37
Spectral Sets

Catalin Badea
Université Lille 1
Bernhard Beckermann
Université Lille 1

Spectral sets and K-spectral sets, introduced by John von Neumann in [vNe51], offer a possibility to estimate the norm of functions of matrices in terms of the sup-norm of the function. Examples of such spectral sets include the numerical range or the pseudospectrum of a matrix, discussed in Chapters 23 and 25. Estimating the norm of functions of matrices is an essential task in numerous fields of pure and applied mathematics, such as (numerical) linear algebra [Gre97, Hig08], functional analysis [Pau02], and numerical analysis. More specific examples include probability [DD99], semi-groups and existence results for operator-valued differential equations, the study of numerical schemes for the time discretization of evolution equations [Cro08], or the convergence rate of GMRES (Section 54.7).

The notion of spectral sets involves many deep connections between linear algebra, operator theory, approximation theory, and complex analysis. For example, one requires simple criteria such that the closed unit disk, the numerical range, or another given set in the complex plane is K-spectral for a given matrix A. In order to study sharpness in matrix norm inequalities, one may look for extremal matrices or operators. It is also of interest to consider joint spectral sets of several matrices. How are notions like functional calculus, similarity, or dilation related to spectral sets? Is the intersection of spectral sets also spectral, and what are optimal constants? How the theory of spectral sets is applied to the approximate computation of matrix functions? The aim of this chapter is to give at least partial answers to these questions, and to present a survey of the modern theory of spectral and K-spectral sets for operators and matrices.

37.1 Matrices and Operators

Though many of the examples presented next are for matrices, it is more natural to present the theory of spectral sets in terms of operators acting on an abstract Hilbert space H. Those readers preferring matrices can always think of the Hilbert space $\mathbb{C}^n$ equipped with the usual scalar product.

For the convenience of the reader, some few basic properties of operator theory are collected below. Standard references are the books [RN55, SNF70, Nik02]. All definitions reduce to known ones in the case of matrices.

Definitions:

For a complex Hilbert space H with scalar product $\langle \cdot, \cdot \rangle$ we denote by $\mathcal{L}(H)$ the normed space of all bounded linear operators on H. The **operator norm** of $A \in \mathcal{L}(H)$ is defined by $\|A\| = \sup\{\|Ax\| : \|x\| = 1\}$. A **contraction** is a linear operator whose operator norm is not greater than one, while a **strict contraction** is an operator A such that $\|A\| < 1$. An operator $A \in \mathcal{L}(H)$ is **normal** if A commutes with its Hilbert space adjoint A^*. The operator A is **unitary** if $AA^* = A^*A = I$, where I represents the identity operator. The operator A is **Hermitian**, or **self-adjoint** if $A^* = A$. We say that the operator $A \in \mathcal{L}(H)$ is **positive semidefinite**, and we write $A \succeq 0$, if $\langle Ax, x \rangle \geq 0$ for each $x \in H$.

The **spectrum** $\sigma(A)$ of A is the set of all complex numbers z such that $A - zI$ is not an invertible operator. The **spectral radius** $\rho(A)$ of the operator A is given by $\rho(A) = \sup\{|\lambda| : \lambda \in \sigma(A)\}$. The **numerical range**, or field of values, of an operator A is defined by $W(A) := \{\langle Ax, x \rangle : \|x\| = 1\}$. The **numerical radius** of $A \in \mathcal{L}(H)$ is defined by $w(A) := \sup\{|\lambda| : \lambda \in W(A)\}$. An operator A is a **numerical radius contraction** if $w(A) \leq 1$.

For $s > 0$, we say that the operator $A \in \mathcal{L}(H)$ belongs to the class C_s of Sz.-Nagy and Foias if the inequality $\frac{2-s}{s}\|\zeta Ax\|^2 + 2\frac{s-1}{s}\mathrm{re}(\langle \zeta Ax, x \rangle) \leq \|x\|^2$ holds true for every $x \in H$ and every complex number ζ with $|\zeta| < 1$. The **operator radius** w_s associated with the class C_s may be defined by $w_s(A) = \inf\left\{r : r > 0, \frac{1}{r}A \in C_s\right\}$.

The following notation will be used throughout this chapter: for a set $M \subset \mathbb{C}$ we denote by ∂M its boundary and by $\overline{M}$ its closure. $\mathbb{D}$ is the open unit disk, $\mathbb{T} = \partial\mathbb{D}$ is the unit circle, and X always denotes a closed subset of $\mathbb{C}$.

Definitions:

$\mathcal{R}(X)$ and $\mathcal{C}(X)$ are the sets of complex-valued **bounded rational functions** on X, and complex-valued **bounded continuous functions** on X, respectively, equipped with the **supremum norm** $\|f\|_X = \sup\{|f(x)| : x \in X\}$.

Facts:

The following facts can be found in [SNF66, SNF70].

1. We have $\|A\|/2 \leq w(A) \leq \|A\|$, and $\|A\|/s \leq w_s(A)$. See also Chapter 25.
2. w_s is a norm on $\mathcal{L}(H)$ if and only if $0 < s \leq 2$.
3. $\lim_{s\to\infty} w_s(A) = \rho(A)$ for every $A \in \mathcal{L}(H)$.
4. The class C_1 is the class of all contractions and $w_1(A) = \|A\|$.
5. The class C_2 is the class of all numerical radius contractions and $w_2(A) = w(A)$.

Examples:

1. The space ℓ^2 of complex square summable sequences $x = (x_0, x_1, x_2, \ldots)$ with scalar product $\langle x, y \rangle = \sum_{j=0}^{\infty} x_j \overline{y_j}$ and norm $\|x\| = \sqrt{\langle x, x \rangle}$ is an example of an infinite dimensional Hilbert space. Here the action of a linear operator can be described by the matrix product Ax with an infinite matrix A. The shift operator S acting on ℓ^2 via $S(z_0, z_1, \ldots) = (0, z_0, z_1, \ldots)$ has the norm given by $\|S\| = 1$, the spectrum $\sigma(S) = \overline{\mathbb{D}}$, and the numerical range $W(S) = \mathbb{D}$.
2. We will sometimes also make use of Banach spaces like the space ℓ^p of complex sequences $x = (x_0, x_1, x_2, \ldots)$ with norm $\|x\| = \left(\sum_{j=0}^{\infty} |x_j|^p\right)^{1/p}$ where again the action of bounded linear operators is described by infinite matrices and the matrix-vector product. If one considers the subspaces of sequences where only the first n

entries are non-zero, then there is a canonical isomorphism with $\mathbb{C}^n$, equipped with the vector Hölder p-norm. Similarly, if the infinite matrix A contains non-zero entries only in the first n rows and columns, then the operator norm $\|A\|_{\mathcal{L}(\ell^p)}$ coincides with the matrix Hölder p-norm of the corresponding principal submatrix of order n.

3. Another example of an infinite dimensional Banach space is the set L^p of complex-valued functions defined on some set X, with $\|f\| := \left(\int_X |f(z)|^p \, d\mu(z)\right)^{1/p}$ for a suitable measure μ on X.
4. Since $f \in \mathcal{R}(X)$ is analytic on a neighborhood of X, we get from the maximum principle for analytic functions that

$$\|f\|_X = \sup\{|f(x)| : x \in X\} = \sup\{|f(x)| : x \in \partial X\}.$$

In particular, $\mathcal{R}(X)$ can be seen as a subalgebra of $\mathcal{C}(\partial X)$.

37.2 Basic Properties of Spectral Sets

Let H be a complex Hilbert space and suppose that A is a bounded linear operator on H. Suppose now that $\sigma(A)$ is included in the closed set X and that $f = p/q \in \mathcal{R}(X)$. As the poles of the rational function f are outside of X, the operator $f(A)$ is naturally defined as $f(A) = p(A)q(A)^{-1}$ (see Chapter 17) or, equivalently, by the Riesz holomorphic functional calculus [RN55].

We can now define the central objects of study of this chapter.

Definitions:

Let H be a complex Hilbert space and suppose that $A \in \mathcal{L}(H)$ is a bounded linear operator on H. Let X be a closed set in the complex plane.

For a fixed constant $K > 0$, the set X is said to be a K-**spectral** set for A if the spectrum $\sigma(A)$ of A is included in X and the inequality $\|f(A)\| \leq K\|f\|_X$ holds for every $f \in \mathcal{R}(X)$.

The set X is a **spectral** set for A if it is a K-spectral set with $K = 1$.

Facts:

Facts requiring proof for which no specific reference is given can be found in [RN55, Chap. XI] or [vNe51].

1. Von Neumann inequalities for closed disks of the Riemann sphere:
   (a) a closed disk $\{z \in \mathbb{C} : |z - \alpha| \leq r\}$ is a spectral set for $A \in \mathcal{L}(H)$ if and only if $\|A - \alpha I\| \leq r$.
   (b) the closed set $\{z \in \mathbb{C} : |z - \alpha| \geq r\}$ is spectral for $A \in \mathcal{L}(H)$ if and only if $\|(A - \alpha I)^{-1}\| \leq r^{-1}$.
   (c) the closed right half-plane $\mathbb{C}_0^+ = \{\mathrm{re}(z) \geq 0\}$ is a spectral set for A if and only if $\mathrm{re}(\langle Av, v\rangle) \geq 0$ for all $v \in H$. More generally, any closed half-plane is spectral for A if and only if it contains the numerical range $W(A)$.
2. Suppose that X is a spectral set for A and let $f \in \mathcal{R}(\sigma(A))$. Then $f(X)$ is spectral for $f(A)$. More generally, if $(f_n) \in \mathcal{R}(X)$, $\lim \|f_n - f\|_X = 0$, and $\lim \|f_n(A) - B\| = 0$, then $f(X)$ is a spectral set for B.
3. Any closed superset of a spectral set is again spectral. Any closed superset of a K-spectral set is again K-spectral.
4. The spectrum $\sigma(A)$ of $A \in \mathcal{L}(H)$ is the intersection of all spectral sets for A.

