\mathbb{N}} \left(\frac{||A^k||}{2}\right)^{1/k} \text{(Definition 23)}, \\ \tau(A) &= \min_{\kappa(X)\leq 2} ||XAX^{-1}|| \text{ (Definition 22)}. \end{aligned}$$

For the case of J_α defined in (2.3), we have shown in Theorem 30 that Crouzeix's conjecture holds for J_α if and only if $c \cdot s(J_\alpha) \leq 1$, where c is a positive constant such that $\varphi(J_\alpha) = cJ_\alpha$ for a bijective conformal mapping φ from $W(J_\alpha)$ to the unit disk. Can we generalize it for any matrix $A \in \mathbb{C}^{n,n}$? If so, how do we define the constant c for A? For this, we assume that Crouzeix's conjecture holds for A; that is,

$$||f(A)|| \leq 2\,||f||_{W(A)} \tag{2.20}$$

for any function f analytic on $W(A)$. Define $\mathcal{H}_A$ by

$$\mathcal{H}_A = \{g, \text{ analytic on } W(A) \text{ such that } g(A) = A\}. \tag{2.21}$$

Then, substituting $f = g^k$, $k \in \mathbb{N}$, in (2.20), we have

$$\frac{||g(A)^k||}{2} \leq ||g^k||_{W(A)} = ||g||_{W(A)}^k$$

and thus

$$\left(\frac{||A^k||}{2}\right)^{1/k} \leq ||g||_{W(A)}.$$

Since $k \in \mathbb{N}$ and $g \in \mathcal{H}_A$ are arbitrary, we have the following relation

$$s(A) \leq \min_{g \in \mathcal{H}_A} ||g||_{W(A)}.$$

Definition 36. For $A \in \mathbb{C}^{n,n}$, we define $\mu(A)$ by

$$\mu(A) = \min_{g \in \mathcal{H}_A} ||g||_{W(A)}.$$

Note that the argument above implies that if Crouzeix's conjecture holds for A, then

$$s(A) \leq \mu(A). \tag{2.22}$$

Comparing the relation $s(A) \leq \mu(A)$ to $c \cdot s(J_\alpha) \leq 1$, we may guess that

$$\mu(J_\alpha) = c^{-1}. \tag{2.23}$$

Before we prove it, we show a method to evaluate $\mu(A)$. The following is Theorem 2.3 in [16].

Theorem 37. *Let $\mathcal{H}^\infty$ be the space of all bounded analytic functions in $\mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$. If $z_1, \ldots, z_n$ are distinct points in $\mathbb{D}$ and $w_1, \ldots, w_n$ are complex numbers, then among all $f \in \mathcal{H}^\infty$ which satisfy $f(z_j) = w_j$ for any j, there is a unique function f of minimal L^∞norm on $\mathbb{D}$. This function has the form $f(z) = \mu B(z)$ where B is a Blaschke product of degree at most $n-1$. The minimal norm $\mu = ||f||_{\mathbb{D}}$ is computed by the following method:*

We define the $n \times n$ matrices A_n, B_n, and C_n by

$$A_n = \begin{pmatrix} 1 & z_1 & \cdots & z_1^{n-1} \\ \vdots & \vdots & & \vdots \\ 1 & z_n & \cdots & z_n^{n-1} \end{pmatrix}, \; B_n = \begin{pmatrix} w_1 z_1^{n-1} & \cdots & w_1 z_1 & w_1 \\ \vdots & \vdots & & \vdots \\ w_n z_n^{n-1} & \cdots & w_n z_n & w_n \end{pmatrix}, \; C_n = A_n^{-1} B_n.$$

C_n is well-defined because A_n is a non-singular Vandermonde matrix. Now define the $2n \times 2n$ block matrix M_{2n} by

$$M_{2n} = \begin{pmatrix} C_n^{re} & C_n^{im} \\ C_n^{im} & -C_n^{re} \end{pmatrix},$$

where C_n^{re} and C_n^{im} are the real and the imaginary parts of C_n, respectively. Then, the minimal norm μ is the largest real eigenvalue of M_{2n}.

Now we give a simple proof of the relation (2.23) using the method described in the theorem above.

Fact 38. *Let φ be the bijective conformal mapping from $W(J_\alpha)$ to $\mathbb{D}$ such that $\varphi(\lambda) = c\lambda$ for any eigenvalue λ of J_α, where c is a positive constant. Then, $\mu(J_\alpha) = c^{-1}$.*

Proof. Note that for any positive constant δ the function ψ defined by $\psi(z) = \varphi(\delta^{-1} z)$ is a bijective conformal mapping from $W(\delta J_\alpha)$ to $\mathbb{D}$ such that $\psi(\lambda) = c\delta^{-1}\lambda$ for any eigenvalue λ of δJ_α. Moreover, since $\mu(\delta J_\alpha) = \delta\mu(J_\alpha)$, we can assume $\rho(J_\alpha) = 1$, if necessary, by using the matrix $J_\alpha/\rho(J_\alpha) = J_{\alpha/\rho(J_\alpha)}$. For any vector $z = (z_1, \ldots, z_n) \in \mathbb{C}^n$, we use the notation $W(z)$ and $D(z)$ for the Wronskian matrix

$$\begin{pmatrix} 1 & z_1 & \cdots & z_1^{n-1} \\ \vdots & \vdots & & \vdots \\ 1 & z_n & \cdots & z_n^{n-1} \end{pmatrix}$$

and the diagonal matrix $\operatorname{diag}(z_1, \ldots, z_n)$, respectively. Note that the eigenvalues of J_α are $e^{ik\theta}$, $k = 0, \ldots, n-1$, where $\theta = 2\pi i/n$. Let $\xi = (1, e^{i\theta}, \ldots, e^{i(n-1)\theta})$ and S be the $n \times n$

matrix $\begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix}$. Then, following the same notations in Theorem 37, we have

$$\begin{aligned} A_n &= W(c\xi), \\ B_n &= D(\xi)A_n S, \\ C_n &= A_n^{-1}B_n = A_n^{-1}D(\xi)A_n S. \end{aligned}$$

