Krylov subspace methods
Connections and open questions

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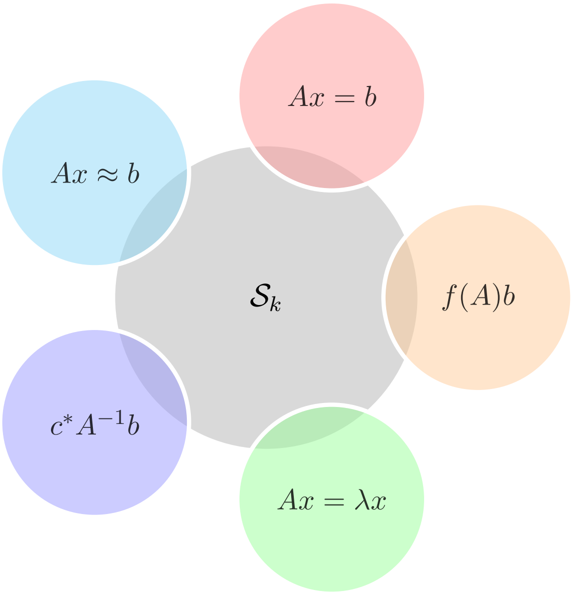

$Ax = b$
$Ax \approx b$
$\mathcal{S}_k$
$f(A)b$
$c^*A^{-1}b$
$Ax = \lambda x$

Krylov subspaces

Given $A \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$,

$$\mathcal{S}_k \equiv \underbrace{\mathrm{span}(v, Av, \ldots, A^{k-1}v)}_{\mathcal{K}_k(A,v)}$$

look for an approximation

$$x_k = p(A)v, \quad p \in \mathcal{P}_{k-1}.$$

"**best**" $x_k \quad \leftrightarrow \quad$ solving **approximation problems**

$Ax = b$

minimal residual approach

$A \in \mathbb{R}^{n\times n}$ nonsingular, $x_0 = 0$, and $\|b\| = 1$

Choose $x_k \in \mathcal{K}_k(A,b)$:

$$\begin{aligned} \| \underbrace{b - Ax_k}_{r_k} \| &= \min_{y\in\mathcal{K}_k} \| b - Ay \| \\ &= \min_{p\in\mathcal{P}_{k-1}} \| b - Ap(A)b \| \\ &\le \min_{p\in\mathcal{P}_{k-1}} \| I - Ap(A) \| . \end{aligned}$$

Approximation problems

normal matrices

Normal matrices

$$\overbrace{\min_{p \in \mathcal{P}_{k-1}} \| b - Ap(A)b \|}^{\text{GMRES}} \quad \leq \quad \overbrace{\min_{p \in \mathcal{P}_{k-1}} \| I - Ap(A) \|}^{\text{ideal GMRES}}$$

$A = Q\Lambda Q^*, \qquad b = Qc, \qquad Q$ unitary

$$\min_{p \in \mathcal{P}_{k-1}} \| c - \Lambda p(\Lambda)c \| \quad \leq \quad \min_{p \in \mathcal{P}_{k-1}} \| I - \Lambda p(\Lambda) \|$$

$$= \quad \min_{p \in \mathcal{P}_{k-1}} \max_{\lambda_i} | 1 - zp(z) |$$

$$= \quad \min_{p \in \mathcal{P}_{k-1}} \| 1 - zp(z) \|_L$$

$L = \{\lambda_1, \ldots, \lambda_n\}$, bound attainable [Greenbaum et al. '94], [Liesen, T. '14]

A classical approximation problem

- f and $\varphi_1, \ldots, \varphi_k$ are given (scalar) functions,
- $\mathcal{V}_k = \mathrm{span}\{\varphi_1, \ldots, \varphi_k\}$
- $\Omega \subset \mathbb{R}$ or $\Omega \subset \mathbb{C}$ compact, $\|g\|_\Omega = \max_\Omega |g(z)|$.

$$\min_{s \in \mathcal{V}_k} \| f(z) - s(z) \|_\Omega$$

Such problems have been studied since the 1850s; numerous results on existence, uniqueness and rate of convergence for $k \to \infty$.

[Chebyshev 1854, Weierstrass 1885, de la Vallée Poussin 1908, Haar 1910, Faber 1920, Remez 1936 . . .]

