Crouzeix's Conjecture and the GMRES Algorithm

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Where in the complex plane does a matrix live?
(A question of L. N. Trefethen)

Translating Matrix Problems into Problems in the Complex Plane

What can eigenvalues do?

- If A is **normal** (e.g., real symmetric) or **near normal** (well-conditioned eigenvectors) then eigenvalues describe behavior in spectral norm perfectly or almost perfectly:

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

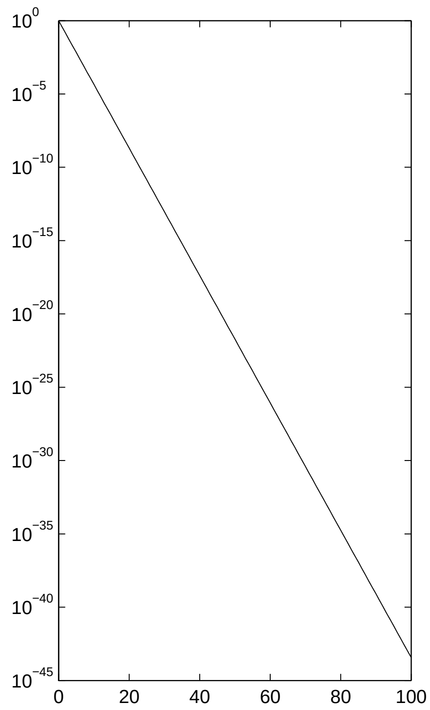
- Even if A is highly **nonnormal** (e.g., not diagonalizable, or diagonalizable but with eigenvectors that are almost linearly dependent), eigenvalues determine the *asymptotic* behavior of many functions of A:

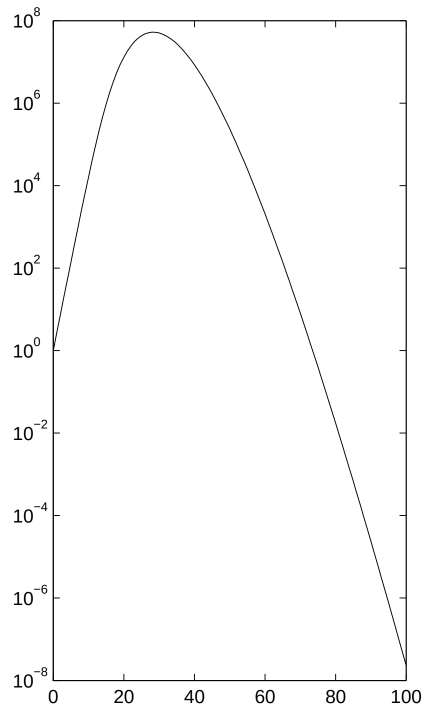
$$\|A^k\| \to 0 \;\text{ as } k \to \infty \;\text{ iff } \rho(A) < 1.$$
$$\|e^{tA}\| \to 0 \;\text{ as } t \to \infty \;\text{ iff } \mathrm{Re}(\sigma(A)) < 0.$$

What can eigenvalues NOT do?

- e^{tA}: Determines the stability of $y' = Ay$.

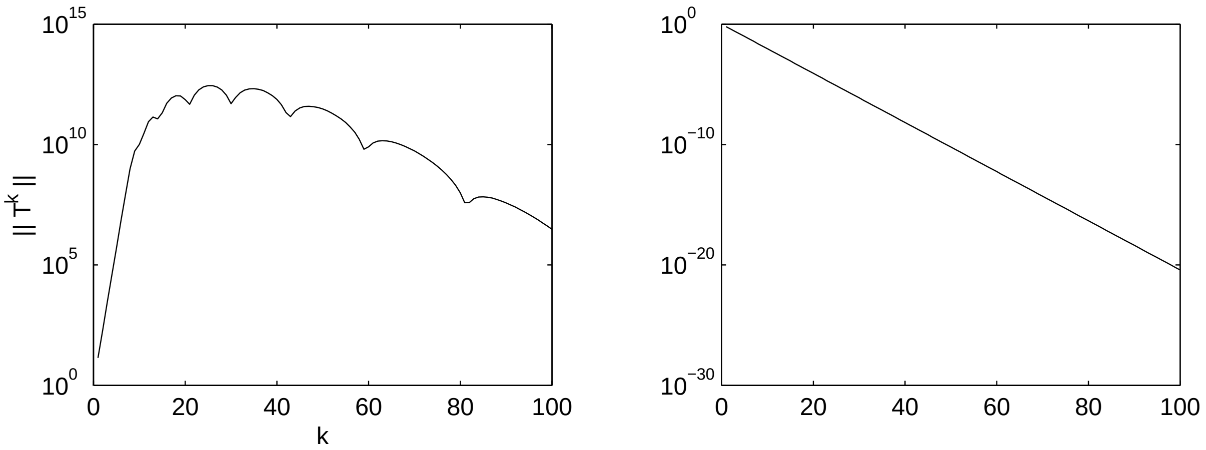
  $\lim_{t\to\infty} \|e^{tA}\| = 0$ if and only if the eigenvalues of A have negative real parts.
  But eigenvalues alone cannot distinguish:





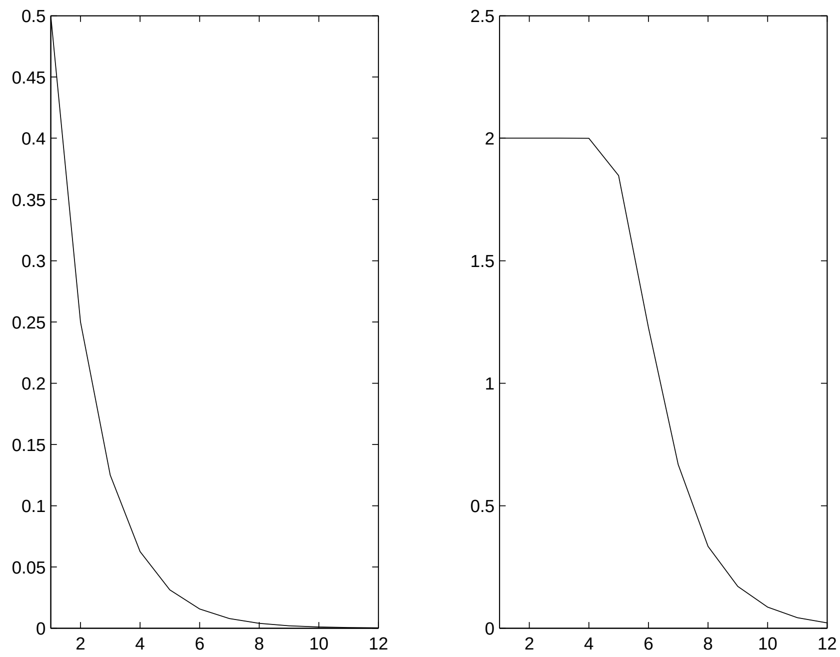
- A^k: Determines stability of finite difference schemes; determines the convergence of stationary iterative methods for linear systems.

  $\lim_{k\to\infty} \|A^k\| = 0$ if and only if $\rho(A) < 1$. But eigenvalues alone cannot distinguish:



- A^k: Markov chains.

  y_0 = initial state; $A^k y_0$ = state after k steps. $A^k y_0 \longrightarrow v$ = eigenvector corresponding to eigenvalue 1. For k large, convergence rate is determined by second largest eigenvalue. But eigenvalues cannot distinguish:



- $\min_{c_1,\ldots,c_k} \|I - \sum_{j=1}^{k} c_j A^j\|$: Residual norm in ideal GMRES.

  Any possible convergence behavior of GMRES can be attained with a matrix having any given eigenvalues. (G., Pták, Strakoš, '96)

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

$$\mathbf{r_0} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad A\mathbf{r_0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ * \end{pmatrix} \perp \mathbf{r_0}, \quad A^2\mathbf{r_0} = \begin{pmatrix} 0 \\ \vdots \\ * \\ * \end{pmatrix} \perp \mathbf{r_0}, \ldots, A^{n-1}\mathbf{r_0} = \begin{pmatrix} 0 \\ * \\ \vdots \\ * \end{pmatrix} \perp \mathbf{r_0}.$$

Given an n by n matrix A, find a set $S \subset \mathbf{C}$ that can be associated with A to give more information than the spectrum alone can provide about the 2-norm of functions of A.