Since $A_n = W(c\xi) = W(\xi)D_c$ and $W(\xi)^{-1} = \frac{1}{n}W(\xi)^*$, where $D_c = D(1, c, \ldots, c^{n-1})$, we have

$$\begin{aligned} C_n &= D_c^{-1}W(\xi)^{-1}D(\xi)W(\xi)D_c S \\ &= D_c^{-1}\begin{pmatrix} & & & 1 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{pmatrix}D_c S \\ &= c^{-1}\begin{pmatrix} & & & c^n \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{pmatrix}S = c^{-1}\begin{pmatrix} c^n & & & \\ & & & 1 \\ & & \iddots & \\ & 1 & & \end{pmatrix}. \end{aligned}$$

Since $\varphi(1) = c \leq 1$, the largest eigenvalue of C_n is c^{-1}. Therefore, $\mu(J_\alpha)$ which is the largest eigenvalue of $M_{2n} = \begin{pmatrix} C_n & O \\ O & -C_n \end{pmatrix}$ is c^{-1}. □

Therefore, when $A = J_\alpha$, the following statement is true:

$$\text{Crouzeix's conjecture holds for } A \iff s(A) \leq \mu(A)$$

We are not sure if the above relation is true in general.

In Theorem 20 or (2.6), we have shown that if $\tau(g(A)) \leq 1$, then Crouzeix's conjecture holds for A, where g is a bijective conformal mapping from $W(A)$ to $\mathbb{D}$. We conjecture that the inequality $\tau(g(A)) \leq 1$ is always true for any $A \in \mathbb{C}^{n,n}$. More generally, we suggest the following:

Conjecture 39. *Let $A \in \mathbb{C}^{n,n}$ and f be an analytic function defined on $W(A)$. Then,*

$$\tau(f(A)) \leq ||f||_{W(A)}.$$

In particular, if we consider the functions $f \in \mathcal{H}_A$ (the set $\mathcal{H}_A$ is defined in (2.21)), then the above conjecture implies that

$$\tau(A) \leq \mu(A), \tag{2.24}$$

which is a stronger result than the inequality $\tau(A) \leq r(A)$ proved by Okubo and Ando in [30] (we mentioned it in the proof of Lemma 25). Since the relation $s(A) \leq \tau(A)$ holds for any A (Lemma 25), if (2.24) is true, then we will have the following relations:

$$\rho(A) \leq s(A) \leq \tau(A) \leq \mu(A) \leq r(A). \tag{2.25}$$

The relation $\mu(A) \leq r(A)$ is clear by definition of $\mu(A)$, and the only things unclear in (2.25) are $s(A) \leq \mu(A)$ and $\tau(A) \leq \mu(A)$. Table 2.2 shows the relation (2.25) for the following test matrices (Many of them could be found in [36]):

- `gallery(3)` generates the matrix $\begin{pmatrix} -149 & -50 & -154 \\ 537 & 180 & 546 \\ -27 & -9 & -25 \end{pmatrix}$ which is badly conditioned; its condition number is 2.7585e+005.

- M_3 is the 3 by 3 Markov matrix

$$M_3 = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \tag{2.26}$$

and M_4 is the 4 by 4 Markov matrix

$$M_4 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \tag{2.27}$$

A (right) Markov matrix is a square matrix of nonnegative real numbers, with each row summing to 1. It is also termed a stochastic matrix (see [26] more).

- W is the N by N Wilkinson matrix $\begin{pmatrix} \frac{1}{N} & 1 & & \\ & \frac{2}{N} & \ddots & \\ & & \ddots & 1 \\ & & & 1 \end{pmatrix}$ ($N = 6$ is used for our test).

Clearly all eigenvalues of the Wilkinson's matrix, the diagonal elements which vary smoothly, are sensitive. If we perturb the $(N, 1)$ entry of W, we will see a dramatic change in the eigenvalues.

- F is the 6 by 6 Frank matrix $\begin{pmatrix} 6 & 5 & 4 & 3 & 2 & 1 \\ 5 & 5 & 4 & 3 & 2 & 1 \\ 0 & 4 & 4 & 3 & 2 & 1 \\ 0 & 0 & 3 & 3 & 2 & 1 \\ 0 & 0 & 0 & 2 & 2 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$. The Frank matrix is an upper

Hessenberg matrix with ill-conditioned eigenvalues. Its determinant is 1, but it is difficult to compute numerically. MATLAB provides the Frank matrix of size n in gallery('frank',n).

Table 2.2: Examples showing $\rho(A) \leq s(A) \leq \tau(A) \leq \mu(A) \leq r(A)$

Matrix	ρ	s	τ	μ	r
`gallery(3)`	3	408.8798	408.8855	409.6984	410.6420
`gallery('grcar',10)`	2.1384	2.5074	2.5488	2.7789	2.8428
M_3	1	1	1	1	1.0083
M_4	1	1	1	1.0290	1.1469
W	1	1.4089	1.4197	1.5516	1.6148
F	12.9736	12.9736	12.9868	13.1034	14.1309
K	1	1.0517	1.1394	1.3922	1.4204
L	15.4509	16.0324	16.3502	16.8123	17.6672

- $K = \begin{pmatrix} 1 & -c & -c & -c & -c & -c \\ & s & -sc & -sc & -sc & -sc \\ & & s^2 & -s^2c & -s^2c & -s^2c \\ & & & s^3 & -s^3c & -s^3c \\ & & & & s^4 & -s^4c \\ & & & & & s^5 \end{pmatrix}$ is the 6 by 6 Kahan matrix, where $s^5 = 0.1$ and $c = \sqrt{1-s^2}$. The Kahan matrix, an upper triangular matrix made up of sines and cosines, was introduced in [24] to show that QR decomposition with column pivoting is not a fail-safe method for determining the rank of the matrix. It is provided by the MATLAB command gallery('kahan',n).

