K-Spectral Sets and the Convergence Rate of GMRES

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Let $A$ be an $n$ by $n$ matrix or a bounded linear operator on a Hilbert space. If $f$ is holomorphic in a region $\Omega \subset \mathbb{C}$ containing the spectrum of $A$, then

$$f(A) = \frac{1}{2\pi i} \int_{\partial \Omega} (zI - A)^{-1} f(z) \, dz.$$
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$$f(A) = \frac{1}{2\pi i} \int_{\partial \Omega} (zI - A)^{-1} f(z) \, dz.$$ 

Can $\|f(A)\| \equiv \sup_{\|w\|_2 = 1} \|f(A)w\|_2$ be related to $\|f\|_\Omega \equiv \sup_{z \in \Omega} |f(z)|$?
Applications

$\|e^{tA}\|$ determines stability of $y'(t) = Ay(t)$, $t > 0$. 
$\lim_{t \to \infty} \|e^{tA}\| = 0$ iff the spectrum $\sigma(A)$ lies in the open left half-plane. But $\sigma(A)$ does not necessarily determine finite time behavior of $\|e^{tA}\|$. 

$\|e^{\Delta t A}j\|$ determines stability of Euler's method for approximating the solution. 
$\lim_{j \to \infty} \|e^{\Delta t A}j\| = 0$ iff $\sigma(I + \Delta t A)$ lies in the open unit disk. But $\sigma(I + \Delta t A)$ does not necessarily determine $\|e^{\Delta t A}j\|$ for finite $j$. 

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Applications

- \( \| e^{tA} \| \) determines stability of \( y'(t) = Ay(t), \ t > 0 \).
  \( \lim_{t \to \infty} \| e^{tA} \| = 0 \) iff the spectrum \( \sigma(A) \) lies in the open left half-plane. But \( \sigma(A) \) does not necessarily determine finite time behavior of \( \| e^{tA} \| \).

- \( \| (I + \Delta t A)^j \| \) determines stability of Euler’s method for approximating the solution.
  \( \lim_{j \to \infty} \| (I + \Delta t A)^j \| = 0 \) iff \( \sigma(I + \Delta t A) \) lies in the open unit disk. But \( \sigma(I + \Delta t A) \) does not necessarily determine \( \| (I + \Delta t A)^j \| \) for finite \( j \).
Applications

- \| (I - M^{-1}A)^j \| measures error at step \( j \) of a simple iteration method for solving \( Ax = b \) with preconditioner \( M \). The error goes to 0 as \( j \to \infty \) iff the spectral radius \( \rho(I - M^{-1}A) < 1 \), but \( \sigma(I - M^{-1}A) \) does not necessarily determine the rate of convergence.
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- The **GMRES** algorithm for solving \(Ax = b\) constructs an approximate solution \(x^{(j)}\) at step \(j\) for which the residual \(r^{(j)} = b - Ax^{(j)}\) satisfies

  \[
  \|r^{(j)}\|_2 = \min_{c_1, \ldots, c_j} \left\| \left( I - \sum_{\ell=1}^{j} c_\ell A^\ell \right) r^{(0)} \right\|.
  \]

  G., Ptak, Strakoš (1996): Any nonincreasing sequence of residual norms can be obtained with a matrix having any given eigenvalues.
If $A$ is diagonalizable, $A = V \Lambda V^{-1}$, then

$$\|f\|_{\sigma(A)} \leq \|f(A)\| \leq \|V\| \cdot \|V^{-1}\| \cdot \|f\|_{\sigma(A)}.$$
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If $\kappa(V) \equiv \|V\| \cdot \|V^{-1}\|$ is of moderate size, then $\|f(A)\|$ is well-approximated by $\|f\|_{\sigma(A)}$. **What if $\kappa(V)$ is huge?**
$\Omega \subset \mathbb{C}$ is a $K$-spectral set for $A$ if $\|f(A)\| \leq K \sup_{z \in \Omega} |f(z)|$ for all rational functions $f$ with no poles in $\Omega$. 

Von Neumann's inequality (1951): If $A$ is a contraction, i.e., $\|A\| \leq 1$, then the unit disk $D$ is a 1-spectral set for $A$; that is, $\|f(A)\| \leq \sup_{z \in D} |f(z)| \equiv \|f\|_D$.