5. [Will67] Any spectral set contains a *minimal spectral set*, i.e., a spectral set having no proper closed subset that is spectral.
6. [vNe51] If the operator $A \in \mathcal{L}(H)$ is normal, then the spectrum $\sigma(A)$ is a (minimal) spectral set for A.
7. [Will67] Let A be a Hilbert space operator, X a set containing $\sigma(A)$, and let z_0 be an interior point of X. If $\|f(A)\| \leq \|f\|_X$ for each rational function $f \in \mathcal{R}(X)$ that vanishes at z_0, then X is a spectral set for A.
8. [Pau02, p. 18] Let A be a Hilbert space operator and let X be a closed set in the complex plane. Let $\mathcal{S} := \mathcal{R}(X) + \overline{\mathcal{R}(X)}$ regarded as a subset of $\mathcal{C}(\partial X)$. If X is spectral for A, then the functional calculus homomorphism from $\mathcal{R}(X)$ to $\mathcal{L}(H)$ defined by $f \mapsto f(A)$ extends to a well defined, *positive map* (i.e., it sends positive functions to positive semidefinite operators) Φ on $\mathcal{S}$, which sends $f + \overline{g}$ to $f(A) + g(A)^*$. Conversely, if Φ is well defined on $\mathcal{S}$, sends $f + \overline{g}$ to $f(A) + g(A)^*$, and is a positive map, then X is spectral for A.
9. Spectral sets and matrices with structure:
   (a) A complex matrix $A \in \mathbb{C}^{n \times n}$ is normal if and only if its set of eigenvalues $\sigma(A)$ is a spectral set for A.
   (b) The unit circle $\mathbb{T}$ is a spectral set for $A \in \mathcal{L}(H)$ if and only if A is unitary.
   (c) The real axis $\mathbb{R}$ is a spectral set for $A \in \mathcal{L}(H)$ if and only if A is self-adjoint (= Hermitian).
   (d) [Will67] Let A be a completely non-normal matrix; that is, the triangular factor in a Schur decomposition of A is not block diagonal. If $\|A\| = 1$, then the closed unit disk is a minimal spectral set.
10. Let $s > 0$. If A belongs to the class C_s, then the closed unit disk is K-spectral for A. [SNF66] We can take $K = 2s - 1$ if $s \geq 1$. [OA75] $K = \max(1, s)$ is the best possible constant.
11. [Nev12] Lemniscates as K-spectral sets: let p be a polynomial with distinct roots and let $A \in \mathcal{L}(H)$. Let $R \geq 0$ satisfy $\|p(A)\| \leq R$ and be such that the lemniscate $\{z \in \mathbb{C} : |p(z)| = R\}$ contains no critical points of p. Then $\{z \in \mathbb{C} : |p(z)| \leq R\}$ is a K-spectral set for A.
12. [KM66] The closed disk $3\overline{\mathbb{D}}$ of radius 3 is spectral for every Banach space contraction: if A is an operator acting on a complex Banach space E such that $\|A\|_{\mathcal{L}(E)} \leq 1$, and p is a polynomial, then $\|p(A)\|_{\mathcal{L}(E)} \leq \sup\{|p(z)| : |z| \leq 3\}$. The constant 3 is the best possible one.

Examples:

1. Suppose that -1 is not in the spectrum of the square matrix A of order n. If the right half-plane $\mathbb{C}_0^+ = \{\mathrm{re}(z) \geq 0\}$ is a spectral set for A, then $\|f(A)\| \leq \|f\|_{\mathbb{C}_0^+} = 1$ for $f(z) = \frac{z-1}{z+1}$ by definition of a spectral set. In order to see that also the converse is true, suppose that $\|f(A)\| \leq 1$. We set $\mathbf{u} = (A + I)\mathbf{v}$, and observe that
$$0 \leq \|\mathbf{u}\|^2 - \|f(A)\mathbf{u}\|^2 = \|(A + I)\mathbf{v}\|^2 - \|(A - I)\mathbf{v}\|^2 = 4\,\mathrm{re}(\langle A\mathbf{v}, \mathbf{v}\rangle).$$
In particular, $\mathbb{C}_0^+$ contains the spectrum of A, and $\mathbb{C}_0^+$ is spectral for A by Fact 37.2.1c.
2. Let $A \in \mathcal{L}(H)$, and $\alpha, \beta, \gamma, \delta \in \mathbb{C}$, $\alpha\delta - \beta\gamma \neq 0$, $-\delta/\gamma \notin \sigma(A)$. Then both $f(z) = \frac{\alpha z + \beta}{\gamma z + \delta}$ and its inverse are rational functions. Applying twice Fact 37.2.2, we see that X is spectral for A if and only if $f(X)$ is spectral for $f(A)$. Thus, for a proof of Fact 37.2.1 one only needs to show that $\|A\| \leq 1$ implies that $\overline{\mathbb{D}}$ is spectral for A; see, for instance, [RN55, Sect. 153].

3. Let the matrix A be block diagonal with $A = \mathrm{diag}(A_1, A_2)$. Then we have $f(A) = \mathrm{diag}(f(A_1), f(A_2))$ and hence X is K-spectral for A if and only if it is K-spectral for A_1 and A_2.
4. If the matrix A can be factorized as $A = CBC^{-1}$, then $f(A) = Cf(B)C^{-1}$. In particular, if X is K-spectral for B, then it is also K'-spectral for A with $K' \leq K \|C\| \|C^{-1}\|$.
5. If the matrix A is not diagonalisable, then no finite set X can be K-spectral for A. For a proof, according to Example 37.2.3 and Example 37.2.4 we may suppose that A is a Jordan block of order ≥ 2. Suppose that $X = \{x_1, ..., x_k\}$ is finite. Direct computations show that $f(A) \neq 0$ for $f(x) = (x - x_1) \cdots (x - x_k)$, and hence X cannot be K-spectral for A.
   It follows that the spectrum $\sigma(A)$ of a matrix A is K-spectral if and only if A is diagonalisable, and in this case we can take as K the condition number of the matrix of eigenvectors. See also Example 37.5.4.
6. From Example 37.2.4 we see that a normal, Hermitian, or unitary matrix A has $\sigma(A), \mathbb{R}$, or $\mathbb{T}$, respectively, as a spectral set. Let us show the converse result claimed in Facts 37.2.9a– 37.2.9c.
   If $\mathbb{R}$ is spectral for A, then according to Facts 37.2.2 and 37.2.3 the right half-plane $\mathbb{C}_0^+$ is spectral for iA and for $-iA$, which together with Fact 37.2.1c implies that $\langle A\mathbf{u}, \mathbf{u}\rangle \in \mathbb{R}$ for all $\mathbf{u}$. Hence, A is Hermitian.
   If $\mathbb{T}$ is spectral for A, then $f(\mathbb{T}) = \mathbb{R}$ is spectral for $f(A)$, $f(z) = \frac{1}{i}\frac{z-1}{z+1}$, according to Fact 37.2.2. Hence, $f(A)$ is Hermitian, implying that A is unitary.
   Finally, suppose that $\sigma(A) = \{\lambda_1, ..., \lambda_n\}$ is spectral for A. Then, denoting by $\ell_1, ..., \ell_n$ the Lagrange interpolation polynomials for $\sigma(A)$, that is, ℓ_j a polynomial of degree $\leq n - 1$ with $\ell_j(\lambda_k) = 0$ for $j \neq k$ and $= 1$ for $j = k$, we find that

$$z = \sum_{j=1}^{n} \lambda_j \ell_j(z) \quad \text{and hence} \quad A = \sum_{j=1}^{n} \lambda_j \ell_j(A).$$

   By Fact 37.2.2, $\ell_j(\sigma(A)) = \{0, 1\} \subset \mathbb{R}$ is spectral for $\ell_j(A)$, implying that $\ell_j(A)$ is Hermitian. From Example 37.2.5 we know that A is diagonalisable, implying that the $\ell_j(A)$ commute, and thus A is normal.
7. The closure X of the ϵ-pseudospectrum of $A \in \mathcal{L}(H)$ is a K-spectral set for $K = \frac{\mathrm{length}(\partial X)}{2\pi\epsilon}$ for any $\epsilon > 0$; see Fact 23.3.5.
8. [BS67, OA75, Cro04a] The disk $\{z \in \mathbb{C} : |z| \leq w(A)\}$ is 2-spectral for A. $K = 2$ is the best possible constant. This follows from Fact 37.2.10.

37.3 Around the von Neumann Inequality

According to Fact 37.2.1a stated for $\alpha = 0$, if A is a Hilbert space contraction and f is a rational function with poles off the closed unit disk, then $\|f(A)\| \leq \|f\|_{\overline{\mathbb{D}}}$. Since polynomials are dense in the *disk algebra* (that is, the Banach algebra of all complex-valued functions which are analytic on $\mathbb{D}$ and continuous up to $\partial\mathbb{D}$), the previous inequality implies that for every contraction on Hilbert space the rational functional calculus extends to a functional calculus on the disk algebra. The inequality $\|f(A)\| \leq \|f\|_{\overline{\mathbb{D}}}$ is known in Operator Theory as the *von Neumann inequality*. The aim of this section is to present several variations and generalizations.

Facts:

1. [Foi57] The von Neumann inequality characterizes Hilbert spaces: if E is a complex Banach space such that $\|p(A)\|_{\mathcal{L}(E)} \leq \|p\|_{\overline{\mathbb{D}}}$ holds for every polynomial p and every $A \in \mathcal{L}(E)$ with $\|A\|_{\mathcal{L}(E)} = 1$, then E is isometrically isomorphic to a Hilbert space (i.e., the norm of E comes from an inner product).
2. [Rov82] Another converse of von Neumann inequality: suppose that f_0 is holomorphic on an open subset G of $\mathbb{D}$ and $\|f_0(A)\| \leq 1$ for every contraction A on a Hilbert space, with spectrum contained in G (the operator $f_0(A)$ being defined by the Riesz holomorphic functional calculus). Then f_0 is the restriction to G of a holomorphic function f defined and bounded by 1 on $\mathbb{D}$.
3. [KM66] The von Neumann inequality for arbitrary matrix norms: let p be a polynomial of degree d with complex coefficients and let A be a complex matrix in $\mathbb{C}^{n\times n}$ with $\|A\| \leq 1$ for some subordinate matrix norm $\|\cdot\|$. Then $\|p(A)\| \leq (\pi n + 1)\,\|\,p\,\|_{\overline{\mathbb{D}}}$.
4. The shift as an extremal operator: define the shift S on a suitable space of sequences by $S(z_0, z_1, \ldots) = (0, z_0, z_1, \ldots)$.
   (a) [PPS02, Dix95] An operator-theoretical interpretation of H. Bohr's inequality: let $r > 0$, let E be a Banach space and let $A \in \mathcal{L}(E)$ be such that $\|A\|_{\mathcal{L}(E)} \leq r$. Then $\|p(A)\|_{\mathcal{L}(E)} \leq \|p(rS)\|_{\mathcal{L}(\ell^1)}$ for every polynomial p. We have $\|p(rS)\|_{\mathcal{L}(\ell^1)} \leq \|p\|_{\overline{\mathbb{D}}}$ if and only if $r \leq 1/3$.
   (b) [Pel81, CRW78, Nik02] Matsaev inequality for some classes of contractions: let p be a real number between 1 and ∞. Let $A : L^p \mapsto L^p$ be an isometry on a L^p space. Then A verifies the Matsaev inequality $\|f(A)\|_{\mathcal{L}(L^p)} \leq \|f(S)\|_{\mathcal{L}(\ell^p)}$ for every polynomial f. This inequality also holds for contractions on L^p which preserve positive functions, or for *disjoint contractions* ($A(f)A(g) = 0$ whenever $fg = 0$), or for operators such that $\|A\|_{\mathcal{L}(L^1)} \leq 1$ and $\|A\|_{\mathcal{L}(L^\infty)} \leq 1$.
   (c) [Dru11] Counterexample to a conjecture of Matsaev: let $f(z) = 1 + 2z - \frac{22}{5}z^2$. There is a 2×2 real matrix A with a real (or complex) Hölder 4-norm bounded above by 1 but with the Hölder 4-norm of $f(A)$ exceeding $\|f(S)\|_{\mathcal{L}(\ell^4)}$.
5. Constrained von Neumann inequalities
   (a) [PY80] Let f and g be two polynomials. Suppose that A is a Hilbert space contraction with spectrum included in $\mathbb{D}$ such that $g(A) = 0$. Then $\|f(A)\| \leq \|f(S^* \mid \ker g(S^*))\|$, where S^* is the backward shift,
   $$S^*(z_0, z_1, z_2, \ldots) = (z_1, z_2, \ldots),$$
   which is the adjoint of S acting on ℓ^2.
   (b) [HdlH92] Let A be a Hilbert space nilpotent contraction with $A^n = 0$, $n \geq 2$. Then
   $$w(A) \leq w(S^* \mid \ker(S^{n*}))) = \cos\frac{\pi}{n+1}.$$
   (c) [BC02] Let $n \geq 2$. Let $A \in \mathcal{L}(H)$ be a contraction such that $A^n = 0$. Then for each $s > 0$ and each polynomial f, we have $w_s(f(A)) \leq w_s(f(S_n^*))$. Here S_n^* denotes the nilpotent Jordan block
   $$S_n^* = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix}$$

which is unitarily equivalent to $S^* \mid \mathbb{C}^n = S^* \mid \ker S^{n*}$. In particular, for any m we have

$$w(A^m) \leq \cos \frac{\pi}{k(m,n)+2}, \quad k(m,n) := [\frac{n-1}{m}].$$

Also, if the degree of the polynomial f is at most $n-1$, then

$$w_s(f(A)) \leq \left(\frac{2}{s} - 1\right) \|f\|_{\mathbb{D}}^s \left[\inf_{\theta \in \mathbb{R}} \sup\{|f(\zeta)| : \zeta \in \mathbb{C}, \zeta^{2n-1} = e^{i\theta}\}\right]^{1-s}$$

if $s \in (0,1]$, and

$$w_s(f(A)) \leq \|f\|_{\mathbb{D}}^{2-s} \left[\inf_{\theta \in \mathbb{R}} \sup\{|f(\zeta)| : \zeta \in \mathbb{C}, \zeta^{2n-1} = e^{i\theta}\}\right]^{s-1}$$

if $s \in [1,2]$.

(d) [BC02] Let $A \in \mathcal{L}(H)$ be a nilpotent Hilbert space operator satisfying

$$I - A^*A \succeq 0, \quad I - 2A^*A + A^{*2}A^2 \succeq 0,$$

and $A^n = 0$, $n \geq 2$. Then

$$w_s(f(A)) \leq w_s(f(B_n^*))$$

for all $s > 0$ and all polynomials f. Here B_n^* is given by the matrix

$$B_n^* = \begin{bmatrix} 0 & \sqrt{\frac{1}{2}} & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & \sqrt{\frac{n}{n+1}} \\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix}$$

which is unitarily equivalent to a compression of the Bergman shift.

(e) [BC02] Suppose $A \in \mathcal{L}(H)$ satisfies $\|A\| \leq 1$, $A^3 = 0$ and $I - 2A^*A + A^{*2}A^2 \succeq 0$. Then

$$w(A) \leq \sqrt{\frac{7}{24}} \quad \text{and} \quad w(A^2) \leq \sqrt{\frac{1}{12}}$$

and these constants are the best possible ones.

(f) [BC02] The link between the extremal operator in the constrained von Neumann inequalities and the Taylor coefficients of rational functions positive on the unit circle $\mathbb{T}$: let $F = P/Q$ be a rational function with no principal part and which is positive on the unit circle. Then the kth Taylor coefficient c_k satisfies $|c_k| \leq c_0 w(R^k)$, where $R = S^* \mid \ker(Q(S^*))$. In particular, if $P(e^{it}) = \sum_{j=-n+1}^{n-1} c_j e^{ijt}$ is a positive trigonometric polynomial, $n \geq 2$, then $|c_k| \leq c_0 \cos(\frac{\pi}{[\frac{n-1}{k}]+2})$ for $1 \leq k \leq n-1$ and, for every distinct numbers k and l among $\{0, \ldots, n-1\}$, there exists $\gamma \in \mathbb{R}$ such that $|c_k| + |c_l| \leq c_0 w(S_n^k + e^{i\gamma} S_n^l)$. We also have

$$|c_k| + |c_l| \leq c_0 \left(1 + \cos \frac{\pi}{[\frac{n-1}{k+l}] + 2}\right)^{1/2} \left(1 + \cos \frac{\pi}{[\frac{n-1}{|k-l|}] + 2}\right)^{1/2}.$$

Examples:

1. [RN55, p. 436] The von Neumann inequality fails for the Hölder 1-norm in $\mathbb{C}^2$ (or in ℓ^1): consider

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad f(z) = \frac{z+a}{1+\overline{a}z}, \quad a = \frac{i}{2}, \quad f(A) = \begin{bmatrix} 4i/5 & 3/5 \\ 3/5 & 4i/5 \end{bmatrix},$$

then $\|A\|_1 = 1$, $\|f\|_{\overline{\mathbb{D}}} = 1$, but $\|f(A)\|_1 = \frac{7}{5} > 1$.

2. [Pau02, p. 23] The Schwarz-Pick lemma as a consequence of von Neumann inequality: Let p be a polynomial such that $\|p\|_{\overline{\mathbb{D}}} < 1$. Let a, b, and c be complex numbers such that $|a| < 1, |c| < 1$, $a \neq c$, and $|b|^2 = (1-|a|^2)(1-|c|^2)$. Consider the 2×2 matrix

$$A = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$$

acting on the Euclidean space $\mathbb{C}^2$. Then $\|A\| = 1$,

$$p(A) = \begin{bmatrix} p(a) & b\frac{p(a)-p(c)}{a-c} \\ 0 & p(c) \end{bmatrix}$$

and the von Neumann inequality $\|p(A)\| \leq \|p\|_{\overline{\mathbb{D}}}$ implies that

$$\left|\frac{p(a)-p(c)}{a-c}\right|^2 \leq \frac{1-|p(a)|^2}{1-|a|^2}\frac{1-|p(c)|^2}{1-|c|^2}.$$

Using the identity $|1-u\overline{v}|^2 = (1-|u|^2)(1-|v|^2) + |u-v|^2$, this can be written as

$$\left|\frac{p(a)-p(c)}{1-\overline{p(c)}p(a)}\right| \leq \left|\frac{a-c}{1-\overline{c}a}\right|.$$

37.4 The Multidimensional von Neumann Inequality

Definitions:

We say that the **multidimensional von Neumann inequality** holds for a fixed n-tuple of commuting operators $A = (A_1, A_2, \ldots, A_n)$ if

$$\|p(A_1, \ldots, A_n)\| \leq \|p\|_{\overline{\mathbb{D}}^n}$$

for every polynomial p in n (commutative) variables.

Facts:

We use [Nik02] as a general reference.

1. The multidimensional von Neumann inequality holds in the following situations:
   (a) [And63] For a pair of commutative Hilbert space contractions ($n = 2$).
   (b) For a commutative family of isometries.
   (c) For a family of *doubly commuting* (i.e., $A_iA_j = A_jA_i$ for all i and j and $A_i^*A_j = A_jA_i^*$ whenever $i \neq j$) contractions.
   (d) [Bre61] For a commutative family A such that $\sum_{j=1}^n \|A_j\|^2 \leq 1$.

2. [AM05] Distinguished varieties: let A_1 and A_2 be two commuting contractive matrices, neither of which has eigenvalues of modulus one. Then there is a polynomial $q \in \mathbb{C}[z,w]$ such that the algebraic set $V = \{(z,w) \in \mathbb{D}^2 : q(z,w) = 0\}$ verifies $\|p(A_1,A_2)\| \leq \|p\|_V$ for any polynomial p in two variables and $\overline{V} \cap \partial(\mathbb{D}^2) = \overline{V} \cap (\partial\mathbb{D})^2$ (the variety exits the bidisk through the distinguished boundary).
3. Extremal n-tuples.
   (a) [Dru78, Pop99, Arv98] The Drury-Arveson space and the von Neumann inequality of Drury-Popescu-Arveson: let $\mathbb{B}^n = \{z \in \mathbb{C}^n : \sum_{j=1}^n |z_j|^2 < 1\}$ be the unit open ball in $\mathbb{C}^n$. Let DA_n be the Drury-Arveson space of all power series g such that
   $$g = \sum_{\alpha \geq 0} a_\alpha z^\alpha, \quad \|g\|^2_{DA_n} = \sum_{\alpha \geq 0} |a_\alpha|^2 \frac{\alpha!}{|\alpha|!} < \infty,$$
   where $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$, $|\alpha| = \sum_{j=1}^n \alpha_j$ and $\alpha! = \prod_{j=1}^n (\alpha_j!)$. The Drury-Arveson space DA_n can be also regarded as the reproducing kernel Hilbert space with kernel
   $$k_\lambda(z) = \frac{1}{1 - \sum_{j=1}^n z_j \overline{\lambda_j}}, \quad z, \lambda \in \mathbb{B}^n.$$
   Let $S_j g(z) = z_j g(z)$, where $z = (z_1, \ldots, z_n)$ and $g \in DA_n$. Let $A = (A_1, \ldots, A_n)$ be a commutative n-tuple on a Hilbert space H such that $I \succeq \sum_{j=1}^n A_j A_j^*$, or equivalently,
   $$\left\| \sum_{j=1}^n A_j x_j \right\|^2 \leq \sum_{j=1}^n \|x_j\|^2$$
   for all $x_j \in H$. Then
   $$\|p(A_1, \ldots, A_n)\| \leq \|p(S_1, \ldots, S_n)\|$$
   for every polynomial p.
   (b) [Dru78] A dual version: let S_j^*, $j = 1, \ldots, n$, be the backward shift operators on the Cauchy dual DA_n^* of the Drury-Arveson space. This means that $g = \sum_{\alpha \geq 0} a_\alpha z^\alpha$ with $\|g\|^2_{DA_n^*} = \sum_{\alpha \geq 0} |a_\alpha|^2 \frac{|\alpha|!}{\alpha!} < \infty$, and $a_\alpha(S_j^* g) = a_{\alpha + \delta_j}(g)$ for all $\alpha \geq 0$, where $\delta_j = (\delta_{jk})_{1 \leq k \leq n}$. Let $A = (A_1, \ldots, A_n)$ be a commutative n-tuple on a Hilbert space H such that $I \succeq \sum_{j=1}^n A_j^* A_j$, or equivalently,
   $$\sum_{j=1}^n \|A_j x\|^2 \leq \|x\|^2$$
   for all $x \in H$. Then
   $$\|p(A_1, \ldots, A_n)\| \leq \|p(S_1^*, \ldots, S_n^*)\|$$
   for every polynomial p.
4. [Mla71] Mlak's von Neumann inequality with operator coefficients: let $C_k : H \mapsto H$ be bounded linear operators, $k = 0, \ldots, n$, and $A \in \mathcal{L}(H)$ be a contraction which double-commutes with the C_k's, i.e., $AC_k = C_k A$ and $AC_k^* = C_k^* A$ for every k. Then
   $$\left\| \sum_{j=0}^n C_j A^j \right\| \leq \sup_{|z| \leq 1} \left\| \sum_{j=0}^n C_j z^j \right\|.$$