- $L = \begin{pmatrix} -5 & 2 & & & & \\ \frac{1}{2} & -7 & 3 & & & \\ & \frac{1}{3} & -9 & 4 & & \\ & & \frac{1}{4} & -11 & 5 & \\ & & & \frac{1}{5} & -13 & 6 \\ & & & & \frac{1}{6} & -15 \end{pmatrix}$ is the 6 by 6 matrix of Lenferink and Spijker, which was devised in [27] to illustrate stability estimates of a type of differential equations.

The relations in (2.25) are true for any 2 by 2 matrix A, since the inequality $\tau(A) \leq \mu(A)$ is proved as follows:

Fact 40. *For any 2 by 2 matrix A, we have $\tau(A) \leq \mu(A)$.*

Proof. Since any 2×2 matrix is unitarily similar to a matrix of the form $\lambda I + J_\alpha$ for $\lambda \in \mathbb{C}$ and $\alpha = (\alpha_1, \alpha_2)$ with $\alpha_1, \alpha_2 \geq 0$, we may assume that $A = \lambda I + J_\alpha$ for such λ, α. Furthermore, we may assume $\alpha_1\alpha_2 = 1$. Denote $s(J_\alpha)$ and $\mu(J_\alpha)$ by s and μ, respectively. As in the proof of Lemma 26, if we define the diagonal matrix $X = \text{diag}(x_1, x_2)$ with $x_1 = \max\{1, s^{-1}\alpha_2\}$ and $x_2 = \max\{1, s^{-1}\alpha_1\}$, then $\kappa(X) \leq 2$ and $||XJ_\alpha X^{-1}|| = s$. For the matrix X, it is easy to check that $XJ_\alpha X^{-1}$ is either $\begin{pmatrix} 0 & s \\ s^{-1} & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & s^{-1} \\ s & 0 \end{pmatrix}$ and that $||XAX^{-1}||$ is the square root of the largest zero of the function

$$P_s(z) = z^2 - (2|\lambda|^2 + \delta_s)z + |\lambda^2 - 1|^2,$$

where $\delta_s = s^2 + s^{-2}$. Meanwhile, by following the algorithm in Theorem 37, we can show that $\mu(A)$ is the largest zero of the function $P_\mu(z^2)$. Since $P_s(z) = 0$ implies that $z^2 - 2|\lambda|^2 z + |\lambda^2 - 1|^2 = \delta_s z$, we have

$$\begin{aligned} & ||XAX^{-1}|| \leq \mu(A) \\ \Longleftrightarrow \quad & \delta_s \leq \delta_\mu \\ \Longleftrightarrow \quad & s \leq \mu \text{ or } s\mu \leq 1 \end{aligned}$$

Since Crouzeix's conjecture holds for J_α, we have $s \leq \mu$. Thus, the inequality $\tau(A) \leq \mu(A)$ holds for any 2×2 matrix A. □

We know from Theorem 20 that Conjecture 39 implies Crouzeix's conjecture for A. The following also shows the result from a different point of view.

Fact 41. *Let $A \in \mathbb{C}^{n,n}$. The following two statements are equivalent.*

(a) Crouzeix's conjecture holds for A; that is, $||f(A)|| \leq 2\,||f||_{W(A)}$ for any function f analytic on $W(A)$.

(b) $s(f(A)) \leq ||f||_{W(A)}$ for any function f analytic on $W(A)$.

Proof. Since $s(B) = \sup_{k\in\mathbb{N}} \left(\frac{||B^k||}{2}\right)^{1/k} \geq \frac{||B||}{2}$, the second statement implies the first one. Assume that the first statement is true. If f is an analytic function on $W(A)$, then for any $k \in \mathbb{N}$ we have

$$||f^k(A)|| \leq 2\,||f^k||_{W(A)} = 2\,||f||^k_{W(A)},$$

or equivalently,

$$\left(\frac{||f^k(A)||}{2}\right)^{1/k} \leq ||f||_{W(A)}.$$

By taking the supremum over $k \in \mathbb{N}$ in the left hand side, we have $s(f(A)) \leq ||f||_{W(A)}$. $\square$

Therefore, since $s(\cdot) \leq \tau(\cdot)$, if Conjecture 39 is true, then Crouzeix's conjecture also holds for A.

Chapter 3

APPLICATION AND SUMMARY

3.1 An application to the analysis of GMRES

The generalized minimal residual method (GMRES) is a Krylov-based iterative method for solving non-hermitian linear systems [32]. In the kth iteration of GMRES the approximate solution to the linear system $Ax = b$ is the vector x_k in the kth Krylov subspace $K_k = \text{span}\{b, Ab, \ldots, A^{k-1}b\}$ that minimizes the two-norm of the residual $r_k = b - Ax_k$. Since the vectors $b, Ab, \ldots, A^{k-1}b$ tend to be nearly linearly dependent for large k, a stable way is needed to find an orthogonal basis of successive Krylov subspaces, and the the Arnoldi process is used for this. It is well known (see [19]) that the relative residual norm at the kth iteration is bounded by

$$\frac{||r_k||}{||r_0||} \leq \min\{||p(A)|| : p \text{ is a polynomial of degree} \leq k,\ p(0) = 1\}. \tag{3.1}$$