Okubo and Ando (1975): If the field of values, or, numerical range $W(A) = \{\langle Aq, q \rangle : q \in \mathbb{C}^n, \|q\|_2 = 1\}$ is a subset of $D$; i.e., if the numerical radius $w(A) = \sup_{z \in W(A)} |z|$ is less than or equal to 1, then $D$ is a 2-spectral set for $A$. In fact, $A$ is 2-similar to a contraction; that is, $A = XCX^{-1}$ where $\|C\| \leq 1$ and $\kappa(X) \equiv \|X\| \cdot \|X^{-1}\| \leq 2$. 

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\( \Omega \subset \mathbb{C} \) is a \( K \)-spectral set for \( A \) if \( \| f(A) \| \leq K \sup_{z \in \Omega} |f(z)| \) for all rational functions \( f \) with no poles in \( \Omega \).

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$K$-Spectral Sets

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*Constant 2 can be attained:*

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

$W(A)$ is disk of radius $1/2$ about $0$.  

$\|A\| = 1 = 2 \max_{z \in W(A)} |z|$.  

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More $K$-Spectral Sets

- $\epsilon$-Pseudospectrum (Trefethen and Embree, 2005):

$$\Lambda_{\epsilon}(A) = \{z \in \mathbb{C} : \|(zl - A)^{-1}\| > \epsilon^{-1}\}$$

is a $|\partial\Lambda_{\epsilon}|/(2\pi\epsilon)$-spectral set for $A$, where $|\partial\Lambda_{\epsilon}|$ is the length of the boundary of $\Lambda_{\epsilon}$. 
More $K$-Spectral Sets

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- Note: If $A = \varphi(B)$ and $\Omega$ is a $K$-spectral set for $B$, then $\varphi(\Omega)$ is a $K$-spectral set for $A$, since

$$\|f(A)\| = \|f(\varphi(B))\| \leq K\|f \circ \varphi\|_\Omega = K\|f\|_{\varphi(\Omega)}.$$  

Enables one to derive many other $K$-spectral sets.
(Eisenstat, Elman, Schultz, 1983). If $0 \notin W(A)$, then

$$\|r^{(j)}\|/\|r^{(0)}\| \leq (1 - d^2/\|A\|^2)^{j/2},$$

where $d$ is the distance from 0 to $W(A)$. 
Convergence of GMRES

- (Eisenstat, Elman, Schultz, 1983). If $0 \not\in \mathcal{W}(A)$, then
  $$\frac{\|r^{(j)}\|}{\|r^{(0)}\|} \leq (1 - \frac{d^2}{\|A\|^2})^{j/2},$$

  where $d$ is the distance from $0$ to $\mathcal{W}(A)$.

- Improvements by Beckermann, Goreinov, Tyrtshnikov, 2005; Beckermann, 2005.
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where $d$ is the distance from 0 to $W(A)$.

- Improvements by Beckermann, Goreinov, Tyrtyshnikov, 2005; Beckermann, 2005.

- Using Crouzeix's conjecture/theorem,

\[ \|r(j)\|/\|r(0)\| \leq 2(\text{or } 11.08) \min_{p \in P_j, p(0)=1} \|p\|_{W(A)}. \]
(Eisenstat, Elman, Schultz, 1983). If $0 \notin W(A)$, then
\[ \| r^{(j)} \| / \| r^{(0)} \| \leq (1 - d^2 / \| A \|^2)^{j/2}, \]
where $d$ is the distance from 0 to $W(A)$.

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- Using Crouzeix’s conjecture/theorem,
\[ \| r^{(j)} \| / \| r^{(0)} \| \leq 2 \text{ (or 11.08)} \min_{p \in P_j} \| p \|_{W(A)} \cdot \min_{p(0)=1} \| p \|_{W(A)}. \]

But none of these help if $0 \in W(A)$. 
If $A$ is nonsingular, then $B = A^{1/m}$ is well-defined and $A = \varphi(B)$, where $\varphi(z) = z^m$. Since $B \to I$ as $m \to \infty$, for large $m$, $W(B)$ will be a small region about 1 that does not contain the origin. When raised to the $m$th power, the points in $\varphi(W(B))$ may wrap around the origin but they will not contain the origin.
Region inside red curve looks a lot like the 0.4-pseudospectrum. If conjecture is true, get a smaller constant \( |\partial \Lambda \epsilon| / (2 \pi \epsilon) \approx 6.\)
Region inside red curve looks a lot like the 0.4-pseudospectrum. If conjecture is true, get a smaller constant(2) than $\frac{|\partial \Lambda_\epsilon|}{(2\pi \epsilon)} \approx 6$. 
If $A$ has the following sparsity pattern

$$
\begin{pmatrix}
0 & * & 0 & \ldots & 0 \\
0 & * & * & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & * & * & \ldots & * \\
* & * & * & \ldots & * 
\end{pmatrix},
$$

and $r^{(0)}$ is a multiple of the first unit vector, then GMRES makes no progress until step $n$. 