- Field of values or Numerical Range:

$$W(A) = \{\langle Aq, q\rangle : \ q \in \mathbf{C^n}, \ \langle q, q\rangle = 1\}.$$

- ϵ-pseudospectrum:

$$\sigma_\epsilon(A) = \{z \in \mathbf{C} : \ z \text{ is an eigenvalue of } A + E \text{ for some } E \text{ with } \|E\| < \epsilon\}.$$

- Polynomial numerical hull of degree k:

$$\mathcal{H}_k(A) = \{z \in \mathbf{C} : \ \|p(A)\| \geq |p(z)| \ \forall p \in \mathcal{P}_k\}.$$

In trying to relate $\|f(A)\|$ to the size of f on any set $S \subset \mathbf{C}$, however, **remember** that there are *infinitely* many functions g such that $g(A) = f(A)$; e.g., any function g of the form

$$g(z) = f(z) + \chi(z)h(z),$$

where χ is the minimal polynomial of A and h is any function analytic in a neighborhood of each eigenvalue of A. These functions all have the same values on $\sigma(A)$, but they differ on other sets $S \subset \mathbf{C}$. Which one should $\|f(A)\|$ be related to?

If you know that $\|f(A)\| \leq C \max_{z \in S} |f(z)|$, then choose a function g whose ∞-norm on S is minimal.

Pick-Nevanlinna Interpolation Problem

$g(A) = f(A)$ if f and g match at the eigenvalues of A and if their derivatives of orders up through $t-1$ match at eigenvalues corresponding to a $t \times t$ Jordan block. Assume for this talk that A is diagonalizable, with distinct eigenvalues $\lambda_1, \ldots, \lambda_n$.

Find the function $g \in \mathcal{H}^\infty(S)$ satisfying $g(\lambda_j) = f(\lambda_j)$, $j = 1, \ldots, n$, for which $\|g\|_{\mathcal{L}^\infty(S)}$ is minimal.

If $S = \mathcal{D}$, this is a **Pick-Nevanlinna interpolation problem**. If S is simply connected (and $S \neq \mathbf{C}$), do a conformal mapping to the unit disk. *Some* results also known for multiply connected regions.

Field of Values or Numerical Range

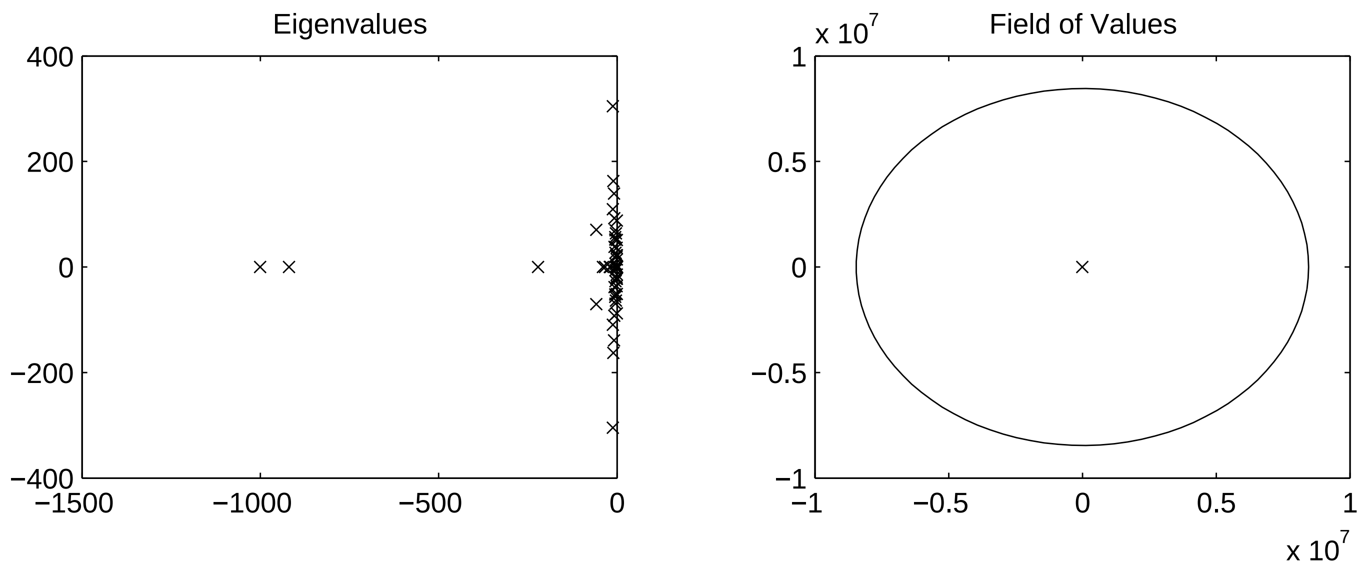
- $W(A) = \{\mathbf{q}^* A\mathbf{q} : \|\mathbf{q}\| = 1\}$ is closed if A is finite dimensional (continuous image of compact unit ball); not necessarily so if A is an operator on infinite dimensional Hilbert space.
- $\sigma(A) \subset \overline{W(A)}$.

