Why Does GMRES Work Well for Second Kind Fredholm Integral Equations?

(a) Because the matrix is well-conditioned.

(b) Because the eigenvalues are nicely distributed.

(c) Neither of the above.

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The GMRES Algorithm for Solving Nonsymmetric Linear Systems $Ax = b$

- Given an initial guess $x^{(0)}$, compute the initial residual $r^{(0)} = b - Ax^{(0)}$. At each step $j = 1, 2, \ldots$, the algorithm chooses $x^{(j)}$ so that $r^{(j)} = (I - AP_{j-1}(A))r^{(0)}$ for a certain $(j-1)$st degree polynomial P_{j-1}, where P_{j-1} is chosen to minimize $\|r^{(j)}\|_2 \equiv \|r^{(j)}\|$:

$$\|r^{(j)}\| = \min_{p_{j-1} \in \mathcal{P}_{j-1}} \|(I - Ap_{j-1}(A))r^{(0)}\|.$$

- To eliminate dependence on direction of initial residual, study the upper bound:

$$\|r^{(j)}\| / \|r^{(0)}\| \leq \min_{p_{j-1} \in \mathcal{P}_{j-1}} \|I - Ap_{j-1}(A)\|.$$

Does GMRES Converge Rapidly for Well-Conditioned Matrices?

(a) NOT NECESSARILY.

- If A is **normal** or **near-normal** ($A = V\Lambda V^{-1}$, where Λ is diagonal and $\|V\| \cdot \|V^{-1}\| \approx 1$) then **eigenvalues** determine the behavior of GMRES.

$$\|I - AP_{j-1}(A)\| \approx \min_{p_{j-1} \in \mathcal{P}_{j-1}} \|I - \Lambda p_{j-1}(\Lambda)\| = \min_{p_{j-1} \in \mathcal{P}_{j-1}} \max_{i=1,\ldots,n} |1 - \lambda_i p_{j-1}(\lambda_i)|.$$

- A **unitary** matrix Q ($Q^* = Q^{-1}$) is **normal** and has **condition number 1** (since its singular values are the square roots of the eigenvalues of $Q^*Q = I$). But if Q has n eigenvalues equally spaced about the unit circle, then a jth degree polynomial with value 1 at the origin cannot be less than 1 in modulus at all of these eigenvalues if $j < n$. Thus GMRES makes **no progress** until step n.

Does GMRES Converge Rapidly for Matrices with 'Nice' Eigenvalues?

(b) NOT NECESSARILY.

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

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

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

Second Kind Fredholm Integral Equations

$(\alpha\mathcal{I} + \mathcal{K})u = g$, where $\alpha \neq 0$ and

$$(\mathcal{K}u)(x) = \int_\Omega k(x,y)u(y)\,dy, \quad x \in \Omega.$$

1. $\Omega \subset \mathbf{R}^d$ is compact, $k \in C(\Omega \times \Omega)$, $\mathcal{K} : C(\Omega) \to C(\Omega)$ is a bounded linear operator and $\|\mathcal{K}\| \leq m(\Omega) \cdot \|k\|_\infty$.
2. $\Omega \subset \mathbf{R}^d$ is measurable, $k \in L^2(\Omega \times \Omega)$, $\mathcal{K} : L^2(\Omega) \to L^2(\Omega)$ is a bounded linear operator and $\|\mathcal{K}\| \leq \|k\|_{L^2(\Omega\times\Omega)}$.

In both cases, $\mathcal{K}$ is **compact**. The nonzero spectrum of $\mathcal{K}$ consists only of eigenvalues, the spectrum is countable and can accumulate only at 0.

Discretized Linear System

- Expect similar properties in discretized linear system $(\alpha I + K)u = g$. $A \equiv \alpha I + K$ has most eigenvalues close to $\alpha \neq 0$, and $\|K\|$ (i.e., the largest singular value of K) is of moderate size.

- Assume wlog $\alpha = 1$. If $\|K\| < 1$, can choose p_{j-1} so that $I - Ap_{j-1}(A) = (-1)^j K^j$. Hence $\|r^{(j)}\| \leq \|K^j\| \leq \|K\|^j$.

- But often $\|K\| > 1$. $K = L + M$, where L has **low rank** and $\|M\| << 1$.

GMRES for $A = I + L + M$, where $\mathbf{Rank}(L) = s << n$ and $\|M\| << 1$

$$\begin{aligned}
\chi_{I+L}(A) &= \prod_{i=0}^{s}\left(I - \frac{1}{1+\lambda_i}(I+L) - \frac{1}{1+\lambda_i}M\right), \\
&= \sum_{\ell=0}^{s}\left[\prod_{i=0}^{\ell-1}\left(I - \frac{1}{1+\lambda_i}(I+L)\right)\right]\cdot\left[\frac{-1}{1+\lambda_\ell}M\right]\cdot \\
&\qquad \left[\prod_{i=\ell+1}^{s}\left(I - \frac{1}{1+\lambda_i}(I+L)\right)\right] + O(\|M\|^2).
\end{aligned}$$

If $\|M\|$ is small enough so that $\|\chi_{I+L}(A)\| < 1$, then

$$\|r^{(j(s+1))}\|/\|r^{(0)}\| \le \|(\chi_{I+L}(A))^j\| \le \|\chi_{I+L}(A)\|^j.$$

Cannot argue that now that L is annihilated, apply $(I - Ap_{j-1}(A)) = (-1)^j K^j = (-1)^j (L+M)^j$ to $\chi_{I+L}(A)$ to reduce residual at rate of GMRES($I + M$).