5. [Lub78] Let $(A_1, \ldots, A_n)$ be commuting contractions on a Hilbert space H. Then the polydisk $\{(z_1, \ldots, z_n) : |z_i| < \sqrt{n}, 1 \le j \le n\}$ is a spectral set for $(A_1, \ldots, A_n)$.
6. [Hir72] The *Poisson radius*: let $A = (A_1, \ldots, A_n)$ be an n-tuple of commuting operators on a Hilbert space H, with spectra included in $\overline{\mathbb{D}}$. Define

$$P_j(rA_j, \zeta_j) = \mathrm{re}\left(\left((\zeta_j I + rA_j)(\zeta_j I - rA_j)^{-1}\right)\right)$$

for $0 \le r < 1$, $\zeta_j \in \mathbb{T}$, $1 \le j \le n$, and the Poisson radius $r_P(A)$ of A as the supremum of $r \in [0, 1)$ such that

$$\frac{1}{n!} \sum_{\sigma} P_{\sigma(1)}(rA_{\sigma(1)}, \zeta_{\sigma(1)}) \ldots P_{\sigma(n)}(rA_{\sigma(n)}, \zeta_{\sigma(n)})$$

is a positive operator for every $\zeta \in \mathbb{T}^n$, where σ runs over all permutations of $(1, \ldots, n)$. Then $0 < r_P(A) \le 1$ and $\|f(r_P(A)A)\| \le \|f\|_{\overline{\mathbb{D}}^n}$ for every polynomial f.
7. [Agl90] The Schur-Agler class: let f be an analytic function of n complex variables $\lambda = (\lambda^1, \cdots, \lambda^n)$. Then $f(rA_1, \ldots, rA_n)$ has norm at most 1 for any $r < 1$ and any collection of n commuting contractions $(A_1, \ldots, A_n)$ on a Hilbert space if and only if there are auxiliary Hilbert spaces H_j, $1 \le j \le n$, and an isometry $V \in \mathcal{L}(\mathbb{C} \oplus H_1 \oplus \cdots \oplus H_n)$ such that, if $H = H_1 \oplus \cdots \oplus H_n$, V is written with respect to $\mathbb{C} \oplus H$ as $V = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, and $\mathcal{E}_\lambda = \lambda^1 I_{H_1} \oplus \cdots \lambda^n I_{H_n}$, then $f(\lambda) = A + B\mathcal{E}_\lambda(I_H - D\mathcal{E}_\lambda)^{-1}C$.
8. [Boz89] Bożejko's von Neumann inequality for non-commuting tuples: let A_k, $1 \le k \le n$, be (not necessarily commuting) contractions on H. Let $f = f(x_1, \ldots, x_n)$ be a polynomial in the noncommutative indeterminates $x_1, \ldots, x_n$. Then

$$\|f(A_1, \ldots, A_n)\| \le \sup\{\|f(U_1, \ldots, U_n)\| : U_j \text{ unitary matrices on } \mathbb{C}^{m \times m}, m \in \mathbb{N}\}.$$

Open Problems:

1. [Dix76] It is not known if for each n there exists a finite constant C_n such that for any commuting contractions $A_1, \ldots, A_n$ and any polynomial f in n variables one has

$$\|f(A_1, \ldots, A_n)\| \le C_n \|f\|_{\overline{\mathbb{D}}^n}.$$

It is generally believed that such a constant C_n does not exist. One knows that C_n must increase faster than any power of n.

Examples:

1. [Var74] The multidimensional von Neumann inequality fails in general for $n \ge 3$ and matrices $A_1, \ldots, A_n \in \mathbb{C}^{d \times d}$.
2. [Var74] The multidimensional von Neumann inequality can fail with $n = 3$ and $d = 5$. The three matrices $A_1, A_2, A_3 \in \mathbb{C}^{5 \times 5}$ are commuting contractions (with respect to the Euclidean norm), and the polynomial $p(z_1, z_2, z_3) = z_1^2 + z_2^2 + z_3^2 - 2z_1z_2 - 2z_1z_3 - 2z_2z_3$ satisfies $\|p\|_{\mathbb{T}^3} = 5$ and $\|f(A_1, A_2, A_3)\| > 5$:

$$A_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 \end{bmatrix},$$

$$A_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \end{bmatrix}.$$

3. [CD75] Denote by $\mathbf{e}_j$, $1 \le j \le 8$, the vectors of the standard orthonormal basis of $\mathbb{C}^8$. Let $p(z_1, z_2, z_3) = z_1 z_2 z_3 - z_1^3 - z_2^3 - z_3^3$. There exist three commuting matrices $A_k \in \mathbb{C}^{8\times 8}$, $k = 1, 2, 3$, such that $\|A_i\| \le 1$ and $\|p(A_1, A_2, A_3)\| \ge 4 > \|p\|_{\mathbb{T}^3}$. The contractions A_i are acting on the orthonormal basis as follows:

$$\begin{aligned} A_1 &: \mathbf{e}_1 \longrightarrow \mathbf{e}_2 \longrightarrow (-\mathbf{e}_5) \longrightarrow (-\mathbf{e}_8) \longrightarrow 0, \mathbf{e}_3 \longrightarrow \mathbf{e}_7 \longrightarrow 0, \mathbf{e}_4 \longrightarrow \mathbf{e}_6 \longrightarrow 0 \\ A_2 &: \mathbf{e}_1 \longrightarrow \mathbf{e}_3 \longrightarrow (-\mathbf{e}_6) \longrightarrow (-\mathbf{e}_8) \longrightarrow 0, \mathbf{e}_2 \longrightarrow \mathbf{e}_7 \longrightarrow 0, \mathbf{e}_4 \longrightarrow \mathbf{e}_5 \longrightarrow 0 \\ A_3 &: \mathbf{e}_1 \longrightarrow \mathbf{e}_4 \longrightarrow (-\mathbf{e}_7) \longrightarrow (-\mathbf{e}_8) \longrightarrow 0, \mathbf{e}_2 \longrightarrow \mathbf{e}_6 \longrightarrow 0, \mathbf{e}_3 \longrightarrow \mathbf{e}_5 \longrightarrow 0 \end{aligned}$$

4. [Var74] Given $K > 0$, there exist a positive integer n, commuting operators $A_1, \ldots, A_n$, and a polynomial p such that $\sum_{j=1}^n \|A_j\|^2 \le 1$ and

$$\|p(A_1, \ldots, A_n)\| > K \sup \left\{ |p(z_1, \ldots, z_n)| : \sum_{j=1}^n |z_j|^2 \le 1 \right\}.$$

37.5 Dilations, Complete Bounds, and Similarity Problems

Definitions:

For a given closed set X of the complex plane, we say that $A \in \mathcal{L}(H)$ has a **normal ∂X-dilation** if there exist a Hilbert space $\mathcal{H}$ containing H and a normal operator N on $\mathcal{H}$ with $\sigma(N) \subset \partial X$ so that

$$f(A) = P_H f(N) \mid_H$$

for every rational function f with poles off X. Here P_H is the orthogonal projection of $\mathcal{H}$ onto H.

If $X = \overline{\mathbb{D}}$, then N is a unitary operator and we say that A has a **unitary (strong) dilation**. Notice that in this chapter, contrary to Chapter 25, a unitary (strong) dilation A is a common dilation of all powers of A.

For a fixed $s > 0$, we say that $A \in \mathcal{L}(H)$ has an **s-unitary dilation** if there exists a Hilbert space $\mathcal{H}$ containing H and a unitary operator U on $\mathcal{H}$ such that

$$A^n = sP_H U^n \mid_H, \quad (n \ge 1).$$

The last two definitions agree in the case $s = 1$.

We denote by $M_n(\mathcal{R}(X))$ the algebra of n by n matrices with entries from $\mathcal{R}(X)$.

Considering the (spectral) Hölder 2-norm for matrices in $\mathbb{C}^{n\times n}$, we can endow $M_n(\mathcal{R}(X))$ with the norm

$$\| (f_{ij})_{1\le i,j\le n} \|_X = \sup\{\| (f_{ij}(x))_{1\le i,j\le n} \| : x \in X\} = \sup\{\| (f_{ij}(x))_{1\le i,j\le n} \| : x \in \partial X\}.$$

In a similar fashion we endow $M_n(\mathcal{L}(H))$ with the norm it inherits by regarding an element $(A_{ij})_{1\le i,j\le n}$ in $M_n(\mathcal{L}(H))$ as an operator acting on the direct sum of n copies of H.

For a fixed constant $K > 0$, the set X is said to be a **complete K-spectral** set for A if $\sigma(A) \subset X$ and the inequality $\|(f_{ij}(A))_{1\le i,j\le n}\| \le K\|(f_{ij})_{1\le i,j\le n}\|_X$ holds for every matrix $(f_{ij}) \in M_n(\mathcal{R}(X))$ and every n.