  Proof for eigenvalues: $A\mathbf{q} = \lambda\mathbf{q}$, $\|\mathbf{q}\| = 1 \quad \Rightarrow \mathbf{q}^* A\mathbf{q} = \lambda$.

- $W(A)$ is a **convex** set (Toeplitz-Hausdorf theorem, 1918).

  Method of Proof: Reduce to the 2 by 2 case.

- If A is normal then $\overline{W(A)}$ is the convex hull of $\sigma(A)$; if A is nonnormal $W(A)$ contains more.



- If $\mathbf{y}' = A\mathbf{y}$ then for certain initial data, $\|\mathbf{y}(t)\|$ initially **increases** if $W(A)$ extends into rhp; $\|\mathbf{y}(t)\|$ decreases monotonically if $W(A)$ lies in lhp.

Proof:

$$\frac{d}{dt}\langle \mathbf{y}(t), \mathbf{y}(t)\rangle = 2\mathrm{Re}\langle \mathbf{y}'(t), \mathbf{y}(t)\rangle = 2\mathrm{Re}\langle A\mathbf{y}, \mathbf{y}\rangle.$$

- If $0 \notin W(A)$, then

$$\min_{c_1} \|I - c_1 A\| \le \sqrt{1 - d^2/\|A\|^2},$$

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

  Proof (that $\min_{c_1} \|(I - c_1 A)\mathbf{r_0}\| \le \sqrt{1 - d^2/\|A\|^2} \cdot \|\mathbf{r_0}\| \quad \forall \mathbf{r_0}$):

$$\mathbf{r_1} = \mathbf{r_0} - \frac{\langle A\mathbf{r_0}, \mathbf{r_0}\rangle}{\langle A\mathbf{r_0}, A\mathbf{r_0}\rangle} A\mathbf{r_0}$$

$$\begin{aligned} \|\mathbf{r_1}\|^2 &= \|\mathbf{r_0}\|^2 - \frac{\langle A\mathbf{r_0}, \mathbf{r_0}\rangle^2}{\langle A\mathbf{r_0}, A\mathbf{r_0}\rangle} = \|\mathbf{r_0}\|^2 \cdot \left(1 - \frac{\langle A\mathbf{r_0}, \mathbf{r_0}\rangle^2}{\|\mathbf{r_0}\|^2 \cdot \|A\mathbf{r_0}\|^2}\right) \\ &\le \|\mathbf{r_0}\|^2 \left(1 - \frac{d^2}{\|A\|^2}\right). \end{aligned}$$

- What if $0 \in W(A)$?

  Then $\min_{c_1} \|I - c_1 A\| = 1$, but might have $\min_{c_1,\ldots,c_k} \|I - \sum_{j=1}^{k} c_j A^j\| < 1$.

Crouzeix's Conjecture:

For any polynomial p (or any function analytic in $W(A)$),

$$\|p(A)\| \leq 2 \max_{z \in W(A)} |p(z)|.$$

- Constant 2 can be attained:

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

  $W(A)$ is disk of radius 1/2 about 0. $\|A\| = 1 = 2 \max_{z \in \mathcal{D}_{1/2}} |z|$.

- For more information and interesting open problems, see:

  `http://perso.univ-rennes1.fr/michel.crouzeix`

Known Results

- Von Neumann's Inequality (1951):

$$\|p(A)\| \leq \max_{z \in \mathcal{D}_{\|A\|}} |p(z)|.$$

- Power Inequality (Berger/Pearcy, 1966):

$$\|A^k\| \leq 2 \max_{z \in W(A)} |z^k|.$$

More precisely, $\nu(A^k) \leq \nu(A)^k$, where $\nu(A)$ is the numerical radius: $\max_{z \in W(A)} |z|$.