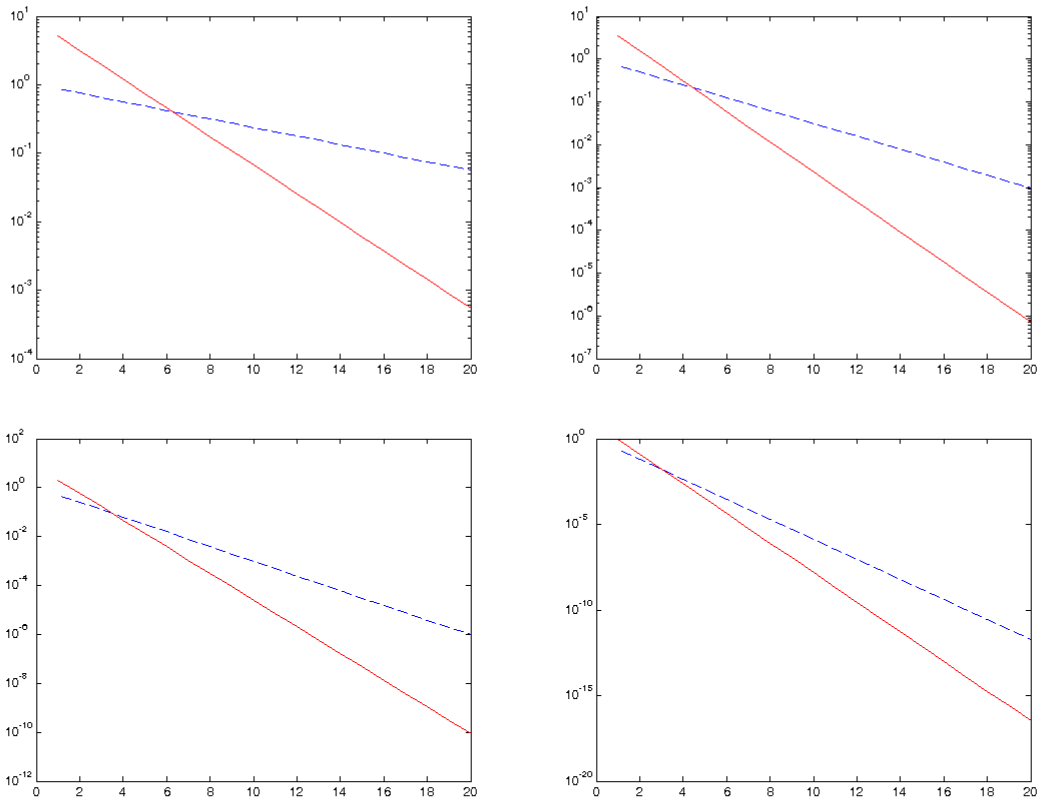
Elman [12] showed a bound for the relative residual norms of GMRES when $0 \notin W(A)$ as follows: if A has a positive definite hermitian part $H(A) = (A + A^*)/2$, then

$$\frac{||r_k||}{||r_0||} \leq \sin^k(\beta), \tag{3.2}$$

where $\cos(\beta) = \lambda_{\min}(H(A))/||A||$. By a simple argument, the expression for $\cos(\beta)$ can be replaced by $\cos(\beta) = \text{dist}(0, W(A))/||A||$ with $\beta \in [0, \pi/2)$ (see [3]). The Crawford number of a given matrix $B \in \mathbb{C}^{n,n}$ is defined as the distance between the origin and the numerical range of B. Denoting the number by $c(B)$, we can express $\lambda_{\min}(H(A))$ and $\text{dist}(0, W(A))$ by $c(H(A))$ and $c(A)$, respectively. The main theorem in [3] is the following:

$$\frac{||r_k||}{||r_0||} \leq 2(1 + \frac{1}{\sqrt{3}})(2 + \gamma_\beta)\gamma_\beta^k, \tag{3.3}$$

Figure 3.1: The bounds in (3.2) and (3.3) for $\beta = \frac{\pi}{3}, \frac{\pi}{4}, \frac{\pi}{6}$, and $\frac{\pi}{12}$; the curve corresponding to (3.2) is dashed.



where $\gamma_\beta = 2\sin(\beta/[4 - 2\beta/\pi])$ for $\beta \in [0, \pi/2)$ with $\cos(\beta) = c(A)/||A||$. Figure 3.1 compares the bounds in (3.2) and (3.3) for some angles β. The following is a rough sketch of the proof in [3] to show (3.3):

1. Assume without loss of generality that the element of $W(A)$ closest to 0 is real positive. In this case, if K_β is the (convex) intersection between the closed unit disk and the half plane $\{\mathrm{Re}(z) \geq \cos(\beta)\}$, then $W(A) \subset ||A|| \cdot K_\beta$.

2. Let $\alpha \in (\beta, \pi/2)$ and consider the linear fractional transformation

$$L(z) = \frac{||A||e^{i\alpha} - z}{z - ||A||e^{-i\alpha}}.$$

The map has the following properties:

- $L(||A|| \cdot K_\alpha) = S_\alpha$, where $S_\alpha = \{z \in \mathbb{C} : 0 \le \arg(z) \le \alpha\}$.
- For any polynomial p, $p \circ L^{-1}$ is a rational function with all poles at $-1 \notin S_\alpha$.
- $W(L(A)) \subset S_\alpha$.

3. In [9], the authors showed that for each $0 \le \alpha \le \pi$

$$W(B) \subset S_\alpha \implies ||f(B)|| \le 2(1 + \frac{1}{\sqrt{3}})||f||_{S_\alpha} \tag{3.4}$$

for all matrices B and all rational functions f having no pole in S_α.