A **complete spectral** set is a complete K-spectral set with $K = 1$.

We also say that A is **power bounded** if $\sup_n \|A^n\| < \infty$.

Two Hilbert space operators A and B are said to be **similar** if there exists an invertible operator L such that $B = L^{-1}AL$.

Facts:

All the following facts except those with a specific reference can be found in [SNF70, Pie01, Pau02]. We denote by A a Hilbert space operator and by X a closed subset of $\mathbb{C}$.

1. [Arv69, Arv72, Pau84b] A has a normal ∂X-dilation if and only if X is a complete spectral set for A.
2. X is completely K-spectral for A if and only if X is completely spectral for an operator $B \in \mathcal{L}(H)$ similar to A, say, $B = L^{-1}AL$, with $\|L^{-1}\|\,\|L\| \le K$.
3. Each completely spectral set for A is spectral. Conversely, a spectral set for A is completely spectral in the following situations:
   (a) If X is a closed disk.
   (b) [Agl85] If X is an annulus.
   (c) [Pau02, Theorem 4.4] If $\mathbb{C}\backslash X$ has only finitely many components and the interior of X is simply connected or, more generally, if $\mathcal{R}(X) + \overline{\mathcal{R}(X)}$ is dense in $\mathcal{C}(\partial X)$.
   (d) [AHR08, DMC05] There is a closed set X in $\mathbb{C}$ having "two holes" and an operator A such that X is spectral for A but not completely spectral. [Pic10] More generally, such a counterexample exists whenever X is a symmetric domain in $\mathbb{C}$ with n holes, $2 \le n < \infty$.
   (e) [DP86, Pau02] Let the boundary of the compact $X \subset \mathbb{C}$ consist of $n+1$ disjoint Jordan curves. If X is a spectral set, then it is a complete $(2n+1)$-spectral set.
4. Each completely K-spectral set for $A \in \mathcal{L}(H)$ is K-spectral. [Pau87] The converse is true whenever A is a 2×2 matrix. [Pie97] However, there exists an example where $\overline{\mathbb{D}}$ is K-spectral for $A \in \mathcal{L}(H)$ but not completely K'-spectral for any K'.
5. A combination of these facts yields several corollaries which historically came first:
   (a) (Sz.-Nagy dilation theorem) Every Hilbert space contraction has a unitary dilation.
   (b) (Berger dilation theorem) Every numerical radius contraction has a unitary 2-dilation.
   (c) (Paulsen criterion) An operator A is similar to a contraction if and only if it has the closed unit disk as a complete K-spectral set.
6. Operators of class C_s:
   (a) [SNF66, OA75] Let $s > 0$. Every operator of class C_s has a unitary s-dilation.
   (b) Let $s > 0$. If A is of class C_s, then $\|f(A)\| \le \max\{|s\cdot f(z)+(1-s)\cdot f(0)| : |z| \le 1\}$ for every polynomial f.
   (c) Let H be a complex Hilbert space of dimension ≥ 2. Then the class C_s increases with s: we have $\mathrm{C}_s \subset \mathrm{C}_{s'}$ and $\mathrm{C}_s \ne \mathrm{C}_{s'}$ for $0 < s < s'$. The set of operators acting on H which belong to one of the classes C_s, for some $s > 0$, is dense in the strong operator topology in the set of all power bounded operators.

7. Unitary dilations for n-tuples:
   (a) [And63] Every pair of commuting contractions on a Hilbert space has a pair of commuting unitary dilations.
   (b) [GR69] Every n-tuple $A = (A_1, \ldots, A_n) \in \mathcal{L}(H)^n$ which is *cyclic commutative*, i.e.,
   $$A_1 A_2 \ldots A_n = A_n A_1 \ldots A_{n-1} = \ldots = A_2 A_3 \ldots A_n A_1,$$
   has a cyclic commutative dilation to an n-tuple of unitaries.
   (c) [Ope06] Let G be an *acyclic* graph on n vertices $\{1, 2, \ldots, n\}$ (this means that it does not contain a cycle as a subgraph). Let $A = (A_1, A_2, \ldots, A_n)$ be an n-tuple of contractions on a Hilbert space that *commute according to* G, that is $A_i A_j = A_j A_i$ whenever (i, j) is an edge of G. Then there exists an n-tuple U of unitaries on a larger Hilbert space that commute according to G such that U dilates A. This property may fail if G contains a cycle.
8. Power boundedness and similarity to a contraction (i.e., $\overline{\mathbb{D}}$ is completely K-spectral):
   (a) [Rot60, Her76, Voi74] Rota type theorems: If $A \in \mathcal{L}(H)$ with $\sigma(A) \subset \mathbb{D}$, then A is similar to a contraction. More general results are true for some closed sets $X \subset \mathbb{C}$ and for operators A with $\sigma(A) \subset X$.
   (b) [Bad03] A Banach space Rota theorem and Matsaev inequality: Let E_1 be a Banach space and suppose that $A \in \mathcal{L}(E_1)$ has $\sigma(A) \subset \mathbb{D}$. Then, for every $p > 1$, there exists a Banach space E_2 which is a quotient of the set $\ell^p(E_1)$ of E_1-valued sequences and an isomorphism $L : E_2 \to E_1$ such that, if $B = L^{-1}AL \in \mathcal{L}(E_2)$, then
   $$\|f(B)\|_{\mathcal{L}(E_2)} \leq \|f(S)\|_{\mathcal{L}(\ell^p(E_1))}$$
   for each polynomial f and, even more generally,
   $$\|(f_{ij}(B))_{1 \leq i,j \leq n}\|_{\mathcal{L}(E_2^n)} \leq \|(f_{ij}(S))_{1 \leq i,j \leq n}\|_{\mathcal{L}(\ell^p(E_1)^n)}$$
   for all matrices of polynomials.
   (c) If A is compact and power bounded, then A is similar to a contraction.
   (d) [Fog64, Leb68, Pie97] There is a Hilbert space operator A which is power bounded but for which the closed unit disk is not K-spectral for any K, and thus A is not similar to a contraction. There is a Hilbert space operator A which is not similar to a contraction but for which the closed unit disk is K-spectral for A, for some K.
   (e) [Pel82, Bou86] Let $A \in \mathcal{L}(H)$ with $M = \sup_n \|A^n\| < \infty$ and let p be a polynomial of degree $d \geq 2$. Then $\|p(A)\| \leq M^2 (\log d) \| p \|_{\overline{\mathbb{D}}}$. A similar result holds for norms of matrices of polynomials, and the $\log d$ term in the inequality is the best one may hope for.
   (f) [Bou86] Bourgain's estimate for matrices similar to contractions: If A is a matrix such that, with the (spectral) Hölder 2-norm, $\|f(A)\| \leq C\|f\|_{\overline{\mathbb{D}}}$ for any polynomial f, then there is an invertible matrix L such that $\|L^{-1}AL\| \leq 1$ and $\|L^{-1}\| \, \|L\| \leq KC^4 \log(n+1)$, where K is a numerical constant independent of n.
   (g) [BePr98] Suppose that $\overline{\mathbb{D}}$ is K-spectral for $A \in \mathcal{L}(H)$. Then there exist Hilbert spaces H_1, H_2, contractions $A_1 \in \mathcal{L}(H_1)$, $A_2 \in \mathcal{L}(H_2)$ and injective linear operators $X_1 : H_1 \mapsto H, X_2 : H \mapsto H_2$ with dense ranges such that $X_1 A_1 = AX_1$ and $A_2 X_2 = X_2 A$. See also Example 37.5.5.

Open Problems:

1. [SNF70] What is the obstruction to an n-tuple of commuting Hilbert space contractions having commuting unitary dilation?

Examples:

1. The (unilateral) backward shift operator $S^* \in \mathcal{L}(\ell^2)$ defined by $(S^*x)_j = x_{j+1}$, $j \in \mathbb{N}$, is easily seen to be a contraction, with spectrum $\sigma(S^*) = \overline{\mathbb{D}}$. Hence, $X = \overline{\mathbb{D}}$ is a (completely) spectral set for S^*. For quadratic summable sequences x indexed by $\mathbb{Z}$, one defines the bilateral backward shift operator B through $(Bx)_j = x_{j+1}$, $j \in \mathbb{Z}$, which is clearly unitary. Since $(B^n x)_j = x_{j+n}$, $j \in \mathbb{Z}$, $n \geq 1$, we see that B is a 1-unitary dilation and thus a unitary dilation of S^*.
2. The notion of (weak or strong) unitary dilation is a nice illustration of why it is important in linear algebra sometimes to have recourse to infinite dimensions: we say that $A \in \mathbb{C}^{n\times n}$ is imbedded in $B \in \mathbb{C}^{m\times m}$ if $B = \begin{bmatrix} A & * \\ * & * \end{bmatrix}$. Given a contraction $A \in \mathbb{C}^{n\times n}$, is there a unitary $B \in \mathbb{C}^{m\times m}$ such that $p(A)$ is imbedded in $p(B)$ for any polynomial p of degree at most k? This property, related with the exactness property for Krylov spaces, reduces to (strong) unitary dilations for $k = \infty$ considered above, and for $k = 1$ to the (weak) unitary dilation considered in Section 25.6. The latter problem has the solution [Hal50]
$$B = \begin{bmatrix} A & (I - AA^*)^{1/2} \\ (I - A^*A)^{1/2} & -A^* \end{bmatrix}.$$
Egérvary [Ege54] showed that such an imbedding is always possible with $m = (k+1)n$: for example, one may imbed the n-dimensional shift in a unitary circulant of order $m = (k+1)n$. It is also known that in general such an imbedding for finite m is impossible for $k = \infty$; see also [LS13, MS13] for more modern aspects of this question.
3. [Par70] Let U and V be two contractions in $\mathcal{L}(H)$ such that U is unitary and $UV \neq VU$. We define three commuting contractions in $\mathcal{L}(H \oplus H)$ by defining
$$A_1 = \begin{bmatrix} 0 & 0 \\ I & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 0 & 0 \\ U & 0 \end{bmatrix}, A_3 = \begin{bmatrix} 0 & 0 \\ V & 0 \end{bmatrix}.$$
Then the commuting triplet $A = (A_1, A_2, A_3)$ verifies the multidimensional von Neumann inequality but does not possess a commuting triplet of (strong) unitary dilations.
4. Let $A \in \mathbb{C}^{n\times n}$ be diagonalizable. Then A is power bounded if and only if $\sigma(A) \subset \overline{\mathbb{D}}$, and in this case A is similar to the contraction given by the Jordan canonical form. Here $\overline{\mathbb{D}}$ is (completely) K-spectral, with K the condition number of the matrix of eigenvectors.
If $A \in \mathbb{C}^{n\times n}$ is not diagonalizable, then $\sigma(A) \subset \mathbb{D}$ still implies (through, e.g., the Cauchy integral formula and the pseudo-spectrum) that $\overline{\mathbb{D}}$ is completely K-spectral for some K. However, in general, the Jordan canonical form is no longer a contraction.
5. [MT07] Let $T \in \mathcal{L}(H)$ and $S \in \mathcal{L}(K)$ be Hilbert space operators. We say that T is a *quasiaffine transform* of S if there exists an injective operator $A : H \mapsto K$ with dense range such that $AT = SA$. We say that T is *quasisimilar* to S if each operator is a quasiaffine transform of the other.
There exists a power bounded operator on a Hilbert space which is not quasisimilar to a contraction.