- Badea (2004), based on Ando (1973):

$$\|p(A)\| \le 2 \max_{z \in \mathcal{D}_{\nu(A)}} |p(z)|.$$

- Crouzeix (2004 $->$):

The conjecture is true for 2 by 2 matrices. For general n by n matrices,

$$\|p(A)\| \le 11.08 \max_{z \in W(A)} |p(z)|$$

If A is a 2 by 2 matrix and $W(A)$ is a disk, then best constant is 2; if $W(A)$ is an ellipse with eccentricity ϵ, then the best constant is

$$2 \exp\left(- \sum_{n \ge 1} \frac{(-1)^{n+1}}{n} \frac{2}{1+\rho^{4n}} \right), \quad \text{where } \rho = \frac{1+\sqrt{1-\epsilon^2}}{\epsilon}$$

Method of Proof: Explicitly map $W(A)$ to $\bar{\mathcal{D}}$.

Badea's Result

Ando: If $\nu(A) \leq 1$, then there is a Hermitian matrix B and a unitary matrix U such that:

$$A = 2\cos(B)U\sin(B).$$

Claim: A is similar to a contraction via a similarity transformation with condition number ≤ 2.

Let $g(x) = \max\{1, 2|\cos x|\}$, and define $H = g(B)$, $T = H^{-1}AH$. Then

$$\|H\| \leq 2, \quad \|H^{-1}\| \leq 1, \quad \|\sin(B)H\| \leq 1, \quad 2\|H^{-1}\cos(B)\| \leq 1.$$

Thus $\|T\| \leq 1$. $\square$

By von Neumann's inequality,

$$\|p(A)\| \leq \|H\| \; \|p(T)\| \; \|H^{-1}\| \leq 2\|p\|_{\mathcal{L}^\infty(\mathcal{D})}.$$

How does **Crouzeix's conjecture** or **Badea's result** help with the analysis of GMRES?

Equivalent statement:

$$\|p(A)\| \leq 2 \min_{\{f \in \mathcal{H}^\infty(S) : f(A) = p(A)\}} \|f\|_{\mathcal{L}^\infty(S)},$$

where $S = W(A)$ (conjecture) or S is a disk containing $W(A)$ (theorem).

The ideal GMRES polynomial is $P_k(z) = 1 - \sum_{j=1}^k c_j z^j$, where $c_1, \ldots, c_k$ minimize $\|P_k(A)\|$, so

$$\|P_k(A)\| \leq 2 \min_{\substack{p \in \mathcal{P}_k \\ p(0)=1}} \min_{\{f \in \mathcal{H}^\infty(S) : f(A) = p(A)\}} \|f\|_{\mathcal{L}^\infty(S)}.$$

Blaschke Products

Let $w_1, \ldots, w_n$ be the values of a kth degree polynomial p with $p(0) = 1$ at the eigenvalues $\lambda_1, \ldots, \lambda_n$ of A. Map S to $\bar{\mathcal{D}}$ via a conformal mapping φ.

The unique function $\tilde{f} \in \mathcal{H}^\infty(\mathcal{D})$ that satisfies $\tilde{f}(\varphi(\lambda_j)) = w_j$, $j = 1, \ldots, n$, and achieves the infimum over all such functions of $\|f\|_{\mathcal{L}^\infty(\mathcal{D})}$ is a scalar multiple of a finite **Blaschke product**:

$$\tilde{f}(z) = \mu e^{i\theta} \prod_{k=0}^{n-1} \frac{z - \alpha_k}{1 - \bar{\alpha}_k z} = \mu \frac{\gamma_0 + \gamma_1 z + \ldots + \gamma_{n-1} z^{n-1}}{\bar{\gamma}_{n-1} + \bar{\gamma}_{n-2} z + \ldots + \bar{\gamma}_0 z^{n-1}}$$

Using second representation, Glader and Lindström showed how to compute $\tilde{f}$ and $\|\tilde{f}\|_{\mathcal{L}^\infty(\mathcal{D})}$ by solving a simple eigenvalue problem. Determine μ, $\gamma_0, \ldots, \gamma_{n-1}$ from conditions $\tilde{f}(\varphi(\lambda_j)) = w_j$, $j = 1, \ldots, n$.

Example Result

Suppose $W(A) \subset \mathcal{D}$. Give sufficient conditions on the eigenvalues of A to guarantee that GMRES$(n-1)$ converges; i.e., that

$$\|P_{n-1}(A)\| \equiv \min_{c_1,\ldots,c_{n-1}} \|I - \sum_{j=1}^{n-1} c_j A^j\| < 1.$$

(Equivalently, give conditions in terms of $\lambda_1/\nu(A), \ldots, \lambda_n/\nu(A)$).

Recall that such conditions are **not possible** in terms of only $\lambda_1, \ldots, \lambda_n$.