4. Combining (2) and (3), we have that for any polynomial p

$$\begin{aligned} ||p(A)|| &= ||(p \circ L^{-1})(L(A))|| \\ &\le 2(1 + \frac{1}{\sqrt{3}})||(p \circ L^{-1})||_{S_\alpha} \\ &= 2(1 + \frac{1}{\sqrt{3}})||p||_{||A|| \cdot K_\alpha}. \end{aligned}$$

Since α is arbitrary in $(\beta, \pi/2)$, we have the following result:

$$||p(A)|| \le 2(1 + \frac{1}{\sqrt{3}})||p||_{||A|| \cdot K_\beta}. \tag{3.5}$$

5. For a compact subset K of the complex plane, define $E_k(K)$ by

$$E_k(K) = \min\{||p||_K : p \text{ is a polynomial of degree} \le k,\ p(0) = 1\}. \tag{3.6}$$

Then from (3.1) and (3.5) we have

$$\frac{||r_k||}{||r_0||} \le 2(1 + \frac{1}{\sqrt{3}})E_k(||A|| \cdot K_\beta).$$

Since $E_k(K)$ is invariant under a scaling of the set K, we can write it as

$$\frac{||r_k||}{||r_0||} \leq 2(1+\frac{1}{\sqrt{3}})E_k(K_\beta).$$

Now it remains to estimate $E_k(K_\beta)$.

6. Let ϕ be the Riemann conformal mapping from $\overline{\mathbb{C}}\backslash K_\beta$ onto the exterior of the closed unit disk with $\phi(\infty)=\infty$ and F_k be the Faber polynomial of the Laurent series of ϕ^k at ∞ (see [34]). Since K_β is convex, we have $||F_k-\phi^k||_{\partial K_\beta} \leq 1$ (Theorem 2 in [25]). If we define the polynomial p_v by $p_v(z)=F_k(z)+v(\phi(0)^k-F_k(0))$ for each $v\in[0,1]$, then we can show that

$$\begin{aligned} E_k(K_\beta) &\leq \min_{v\in[0,1]} \frac{||p_v||_{K_\beta}}{|p_v(0)|} \\ &\leq \gamma_\beta^k \min_{v\in[0,1]} \frac{2+v\gamma_\beta}{1-(1-v)\gamma_\beta^{k+1}} \\ &\leq \gamma_\beta^k(2+\gamma_\beta). \end{aligned}$$

These bounds are linear, but if Crouzeix's conjecture were proved they could be replaced by more realistic, nonlinear estimates of $E_k(W(A))$. Of course, using Theorem 15, one can replace these bounds by 11.08 $E_k(W(A))$.

3.2 *Another estimation using* $e^{W(\ln A)}$

The bound in (3.3) needs the condition $0 \notin W(A)$. What if 0 is in $W(A)$? Can we find a subset S of the complex plane such that $0 \notin S$ and $||p(A)|| \leq 2\,||p||_S$ for every polynomial p?

Theorem 42. *(Theorem 1 in [5]) Assume that* $A \in \mathbb{C}^{n,n}$ *is nonsingular. Then*

$$\lim_{k\to\infty} W(A^{1/k})^k = e^{W(\ln A)},$$

for any branch cut of $\ln(z)$ *and* $z^{1/k}$ *at the origin which does not meet the spectrum of* A.

Proof. Choose a branch cut at the origin on which no eigenvalue of A lies. Since

$$\begin{aligned} & \lim_{k\to\infty} W(A^{1/k})^k = e^{W(\ln A)} \\ \iff \quad & \lim_{k\to\infty} k \ln W(A^{1/k}) = W(\ln A) \\ \iff \quad & \lim_{h\to 0} \frac{\ln W(A^h)}{h} = W(\ln A), \end{aligned}$$

it is enough to show that

$$\lim_{h\to 0} \frac{\ln(q^* A^h q)}{h} = q^*(\ln A) q$$

for any unit vector q. Note that since $q^* A^h q \to q^* q = 1$ as $h \to 0$, $\ln(q^* A^h q)$ is well-defined for h sufficiently small. Since $\ln(q^* q) = 0$, the left hand side above can be expressed as

$$\frac{d}{dh} \ln(q^* A^h q)|_{h=0}.$$

Fix a vector $q \in \mathbb{C}^n$ with $q^* q = 1$. Then

$$\frac{d}{dh} \ln(q^* A^h q)|_{h=0} = \frac{q^*(\ln A) A^h q}{q^* A^h q}|_{h=0} = q^*(\ln A) q.$$

□

Remark 43. Since $A^{1/k}$ converges to the n by n identity matrix I as k goes to infinity, $W(A^{1/k})$ for k large will be a small region which is close to $\{1\} = W(I)$. Thus, $W(A^{1/k})$ (and $W(A^{1/k})^k$) does not contain the origin for k sufficiently large.

Theorem 44. *Assume that Crouzeix's conjecture holds for (invertible) matrices. Using a branch cut of* $\ln(z)$ *at the origin on which eigenvalues of a given invertible matrix* A *do not lie, we have that for any polynomial* p*,*

(a) $||p(A)|| \leq 2\,||p||_{W(A^{1/k})^k}$ *for any* $k \in \mathbb{N}$*;*

(b) $||p(A)|| \leq 2\,||p||_{e^{W(\ln A)}}$.