6. [Pie97, DP97, Bad03, BP01, Ric02] Let $\alpha = (\alpha_0, \alpha_1, \dots)$ be a sequence in ℓ^2 and set
$$R(\alpha) = \begin{bmatrix} S^* & Y(\alpha) \\ 0 & S \end{bmatrix} \in \mathcal{L}(\ell^2(H) \oplus \ell^2(H)),$$
where S is the shift on the Hilbert space $\ell^2(H)$ of H-valued square summable sequences, H is of infinite dimension, and $Y(\alpha) = \Big[\alpha_{i+j} C_{i+j}\Big]_{i,j\geq 0}$, where the C_j's are operators verifying the *canonical anticommutation relations* $C_i C_j + C_j C_i = 0$ and $C_i C_j^* + C_j^* C_i = \delta_{ij} I$.
Then the operator $R(\alpha)$ is polynomially bounded if and only if $\sup_{k\geq 0}(k+1)^2 \sum_{i\geq k} |\alpha_i|^2$ is finite, and $R(\alpha)$ is similar to a contraction if and only if $\sum_{k\geq 0}(k+1)^2|\alpha_k|^2$ is finite.

37.6 Intersections of Spectral and K-Spectral Sets

In this part we will discuss intersections of spectral sets, including the annulus problem of Shields [Shi74]. It is known that the intersection of two spectral sets is not necessarily a spectral set, see [Will67, Mis84, Pau02] and Example 37.6.1. However, the same question for K-spectral sets remains open, although the previous examples indicate that one may not use the same constant. We refer to [Pau88] and the book [Pau02] for modern surveys of known properties of K-spectral and complete K-spectral sets.
Facts:

1. [DP86, Pau02] If two K-spectral sets have disjoint boundaries, then their intersection is a K'-spectral set for some K'.
2. [Sta86a] The intersection of a simply connected spectral set X of $A \in \mathcal{L}(H)$ whose interior has finitely many components with the closure a simply connected open set G containing the spectrum of A is a K'-spectral set for A for some K'. Weaker versions of this statement concerning the connectivity of X and/or G have been given in [Sta86b, Lew90].
3. [Lew90] The intersection of a (complete) K-spectral set for a bounded linear operator A with the closure of any open set containing the spectrum of A is a (complete) K'-spectral set for A for some K'.
4. [BBC09] Let $A \in \mathcal{L}(H)$, and consider the intersection $X = D_1 \cap D_2 \cap \cdots \cap D_n$ of n disks of the Riemann sphere $\overline{\mathbb{C}}$, each of them being spectral for A. Then X is a complete K-spectral set for A, with a constant $K \leq n + n(n-1)/\sqrt{3}$.
   (a) [Cro07] If in this result we add the requirement that the disks D_j and thus X are convex, then X is a complete 11.08-spectral set for A.
   (b) For $n = 2$ we obtain the constant $K = 2 + 2/\sqrt{3}$ for various configurations as shown in Figure 37.1, in particular for a strip/sector obtained by the intersection of two half-planes and discussed in Example 37.7.3a, or the lens-shaped intersection of two disks [BC06].
5. [Shi74] For $R > 1$, consider the annulus $X = X(R) = \{z \in \mathbb{C} : R^{-1} \leq |z| \leq R\}$, and denote by $K(R)$ (and by $K_{cb}(R) \geq K(R)$, respectively), the smallest constant K such that X is a K-spectral set (and a complete K-spectral set, respectively) for any invertible $A \in \mathcal{L}(H)$ verifying $\|A\| \leq R$ and $\|A^{-1}\| \leq R$. Then
   (a) [Shi74] $K(R) \leq 2 + \sqrt{\frac{R^2+1}{R^2-1}}$;
   (b) [BBC09] $K_{cb}(R) \leq 2 + \frac{R+1}{\sqrt{R^2+R+1}} \leq 2 + \frac{2}{\sqrt{3}}$. The first upper bound is sharper than Fact 37.6.5a for $R \leq 3.1528$;

(c) [BBC09] $K(R) \geq \frac{4}{3}$.

(d) [BBC09] $K_{cb}(R) \leq \max\{3, 2 + \sum_{n=1}^{\infty} \frac{4}{R^{2n}+1}\}$, being sharper than Fact 37.6.5a for $R \geq 1.8544$, and sharper than Fact 37.6.5b whenever $R \geq 1.9879$. It follows in particular that $K(R) \leq 3$ for $R \geq 2.0953$.

(e) [Cro12a] $K_{cb}(R) \leq 2 + \frac{1}{\pi} \int_0^{\pi} \left| \frac{R^2 + \exp(i\theta)}{R^2 - \exp(i\theta)} \right| d\theta$, being always sharper than Fact 37.6.5a, sharper than Fact 37.6.5b for $R \geq 1.6405$, and sharper than Fact 37.6.5d whenever $R \leq 2.0462$.

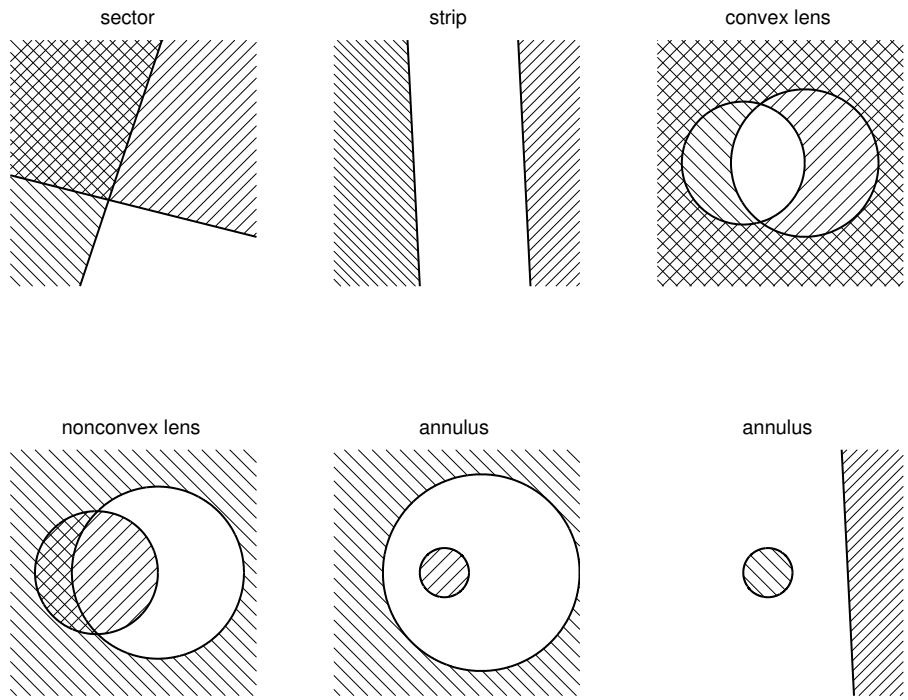

FIGURE 37.1 Six different configurations (in white) of intersections of two disks of the Riemann sphere.

Examples:

Consider the matrix

$$A = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix} \in \mathbb{C}^{2\times 2}, \quad \gamma = R - \frac{1}{R}, \quad R > 1,$$

with $\|A\| = \|A^{-1}\| = R$ such that both sets $\{|z| \leq R\}$ and $\{|z| \geq 1/R\}$ are spectral for A, and consider the intersection $X(R) = \{z \in \mathbb{C} : R^{-1} \leq |z| \leq R\}$.

1. [Mis84] The example of the function $f(z) = z - 1/z$, which verifies $\|f(A)\|/\|f\|_{X(R)} = 2\frac{R^2-1}{R^2+1}$, shows that $X(R)$ is not a spectral set for $R > \sqrt{3}$.
2. We get a sharper statement for the function $f(z) = g(z) - g(1/z)$, $g(z) = R\frac{z-1}{R^2-z}$, leading to

$$\|f(A)\| = 2, \quad \|f\|_{X(R)} = \frac{1 + R^2 + 2R}{1 + R^2 + R} < \frac{4}{3}.$$

Thus, $X(R)$ is even not $\frac{3}{2}$-spectral for A for any $R > 1$. Compared with Fact 37.6.5c we thus have shown the improved lower bound $K(R) \geq 2\frac{1+R^2+R}{1+R^2+2R} > \frac{3}{2}$.

3. Let the boundary of the compact $X \subset \mathbb{C}$ consist of $n+1$ disjoint analytic Jordan curves. Then X is K-spectral for the above matrix A if and only if [Mis84]

$$K \geq \gamma\,\Gamma(X), \quad \Gamma(X) = \sup\Big\{ \frac{|f'(1)|}{\|f\|_X} : f \text{ analytic on the interior of } X,\ f(1) = 0 \Big\}.$$

For the annulus $X(R) = \{z \in \mathbb{C} : R^{-1} \leq |z| \leq R\}$ of the preceding example, the quantity $\Gamma(X(R))$ is computable [BBC09], leading to the lower bound of Fact 37.6.5c. Moreover, given $r \in (1, R)$, using the Schwarz lemma we also conclude that both sets $\{z : |z| \leq r\}$ and $\{z : |z| \geq 1/r\}$ are K-spectral for A with $K = (R - R^{-1})/(r - r^{-1})$ but not their intersection $X(r)$, at least for those r not too far from R.

37.7 The Numerical Range as a K-Spectral Set

Recall that the numerical range is given by $W(A) := \{\langle Ax, x\rangle : \|x\| = 1\}$. It has been conjectured [FW72] that the closure of the numerical range is a complete K-spectral set for A. This was proved in [DD99]. Here we report about recent results along these lines, including the existence of a universal such constant K shown by Crouzeix [Cro07]. For applications in numerical linear algebra of results of this type, see for instance the discussions in [Eie93, Gre97, TT99].