Some Other Approaches

- Ideally, would like some info about the *eigenvectors* of A; e.g., $\|V\| \cdot \|V^{-1}\|$ of moderate size. In the absence of this, ...
- 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:

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

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.

Estimates Based on Other Sets in the Complex Plane

- Von Neumann's Inequality (1951):

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

- Badea (2004), based on Okubo and Ando (1975):

$$\|p(A)\| \leq 2 \max_{z \in \mathcal{D}_{W(A)}} |p(z)|,$$

where $\mathcal{D}_{W(A)}$ is any disk enclosing the field of values $W(A)$.

- Crouzeix (2004 $-$ >):

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

Conjecture is that 11.08 can be replaced by 2. Conjecture has been proved for 2 by 2 matrices (C.), for 3 by 3 nilpotent matrices (C.), and for perturbed Jordan blocks of dimension $n > 5$ (G.).

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:

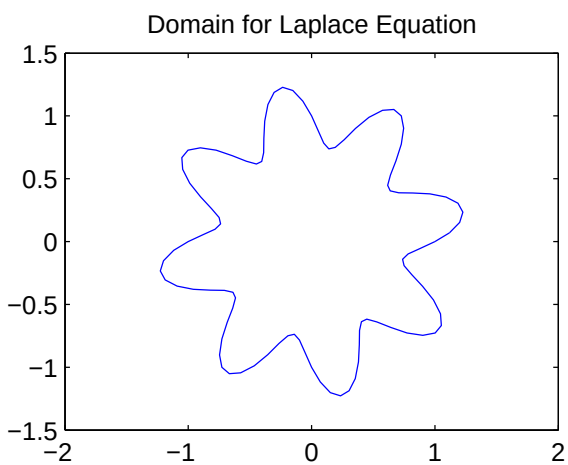
  `http://perso.univ-rennes1.fr/michel.crouzeix`

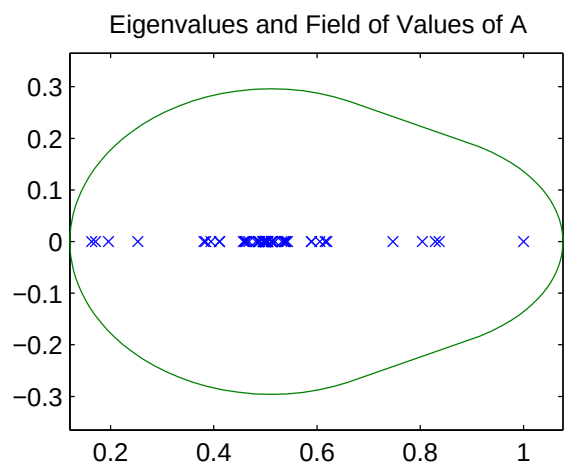
Are Any of These Estimates Useful for Analysis of GMRES Applied to Second Kind Fredholm Integral Equations?

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

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

where d is the distance from 0 to $W(A)$. This was already known but now can be improved.





- Often, $W(A)$ contains the origin, so $\max_{z \in W(A)} |1 - z p_{j-1}(z)| \geq 1$ $\forall p_{j-1} \in \mathcal{P}_{j-1}$.

- However, there are *infinitely* many analytic functions q such that $q(A) = I - A p_{j-1}(A)$; take $q(z) = (1 - z p_{j-1}(z)) + \chi(z) h(z)$, where χ is the minimal polynomial of A and h is any function analytic in the desired region $S = W(A)$ or $\mathcal{D}_{W(A)}$ or $\mathcal{D}_{\|A\|}$. To obtain the best estimate of $\|p(A)\|$ take q to be the function of minimal ∞-norm on S that satisfies $q(A) = p(A)$.

  When $S = \mathcal{D}$, this is a **Pick-Nevanlinna** interpolation problem. When S is simply connected, do a conformal mapping to $\mathcal{D}$. Interesting mathematically; probably too complicated to be used much in practice.

Conclusions

- Most published results about convergence of GMRES for second kind Fredholm integral equations deal with *operator* equations and establish superlinear convergence asymptotically. But in finite dimensional case, GMRES finds the *exact* solution after at most n steps. Need more results about what happens before this.
- It would be nice if one could translate matrix approximation problems (e.g., how rapidly does GMRES reduce the residual norm) into approximation problems in the complex plane. It leads to interesting mathematics but may be too complicated to be useful in practice. Must keep in mind that for any given p there are infinitely many functions q such that $q(A) = p(A)$. The *minimal norm interpolating function* is an important 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.