Proof. Let $g(z) = z^k$. Then

$$\begin{aligned} ||p(A)|| &= ||(p \circ g)(A^{1/k})|| \\ &\leq 2\,||p \circ g||_{W(A^{1/k})}, \text{ since Crouzeix's conjecture holds for } A \\ &= 2\,||p||_{W(A^{1/k})^k}. \end{aligned}$$

The second result follows from (a) and Theorem 42. □

Figure 3.2 shows examples of $W(A)$ and $e^{W(\ln A)}$, where $W(A)$ contains the origin. In the figure, the boundaries of $e^{W(\ln A)}$ are dotted red lines. The test matrices used are the following:

- Grcar matrix of size 10.
- iM_3, where M_3 is the 3 by 3 Markov matrix defined in (2.26).
- $e^{\pi i/4}M_4$, where M_4 is the 4 by 4 Markov matrix defined in (2.27).
- $B = \begin{pmatrix} E_1 & & \\ & \ddots & \\ & & E_5 \end{pmatrix}$, where $E_j = \begin{pmatrix} 1 & j-1 \\ 0 & 1 \end{pmatrix}$; the minimal polynomial of the matrix has degree 2 but which is ill-conditioned, with singular values spread over a wide range [28].
- $V = SDS^{-1}$, where $S = \begin{pmatrix} 1 & \beta & & \\ & \ddots & \ddots & \\ & & \ddots & \beta \\ & & & 1 \end{pmatrix}$ and $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$ (see Chapter 6 in [37]); in this case, $n = 10$, $\beta = 0.9$, and $\lambda_j = j - 0.5$.
- 'Dramadah' is a matrix of zeros and ones for which the Frobenius norm of the inverse is relatively large, which is generated by the MATLAB command `gallery('dramadah',10,3)`.

- J is a 3 by 3 perturbed Jordan block $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0.9134 & 0 & 0 \end{pmatrix}$.

- C =-gallery('chebspec',10,1) is a Chebyshev spectral differentiation matrix of order 10.

For any test matrix A in Figure 3.2, $e^{W(\ln A)}$ does not wind completely around the origin. Meanwhile, Figure 3.3 shows examples that $e^{W(\ln A)}$ is not simply connected, where the right hand sides are the zoomed images around the origin. The following test matrices are used:

- J is a 3 by 3 perturbed Jordan block $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0.1419 & 0 & 0 \end{pmatrix}$.

- $A = i \begin{pmatrix} 1 & \epsilon & 0 & 0 \\ 0 & -1 & 1/\epsilon & 0 \\ 0 & 0 & 1 & \epsilon \\ 0 & 0 & 0 & -1 \end{pmatrix}$, where $\epsilon = 0.3$ (see [19, Chapter 3]).

If Crouzeix's conjecture holds, then the relative GMRES residuals are bounded by

$$\frac{||r_k||}{||r_0||} \leq 2E_k(W(A)). \tag{3.7}$$

Many GMRES estimations in the case that $W(A)$ does not contain the origin are based on (3.7) (the constant 2 and the set $W(A)$ may be replaced by another constant and a set containing $W(A)$, respectively). Meanwhile, from Theorem 44, the GMRES bounds can be the following:

$$\frac{||r_k||}{||r_0||} \leq 2E_k(e^{W(\ln A)}). \tag{3.8}$$

If $W(A)$ contains the origin, then we may use the bound above so that we can follow the arguments used to estimate GMRES residual bounds where the numerical range is assumed not to contain the origin. Furthermore, many numerical tests show the relation

$$E_k(e^{W(\ln A)}) \leq E_k(W(A)). \tag{3.9}$$

For a given subset S of $\mathbb{C}$, $E_k(S)$ can be evaluated numerically, say, by using the SDPT3 [35] which is a MATLAB software for semidefinite programming problems.

Figure 3.4 shows examples of $e^{W(\ln A)}$ for the following matrices, where $W(A)$ does not contain the origin :

- C is a Toeplitz matrix with singular values near π defined by `gallery('parter',6)`.
- V is the matrix used in Figure 3.2 with $\lambda_j = j$.
- T is a tridiagonal matrix defined by `gallery('tridiag',c,d,e)` with subdiagonal `c`, diagonal `d`, and superdiagonal `e`; in this case T is a 5 by 5 matrix for `c`, `d`, and `e` randomly chosen.

In Figure 3.4, the left hand sides are the boundaries of $W(A)$ (red one) and $e^{W(\ln A)}$ (dotted blue one), and the right hand sides show $E_k(W(A))$ (red disk) and $E_k(e^{W(\ln A)})$ (blue square) for each $k = 2, \ldots, 20$, which shows the relation (3.9) clearly.

3.3 Summary and Future Research

It is conjectured that the numerical range of a given square matrix A is 2-spectral. The conjecture is not proved or disproved for general matrices even in dimension 3. In this thesis, we showed in detail that the conjecture holds for a class of matrices, using a sufficient condition (in Theorem 20) for the conjecture. We believe that the sufficient condition holds in general but we have been unable to prove it. Moreover, while working on the conjecture, we defined three constants for a given matrix and showed their relation (partly unproved) in (2.25). Studying the relation in itself seems to be also interesting.

The validity of the conjecture can be used to improve Elman's bound which is an upper bound for the relative residual norms of the generalized minimal residual method, assuming that the numerical range of the coefficient matrix A does not contain the origin. Meanwhile,