Facts:

1. Estimates depending on the shape of X: For every bounded linear operator $A \in \mathcal{L}(H)$, every compact convex set X containing the numerical range is a complete K-spectral set for A, where
   (a) [DD99] $K = 3 + (2\pi\,\text{diameter}(X)^2/\,\text{area}(X))^3$.
   (b) [PS05] $K = 1+2/(1-q(X))$, with $q(X) \in [0,1]$ being C. Neumann's configuration constant of X (the oscillation norm of the underlying Neumann-Poincaré singular integral operator [Kra80]). We have $q(X) = 1$ if and only if X is a triangle or a quadrilateral.
   (c) [BCD06, Theorem 2.3] $K = 2 + \pi + TV(\log(r))$, if the boundary of X is parametrized by $[0, 2\pi] \ni t \mapsto \omega + r(t)e^{it}$, $r(t) \geq 0$.
2. Universal estimates:
   (a) [Cro07, Theorem 1] There exists a universal constant $K = K_{Crouzeix} \in [2, 11.08]$ such that for every bounded linear operator $A \in \mathcal{L}(H)$, the closure of the numerical range $\overline{W(A)}$ is a complete K-spectral set for A.
   (b) [Cro04a, Theorem 1.1] $W(A)$ is completely 2-spectral for every 2×2 matrix A.
3. Mapping theorems for the numerical range: let $A \in \mathcal{L}(H)$, and let f be analytic on $\mathbb{D}$, and continuous up to $\partial\mathbb{D}$.
   (a) [BS67] $w(A) \leq 1$ if and only if for all $z \in \mathbb{C}$

$$\|A - zI\| \leq 1 + \sqrt{1 + |z|^2} = \left\| \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} - zI \right\|.$$

   (b) [BS67] If $w(A) \leq 1$, $\|f\|_{\mathbb{D}} \leq 1$, and $f(0) = 0$ then $w(f(A)) \leq 1$.

(c) [Dru08] If $w(A) \leq 1$, $\|f\|_{\mathbb{D}} \leq 1$, and $|f(0)| < 1$, then $W(A)$ is a subset of the convex hull of the union of the disks $\overline{\mathbb{D}}$ and $\{z \in \mathbb{C} : |z - f(0)| \leq 1 - |f(0)|^2\}$. Furthermore, $\|f(A)\| \leq \nu(|f(0)|)$, where

$$\nu(\alpha) = \left(2 - 3\alpha^2 + 2\alpha^4 + 2(1-\alpha^2)(1-\alpha^2+\alpha^4)^{1/2}\right)^{1/2}.$$

(d) [Dru08] If $w(A) \leq 1$, then $w(f(A)) \leq \frac{5}{4}\|f\|_{\overline{\mathbb{D}}}$, and $\frac{5}{4}$ is the best possible constant.

(e) [Kat65] If r is a rational function with $r(\infty) = \infty$, and if $X = \{z \in \mathbb{C} : |r(z)| \leq 1\}$ is a convex set containing $W(A)$, then $w(r(A)) \leq 1$.

Open Problems:

1. [Cro07] Is $K_{Crouzeix} = 2$? At least if we restrict ourselves to 3×3 matrices?

Examples:

1. [Cla84] The spectrum of the Toeplitz operator T_ϕ acting on the Hardy space H^2 with symbol $\phi(w) = aw + bw^{-1}$, $0 < b < a$, is a convex set whose boundary is an ellipse with semi-axes $a \pm b$. The spectrum coincides with the closure of the numerical range $W(T_\phi)$. This set is not spectral but K-spectral for T_ϕ with $K = \sqrt{1 + |b/a|^2}$. Other classes of symbols with similar properties are given in [Cla84].
2. [PS05] The configuration constant of Fact 37.7.1b can be estimated for (smooth) X: $q(X) \leq 1 - \frac{1+e}{2}\sqrt{1-e^2}$ for ∂X an ellipse with eccentricity $e < 1$ and $q(X) \leq 1 - \frac{\text{length}(\partial X)}{2\pi R}$, with R the maximum radius of curvature.
3. K-spectral sets containing the numerical range: let $A \in \mathcal{L}(H)$, and let $X \subset \mathbb{C}$ be closed and convex containing $W(A)$.
   (a) [CD03, BCD06, BC07] If X is a convex sector or a strip, then X is $(2 + \frac{2}{\sqrt{3}})$-spectral for A.
   (b) [Cro04b, BC07] If the boundary of X is a parabola or a hyperbola, then X is $(2 + \frac{2}{\sqrt{3}})$-spectral for A.
   (c) [BC07, Theorem 1] If the boundary of X is an ellipse with eccentricity $e \leq 1$, then X is $(2 + \frac{2}{\sqrt{4-e^2}})$-spectral for A.
   (d) For an equilateral triangle, we have $K = 2+\pi+6\log(2)$ according to Fact 37.7.1c, and for a square $K = 2 + \pi + 4\log(2)$.
4. [Cro12b] For the 3×3 matrix

$$A = \begin{bmatrix} 0 & 2 & 0 \\ \epsilon & 0 & (1-\epsilon^2)/\sqrt{2} \\ 0 & 0 & (1-\epsilon^2)/\sqrt{2} \end{bmatrix}$$

   and sufficiently small $\epsilon > 0$, the numerical range $W(A)$ is 2-spectral for A but not completely 2-spectral for A.
5. [GC12] Crouzeix's conjecture is known to hold for generalized Jordan blocks where one replaces in a Jordan block of arbitrary size the lower left entry 0 by an arbitrary scalar.
6. For $f(z) = z$ we recover from Fact 37.7.2 the well-known link between numerical radius and Euclidean norm, namely $[1, 2] \ni \|A\|/w(A) = \|f(A)\|/\sup_{z \in W(A)} |f(z)| \leq K_{Crouzeix}$.

7. Consider $A = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \in \mathbb{C}^{2\times 2}$, $f(A) = \begin{bmatrix} f(0) & 2f'(0) \\ 0 & f(0) \end{bmatrix}$. Here $W(A)$ is the closed unit disk and, for $f(z) = z$,

$$\|f(A)\| \Big/ \sup_{z\in W(A)} |f(z)| = 2 \le K_{Crouzeix}.$$

8. [Cro04a, Sect. 2] Consider $A = \begin{bmatrix} 1 & \rho - \frac{1}{\rho} \\ 0 & -1 \end{bmatrix} \in \mathbb{C}^{2\times 2}$ with $\rho > 1$. According to Fact 25.1.7, $W(A)$ is compact, with its boundary given by an ellipse with foci ± 1 and minor axis $\rho - 1/\rho$. The matrix can be diagonalized as

$$A = LBL^{-1}, \quad B = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad L = \begin{bmatrix} 1 & -\frac{\rho-1/\rho}{\rho+1/\rho} \\ 0 & \frac{2}{\rho+1/\rho} \end{bmatrix}, \quad \|L\|\,\|L^{-1}\| = \|A\| = \rho.$$

Thus

$$\frac{\|f(A)\|}{\sup\limits_{z\in W(A)} |f(z)|} \le \rho \frac{\|f(B)\|}{\sup\limits_{z\in W(A)} |f(z)|} = \rho \frac{\max\{|f(-1)|, |f(1)|\}}{\sup\limits_{z\in W(A)} |f(z)|}.$$

By [Cro04a, Theorem 2.1] and some elementary calculus, the right-hand side of this expression is maximized for the function f_0 mapping conformally $W(A)$ on the closed unit disk, with $f_0(0) = 0$, $f_0'(0) > 0$. Thus, $W(A)$ is a K-spectral set for A with optimal constant $K = \rho\, f_0(1) = \|f_0(A)\| \in (1, 2)$, the last two relations following from the fact that an explicit formula for f_0 is known [Cro04a, Eq. (2.2)].

37.8 Applications to the Approximate Computation of Matrix Functions

Facts:

Notation: $A \in \mathbb{C}^{n\times n}$, $\mathbb{E} \subset \mathbb{C}$ compact convex, being $K(\mathbb{E})$–spectral for A, f a function being analytic on $\mathbb{E}$.

1. Polynomial approximation through Taylor sums.
A popular method [Hig08, Sect. 4.3] for approximately computing (entire) functions of matrices is to approach the Taylor series $f(z) = \sum_{j=0}^{\infty} c_j z^j$ by its mth partial sum $S_m(z) = \sum_{j=0}^{m} c_j z^j$, with the error estimate [Mat93, Cor. 2]

$$\|(f - S_m)(A)\| \le \frac{1}{(m+1)!} \max_{0\le t\le 1} \|A^{m+1} f^{(m+1)}(tA)\|.$$

Here the right-hand side can by bounded in terms of $\mathbb{E}$ by the techniques of the preceding subsections, see, e.g., Example 37.2.8 or Fact 37.7.2.

2. Polynomial approximation through Faber sums.
Instead of Taylor sums, following [Hig08, Sect. 4.4.1] and Section 17.7 one may also consider best polynomial approximants p_m of f on $\mathbb{E}$, leading to the error estimate

$$\|(f - p_m)(A)\| \le K(\mathbb{E})\, \rho_m(f, \mathbb{E}), \quad \rho_m(f, \mathbb{E}) = \min_{\deg p \le m} \max_{z\in\mathbb{E}} |f(z) - p(z)|.$$