If $\Omega$ is a $K$-spectral set for $A$, then there is no polynomial $p$ of degree $< n$ with $p(0) = 1$ such that $\|p\|_\Omega < 1/K$. 

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GMRES Provides Information about $K$-Spectral Sets

If $A$ has the following sparsity pattern

$$
\begin{pmatrix}
0 & * & 0 & \ldots & 0 \\
0 & * & * & \ldots & 0 \\
0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ldots & \vdots \\
0 & * & * & \ldots & * \\
* & * & * & \ldots & * \\
\end{pmatrix},
$$

and $r^{(0)}$ is a multiple of the first unit vector, then GMRES makes no progress until step $n$.

$\implies$ If $\Omega$ is a $K$-spectral set for $A$, then there is no polynomial $p$ of degree $< n$ with $p(0) = 1$ such that $\|p\|_\Omega < 1/K$. 
Companion Matrix With Eigenvalues Near 1

Eigenvalues and Field of Values of $A$

$$\begin{bmatrix} A^{(1/6)} \end{bmatrix}^6$$

Points Nearest 0

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Conjecture: For all polynomials $p$,

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

- Holds if $W(A)$ is a disk or if $W(A)$ is replaced by the smallest disk enclosing $W(A)$. (Badea, 2004; using Okubo and Ando, 1975)
Crouzeix’s Conjecture: Current Status

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- Holds if 2 is replaced by 11.08. (Crouzeix, 2007)
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- Holds for 2 by 2 matrices. (Crouzeix, 2004)
Holds for diagonally scaled perturbed Jordan blocks. (G. and Choi, 2012)

\[
\begin{pmatrix}
0 & \alpha_1 \\
0 & \ddots & \ddots \\
\alpha_n & & 0
\end{pmatrix}
\]
Holds for diagonally scaled perturbed Jordan blocks. (G. and Choi, 2012)

\[
\begin{pmatrix}
0 & \alpha_1 \\
0 & \alpha_2 & \ddots \\
& \ddots & \ddots & \ddots \\
& & \alpha_{n-2} & \alpha_{n-1} & 0 \\
& & & \alpha_n
\end{pmatrix}
\]

Holds for 3 by 3 nilpotent matrices. (Crouzeix, 2012)
Let $g$ be a bijective conformal mapping from $W(A)$ to $D$. Crouzeix's conjecture is equivalent to: $D$ is a 2-spectral set for $g(A)$. This is implied by: $g(A)$ is 2-similar to a contraction, since if $g(A) = XCX^{-1}$, where $\|C\| \leq 1$ and $\kappa(X) \leq 2$, then by von Neumann’s inequality

\[
\|p(A)\| = \|(p \circ g^{-1})(g(A))\| = \|X(p \circ g^{-1})(C)X^{-1}\| \\
\leq 2 \cdot \|p \circ g^{-1}\|_D = 2 \cdot \|p\|_W(A).
\]
Advantage of showing that $g(A)$ is 2-similar to a contraction:

- For a given matrix $A$, one can (probably) *prove* $\|p(A)\| \leq 2\|p\|_{W(A)} \ \forall p$ with a careful numerical computation. Compute $W(A)$ and $g : W(A) \to D$, and look for smallest norm matrix to which $g(A)$ is 2-similar (perhaps using constrained optimization code to minimize $\|X^{-1}g(A)X\|$ s.t. $\kappa(X) \leq 2$).
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- For a given matrix $A$, one can (probably) prove $\|p(A)\| \leq 2\|p\|_{W(A)} \forall p$ with a careful numerical computation. Compute $W(A)$ and $g : W(A) \to \mathcal{D}$, and look for smallest norm matrix to which $g(A)$ is 2-similar (perhaps using constrained optimization code to minimize $\|X^{-1}g(A)X\|$ s.t. $\kappa(X) \leq 2$).