Figure 3.2: Examples of $W(A)$ and $e^{W(\ln A)}$

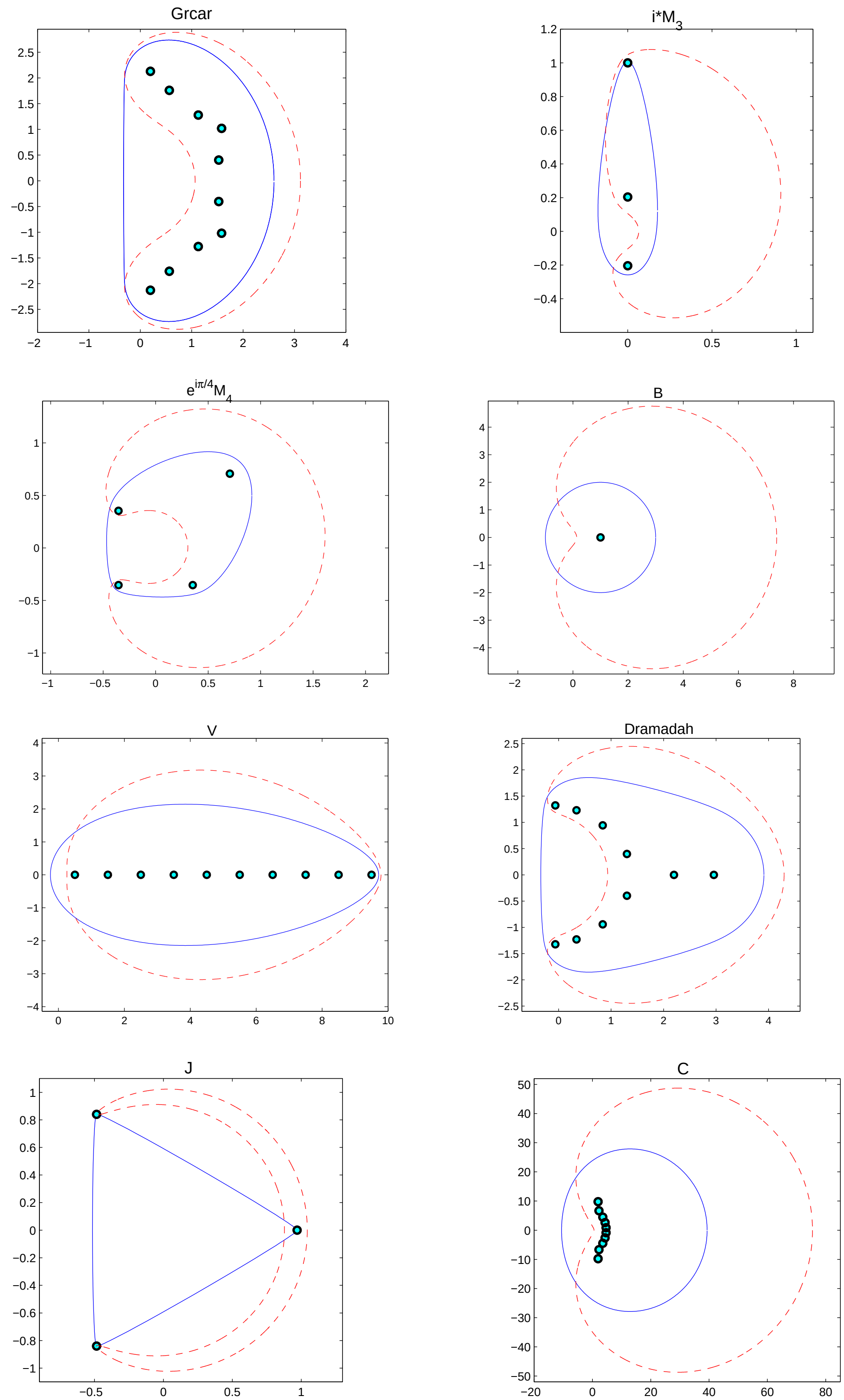


Figure 3.3: Examples for which $e^{W(\ln A)}$ are not simply connected.