According to [KP67, Theorem 4], this rate $\rho_m(f, \mathbb{E})$ is achieved up to some factor $\alpha \log(m) + \beta$ with explicit $\alpha, \beta > 0$ not depending on f nor on $\mathbb{E}$ by taking as p_m the

mth partial Faber series, which is defined as follows: let $\phi = \psi^{-1}$ map conformally the exterior of $\mathbb{E}$ onto the exterior of the closed unit disk $\mathbb{D}$, then the mth Faber polynomial F_m is defined as the polynomial part of the Laurent expansion of ϕ^m at ∞, and f has the Faber series

$$\sum_{j=0}^{\infty} f_j F_j(z), \quad f_m = \frac{1}{2\pi i}\int_{|w|=1} \frac{f(\psi(w))}{w^{m+1}} dw,$$

absolutely converging to f uniformly in $\mathbb{E}$ [KP67, Theorem 5]. Notice that for $\mathbb{E}$ a disk centered at 0 we recover Taylor series, and for $\mathbb{E} = [-1, 1]$ Chebyshev orthogonal series [Tre12]. By [BR09, Sect. 3] one has the a posteriori bound $|f_{m+1}| \le \rho_m(f, \mathbb{E}) \le 2(|f_{m+1}|+|f_{m+2}|+\ldots)$. Estimates for the Faber coefficients of the exponential function can be found in [BR09, Sect. 4].
The Faber operator [Gai87]

$$\mathcal{F}(F)(z) = \sum_{j=0}^{\infty} f_j F_j(z), \quad F(w) = \frac{f_0}{2} + \sum_{j=1} f_j w^j$$

for functions F analytic on $\mathbb{D}$ maps polynomials of degree m to polynomials of degree m, in particular $\mathcal{F}(w^m)(z) = F_m(z)$ for $m \ge 1$. According to [Bec05], [BR09, Theorem 2.1]

$$\|\mathcal{F}(F)(A)\| \le 2 \max_{w\in\mathbb{D}} |F(w)|,$$

allowing to relate best polynomial approximation of f on $\mathbb{E}$ to $\rho_m(\mathcal{F}^{-1}(f), \mathbb{D})$, and to derive error estimates for matrix functions which do not involve $K(\mathbb{E})$, e.g., for the mth partial Faber sum p_m [BR09, Theorem 3.2]

$$\|(f - p_m)(A)\| \le 2 \sum_{j=m+1}^{\infty} |f_j|.$$

3. Polynomial Arnoldi method.

   The Arnoldi process is a popular method for approaching $f(A)b$ for some fixed vector $b \ne 0$ and large sparse A [Hig08, Sect. 13.2]. The mth approximant is given by the projection formula $V_m f(V_m^* A V_m) V_m^* b$, where $V_m \in \mathbb{C}^{n\times m}$ with columns spanning an orthonormal basis of the Krylov subspace $\mathrm{Span}\{b, Ab, \ldots, A^{m-1}b\}$. Typically, $m \ll n$, and hence $f(V_m^* A V_m)$ can be computed by some direct method. According to [Hig08, Lemma 13.4], this method is exact for f a polynomial of degree $\le m-1$, and hence

$$\epsilon_m := \frac{\|f(A)b - V_m f(V_m^* A V_m) V_m^* b\|}{\|b\|} \le \|(f-p)(A)\| + \|(f-p)(V_m^* A V_m)\|$$

   for any polynomial p of degree $\le m-1$. Supposing that $W(A) \subset \mathbb{E}$ (and thus $W(V_m^* A V_m) \subset \mathbb{E}$), we obtain by means of the techniques of Fact 37.8.2 that $\epsilon_m \le 2\, K_{Crouzeix}\, \rho_{m-1}(f, \mathbb{E})$ or $\epsilon_m \le 4\, \rho_{m-1}(\mathcal{F}^{-1}(f), \mathbb{D}) \le 4 \sum_{j=m}^{\infty} |f_j|$, see [BR09, Proposition 3.1 and Theorem 3.2].

4. Rational approximants with free poles via (Faber-)Padé approximants.

   Another popular approach (see [Hig08, Sect. 4.4.2] and Section 17.7) for approaching matrix functions for functions f with singularities is to replace f by the rational function p/q with p, q polynomials of degree at most k, and m, respectively, $k \ge m-1$, such that the first $k+m+1$ terms in the Taylor expansion of $f - p/q$ at zero vanish. Here one hopes that the poles of this $[k|m]$ Padé approximant p/q do mimic the

singularities of f. Though this approach is also applied for entire functions like the exponential function [Hig08, Sect. 10.7.4], the error is best understood for Markov functions

$$f(z) = c + \int_\alpha^\beta \frac{d\mu(x)}{z-x}, \quad c \in \mathbb{R}, \quad \mu \text{ some positive measure},$$

where we suppose that $\beta < -w(A)$. This includes (up to some variable transformations) functions like $\log(z)$, $1/\sqrt{z}$ or more generally pth roots, $\mathrm{sign}(z)$, $\tanh(z)$, and others [BGM81, BR09]. By [ST92, Lemma 6.2.1], the denominator q has all its roots in $[\alpha, \beta]$, and the error may be represented as

$$f(z) - \frac{p}{q}(z) = \frac{z^{m+n+1}}{q(z)^2} \int_\alpha^\beta \frac{q(x)^2}{x^{m+n+1}} \frac{d\mu(x)}{z-x}.$$

Then the error on the disk $\{z \in \mathbb{C} : |z| \leq w(A)\}$ is minimal for $z = -w(A)$, and, using Example 37.2.8,

$$\|(f - \frac{p}{q})(A)\| \leq 2\,|(f - \frac{p}{q})(-w(A))|.$$

In general, sharper error bounds are obtained for $k \geq m$ by combining the above techniques with those of Fact 37.8.2, where we suppose in addition that $\mathbb{E}$ is symmetric with respect to the real axis. We first notice that, with f, also $\mathcal{F}^{-1}(f)$ is a Markov function [BR09, Theorem 6.1(a)]. Denoting by P/Q the $[k|m]$ Padé approximant of $\mathcal{F}^{-1}(f)$, the function $\mathcal{F}(P/Q)$ is rational with numerator degree $\leq k$ and denominator degree $\leq m$, called the $[k|m]$ Faber-Padé approximant [Ell83]. For $\mathbb{E} = [-1, 1]$ one recovers the so–called non-linear Chebyshev-Padé approximant [Sue09]. As above, we may bound for Markov functions the error through

$$\|\Big(f - \mathcal{F}(\frac{P}{Q})\Big)(A)\| \leq 2\,|\Big(\mathcal{F}^{-1}(f) - \frac{P}{Q}\Big)(-1)|.$$

5. Rational approximation with prescribed poles and rational Arnoldi.

   There exists a variant of the polynomial Arnoldi method Fact 37.8.3 where the columns of $Q_m \in \mathbb{C}^{n\times m}$ give an orthonormal basis of the rational Krylov subspace

$$q(A)^{-1}\mathrm{Span}\{b, Ab, \ldots, A^{m-1}b\}$$

   for some fixed polynomial $q(z) = \prod_j (z - z_j)$ of degree $\leq m-1$ (and hence for $q = 1$ we recover the polynomial Arnoldi method). The computation of V_m and $V_m^* A V_m$ by some rational variant of the Arnoldi process [BR09] requires $(A - z_j I)^{-1} a$ for some vectors a, and this task of solving shifted linear systems is particularly trackable if q has a small number of multiple poles. As before we obtain

$$\widetilde{\epsilon}_m := \frac{\|f(A)b - V_m f(V_m^* A V_m) V_m^* b\|}{\|b\|} \leq \|(f - \frac{p}{q})(A)\| + \|(f - \frac{p}{q})(V_m^* A V_m)\|$$

   for any polynomial p of degree $\leq m-1$ [BR09, Theorem 5.2]. Let $W(A) \subset \mathbb{E}$, and suppose that $\mathbb{E}$ is symmetric with respect to the real axis, and $z_j \notin \mathbb{E}$. For estimating the error we are left with the task of approaching f on $\mathbb{E}$ by a rational function with fixed denominator p/q. Notice that $p/q = \mathcal{F}(P/Q)$ with P a polynomial of degree at most $\leq m-1$, and $Q(w) = \prod_j (w - \phi(z_j))$ [Ell83]. Hence, $\widetilde{\epsilon}_m \leq 4\,\rho_{m-1}^Q(\mathcal{F}^{-1}(f), \mathbb{D})$, where

$$\rho_{m-1}^q(f, \mathbb{E}) = \min_{\deg p \leq m-1} \max_{z\in\mathbb{E}} |f(z) - \frac{p}{q}(z)|,$$

see [BR09, Theorem 5.2]. For Markov functions f as in Fact 37.8.4, lower and upper bounds for $\rho^Q_{m-1}(\mathcal{F}^{-1}(f),\mathbb{D})$ are given in [BR09, Theorem 6.2], in particular the simple explicit bound

$$\rho^Q_{m-1}(\mathcal{F}^{-1}(f),\mathbb{D}) \le \frac{1}{|\phi(\beta)|}\ \max_{z\in\mathbb{E}}|f(z)-f(\infty)|\ \max_{w\in[\phi(\alpha),\phi(\beta)]}\Big|\prod_j \frac{w-\phi(z_j)}{1-w\overline{\phi(z_j)}}\Big|.$$

Poles z_j minimizing the right-hand side should therefore be in $[\alpha,\beta]$, the set of singularities of f, and various configurations of poles minimizing the right-hand side have been considered in [BR09, Sect. 6].

6. Error bounds for GMRES and FOM for solving systems of linear equations.

   Both GMRES and FOM are iterative Krylov subspace methods for solving systems $Ax=b$ with A large and sparse (see Chapter 54). Here we may apply the techniques of the preceding sections for the Markov function $f(z)=1/z$ provided that $0\notin\mathbb{E}$, $\mathbb{E}$ containing $W(A)$. The residual of the mth iterate x_m^{GMRES} of GMRES with starting residual $r=b-Ax_0^{GMRES}$ satisfy [Bec05]

$$\frac{\|b-Ax_m^{GMRES}\|}{\|r\|} = \min_{\deg p\le m}\frac{\|p(A)r\|}{|p(0)|\,\|r\|} \le \min\{1,\frac{2}{|F_m(0)|}\} \le \frac{2+1/|\phi(0)|}{|\phi(0)|^m}$$

   with F_m the mth Faber polynomial of $\mathbb{E}$, and ϕ mapping conformally the exterior of $\mathbb{E}$ onto the exterior of the unit disk. The asymptotic convergence factor $1/|\phi(0)|<1$ can be computed for various shapes of $\mathbb{E}$. For instance [Bec05, BGT06], for positive definite $A+A^*$ considering the lens $\mathbb{E}=\{z\in\mathbb{C}:\mathrm{re}(z)\ge\mathrm{dist}(0,W(A)),|z|\le w(A)\}$ we get $1/|\phi(0)| = 2\sin(\beta/(4-2\beta/\pi)) < \sin(\beta)$, with the angle $\beta\in(0,\pi/2)$ being defined by $\cos(\beta)=\frac{\mathrm{dist}(0,W(A))}{w(A)}$.

   The mth iterate of FOM (with starting vector x_0^{FOM} is a special case of the polynomial Arnoldi method Fact 37.8.3, namely $x_m^{FOM}=V_m(V_m^*AV_m)^{-1}V_m^*b$ or $f(z)=1/z$, and thus

$$\frac{\|x_m^{FOM}-A^{-1}b\|}{\|b\|} \le 4\eta_{m-1}(\mathcal{F}^{-1}(f),\mathbb{D}) \le \frac{4|\phi(0)|^{-m}}{\mathrm{dist}(0,\mathbb{E})}.$$

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