Let $p_{n-1}(z) = \prod_{j=1}^{n-1}(1 - \frac{z}{\lambda_j})$. Then $p_{n-1}(\Lambda) = \mu e^{i\theta} B(\Lambda)$, where

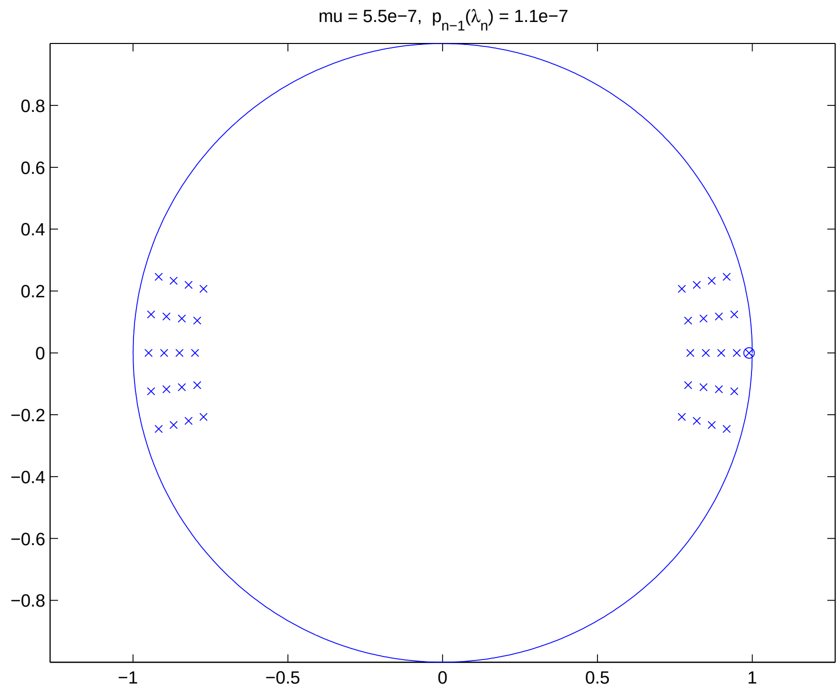
$$B(z) = \frac{\prod_{j=1}^{n-1}(z - \lambda_j)}{\prod_{j=1}^{n-1}(1 - \bar{\lambda}_j z)}.$$

The condition $p_{n-1}(\lambda_n) = \mu e^{i\theta} B(\lambda_n)$ implies

$$\mu = \left| \frac{\left[\prod_{j=1}^{n-1}(1 - \frac{\lambda_n}{\lambda_j})\right] \left[\prod_{j=1}^{n-1}(1 - \bar{\lambda}_j \lambda_n)\right]}{\prod_{j=1}^{n-1}(\lambda_n - \lambda_j)} \right| = \left| \prod_{j=1}^{n-1} \left(\frac{1 - \bar{\lambda}_j \lambda_n}{\lambda_j} \right) \right|.$$

Result holds if

$$\left| \prod_{j=1}^{n-1} \left(\frac{1 - \bar{\lambda}_j \lambda_n}{\lambda_j} \right) \right| < .5.$$



For example, suppose λ_n is close to 1 and other evals occur in $\pm$ pairs: $\lambda_j = -\lambda_{n-j}$, $j = 1, \ldots, n-1$. Assume $\lambda_j = r_j e^{i\theta_j}$, where $\theta_j \in [-\pi/12, \pi/12] \cup [\pi - \pi/12, \pi + \pi/12]$ and $r_j \geq .8$. Then each pair of factors in expression for μ is less than .74, so $\mu < .5$ if 3 or more pairs ($n \geq 7$).

To get good bounds with this approach, mapped evals must be near $\partial\mathcal{D}$. This may not be the case if S is the smallest disk containing $W(A)$. But **if $W(A)$ is long and narrow**, and **if Crouzeix's conjecture is true**, then mapped eigenvalues probably will be near $\partial\mathcal{D}$ (crowding phenomenon).

Conclusions

- It is helpful if one can translate matrix approximation problems into approximation problems in the complex plane.
- Must keep in mind that for any given f there are infinitely many functions g such that $g(A) = f(A)$. The *minimal norm interpolating function* is a useful one.
- No one yet has succeeded at proving or disproving Crouzeix's conjecture. Exploring the implications will lead to useful results if conjecture is true,... or might lead to finding a contradiction.