- If computed $\|X^{-1}g(A)X\| < 1$, use sufficiently high precision to argue that rounding errors, errors in computing $W(A)$, $g$, etc., could not possibly result in computed $g(A)$ being 2-similar to a matrix of norm $\ldots$, when true $g(A)$ is not 2-similar to any matrix with norm $\leq 1$. 
Examples of $A$ and $g(A)$

Eigenvalues and Field of Values of $A$

Random 5x5 Matrix

$\text{normC} = 0.93842, \text{condX} = 2$

Eigenvalues and Field of Values of $g(A)$

Random 6x6 Upper Triangular Matrix

$\text{normC} = 0.95863, \text{condX} = 2$
What about Lower Bounds?

Can one find sets $\Omega \subset \mathbb{C}$ such that $\|p(A)\| \geq k \cdot \|p\|_{\Omega}$ for all polynomials $p$?
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**NO.** Not if \( \Omega \) contains more than \( \sigma(A) \) since the minimal polynomial \( \chi(z) \) satisfies \( \|\chi(A)\| = 0 \) but \( \chi(z) \) is 0 only at eigenvalues of \( A \).
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- Limit the class of polynomials to those of degree $j$ or less. The *polynomial numerical hull of degree $j$* is 
  $$
  \{z \in \mathbb{C} : \|p(A)\| \geq |p(z)| \ \forall p \in P_j\}.
  $$
  (Nevanlinna, 1993; G., 2002)
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  \[ \{ z \in \mathbb{C} : \|p(A)\| \geq |p(z)| \ \forall p \in \mathcal{P}_j \} \]. (Nevanlinna, 1993; G., 2002)

  - $\mathcal{W}(A) = \mathcal{H}_1(A) \supset \mathcal{H}_2(A) \supset \ldots \supset \mathcal{H}_{n-1}(A) \supset \mathcal{H}_n(A) = \sigma(A)$. 

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  $$\{z \in \mathbb{C} : \|p(A)\| \geq |p(z)| \ \forall p \in \mathcal{P}_j\}. \text{ (Nevanlinna, 1993; G., 2002)}$$
  - $W(A) = \mathcal{H}_1(A) \supset \mathcal{H}_2(A) \supset \ldots \supset \mathcal{H}_{n-1}(A) \supset \mathcal{H}_n(A) = \sigma(A)$.
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  - $W(A) = \mathcal{H}_1(A) \supset \mathcal{H}_2(A) \supset \ldots \supset \mathcal{H}_{n-1}(A) \supset \mathcal{H}_n(A) = \sigma(A)$.
  - GMRES makes some progress after $j$ steps iff $0 \notin \mathcal{H}_j(A)$.
  - If $A$ is $n$ by $n$ and has sparsity pattern discussed before, then $0 \in \mathcal{H}_{n-1}(A)$. 
What about Lower Bounds?

Instead of requiring \( \|p(A)\| \geq k \cdot \|p\|_\Omega \), require
\[ \|p(A)\| \geq k \cdot \|\varphi_p\|_\Omega, \]
where \( \|\varphi_p\|_\Omega \) is minimal among all functions \( \varphi \) satisfying \( \varphi(A) = p(A) \). For \( \Omega = D \), \( \varphi_p \) is a scalar multiple of a finite Blaschke product.
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If

\[
A = \begin{pmatrix}
1 & & \\
& \ddots & \\
& & 1 \\
\nu & & 1
\end{pmatrix}, \quad 0 \leq \nu \leq 1,
\]

then \( \|p(A)\| = \|\varphi_p\|_\mathcal{D} \). (G., 2009)
Still not clear what is the best way to describe the behavior of GMRES. Or to deal with other applied problems involving nonnormal matrices.
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Crouzeix’s conjecture (\( \| p(A) \| \leq 2 \| p \|_{W(A)} \)) is *fascinating*.

- Probably best to try to prove: If \( g \) is a bijective conformal mapping from \( W(A) \) to \( D \), then \( g(A) \) is 2-similar to a contraction.
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Probably best to try to prove: If $g$ is a bijective conformal mapping from $W(A)$ to $D$, then $g(A)$ is 2-similar to a contraction.

When is a matrix 2-similar to a contraction? What is the smallest norm matrix to which a given matrix is 2-similar? Numerical analysts should study canonical forms for similarity transformations with bounded condition numbers.