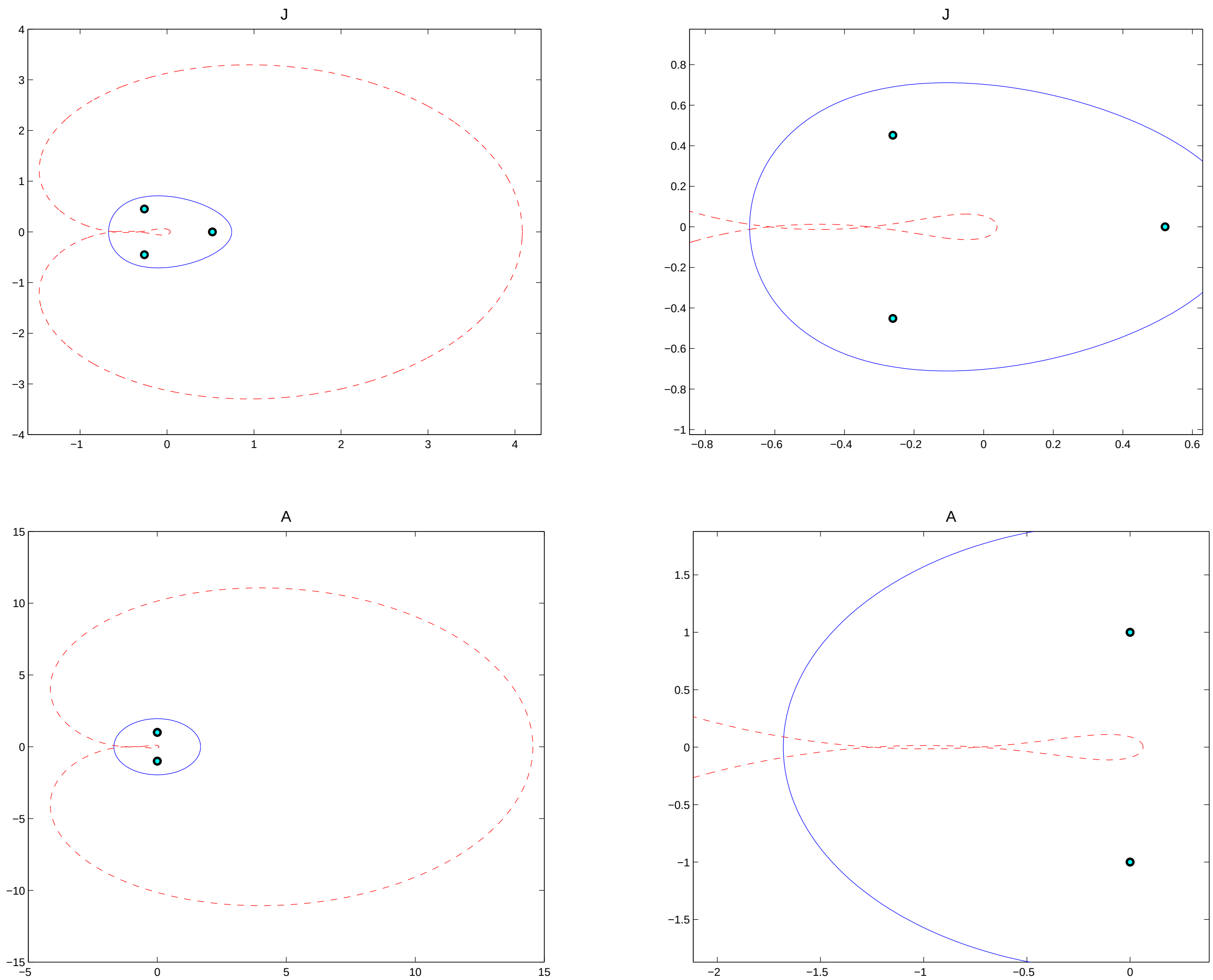
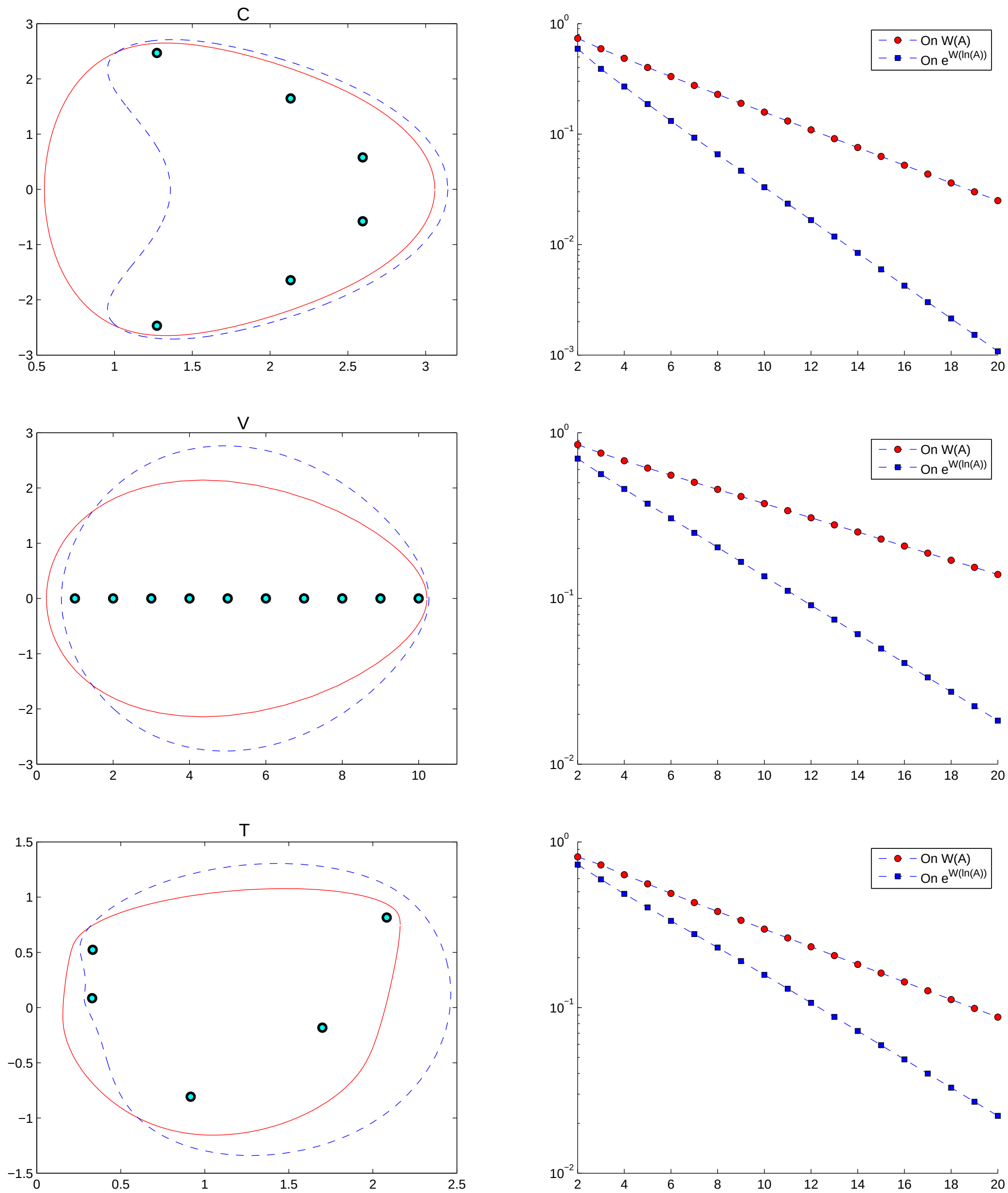


Figure 3.4: $E_k(W(A))$ v.s. $E_k(W(\ln A))$ when $0 \notin W(A)$



if $0 \in W(A)$, then we may use $e^{W(\ln A)}$ as a different K-spectral set. Finding analytic bounds using the set $e^{W(\ln A)}$ is one area of future research.

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