- f and $\varphi_1, \dots, \varphi_k$ are given (scalar) functions,
- $\mathcal{V}_k = \text{span}\{\varphi_1, \dots, \varphi_k\}$,
- $\Omega \subset \mathbb{R}$ or $\Omega \subset \mathbb{C}$ compact.

$$\min_{s \in \mathcal{V}_k} \| f(z) - s(z) \|_\Omega$$

Take $f \equiv 1$, $\mathcal{V}_k = \text{span}\{z, \dots, z^k\}$, $\Omega = \{\lambda_1, \dots, \lambda_n\}$,

$$\min_{p \in \mathcal{P}_{k-1}} \| 1 - zp(z) \|_\Omega$$

Solution of the problem

- Characterization [Kolmogorov '48], [Chebyshev], [Rivlin, Shapiro '61]

$$\| f - s_* \|_\Omega \quad = \quad \min_{s \in \mathcal{V}_k} \| f - s \|_\Omega$$

- There is a subset $S \subseteq \Omega$ consisting of ℓ points such that

$$\min_{s \in \mathcal{V}_k} \| f - s \|_S \quad = \quad \min_{s \in \mathcal{V}_k} \| f - s \|_\Omega$$

and $\ell = k + 1$ if $\Omega \subset \mathbb{R}$, and $\ell \leq 2k + 1$ if $\Omega \subset \mathbb{C}$.

- Chebyshev **alternation points** $\rightarrow$ Remez algorithm [Remez 1936]

Ideal GMRES

as a function of A's eigenvalues? (real case)

$\Omega = \{\lambda_1, \ldots, \lambda_n\}$,

$$M_k^\Omega \equiv \min_{p \in \mathcal{P}_{k-1}} \| 1 - zp(z) \|_\Omega .$$

Real case: $\exists\, S = \{\lambda_1^S, \ldots, \lambda_{k+1}^S\} \subseteq \Omega$:

$$M_k^\Omega = M_k^S \quad = \quad \frac{1}{\sum_{j=1}^{k+1} \prod_{\substack{i=1 \\ i \neq j}}^{k+1} \frac{|\lambda_i^S|}{|\lambda_i^S - \lambda_j^S|}} .$$

[Greenbaum '79; Liesen, T. '04]

Ideal GMRES

as a function of A's eigenvalues? (complex case)

$S \subseteq \Omega$ for which $M_k^\Omega = M_k^S$ might contain $2k+1$ points.

We proved that $\exists S \subseteq \Omega$, $|S| = k+1$: [Liesen, T. '04]

$$M_k^S \;\le\; M_k^\Omega \;\le\; \underbrace{\sqrt{(k+1)(n-k)}}_{\text{conjecture } \frac{4}{\pi}} \; M_k^S \,.$$

and M_k^S can be expressed explicitly.

Conjecture: $k+1$ points are sufficient to characterize M_k^Ω also in the **complex case**, up to the constant of $\frac{4}{\pi}$.

Open question

- f and $\varphi_1, \ldots, \varphi_k$ are given (scalar) functions,
- $\mathcal{V}_k = \mathrm{span}\{\varphi_1, \ldots, \varphi_k\}$,
- $\Omega \subset \mathbb{C}$ compact.

Showing that $\exists S \subseteq \Omega$ containing $k+1$ points s.t.

$$\min_{s \in \mathcal{V}_k} \| f - s \|_\Omega \leq \frac{4}{\pi} \min_{s \in \mathcal{V}_k} \| f - s \|_S$$

would be a nice contribution to approximation theory.

Could lead, e.g., to a simpler Remez-like algorithm in $\mathbb{C}$.

Approximation problems

nonnormal matrices

$Ax = b$

minimal residual approach

$A \in \mathbb{R}^{n\times n}$ nonsingular, $x_0 = 0$, and $\|b\| = 1$

Choose $x_k \in \mathcal{K}_k(A, b)$:

$$
\begin{aligned}
\| \underbrace{b - Ax_k}_{r_k} \| &= \min_{p\in\mathcal{P}_{k-1}} \| b - Ap(A)b \| \\
&\leq \min_{p\in\mathcal{P}_{k-1}} \| I - Ap(A) \| \\
&\leq \kappa(X) \min_{p\in\mathcal{P}_{k-1}} \| I - \Lambda p(\Lambda) \| ,
\end{aligned}
$$

where $A = X\Lambda X^{-1}$ is Jordan decomposition.

Do eigenvalues determine convergence?

The last bound is usually **useless**,

$$\|r_k\| \quad \leq \quad \kappa(X) \min_{p \in \mathcal{P}_{k-1}} \| \, I - \Lambda p(\Lambda) \, \| \, .$$

Theorem [Greenbaum, Pták, Strakoš '96]

Given a nonincreasing positive sequence

$$f_0 \geq f_1 \geq \cdots \geq f_{n-1} > 0$$

and a set of nonzero complex numbers $\{\lambda_1, \ldots, \lambda_n\}$, there exists a matrix A with eigenvalues $\lambda_1, \ldots, \lambda_n$ and a right-hand side b with $\|b\| = f_0$ such that the residuals r_k of GMRES(A, b) satisfy

$$\|r_k\| = f_k, \qquad k = 1, 2, \ldots, n-1 \, .$$

Ideal GMRES bound

$$\| \underbrace{b - Ax_k}_{r_k} \| = \min_{p \in \mathcal{P}_{k-1}} \| b - Ap(A)b \|$$

$$\leq \min_{p \in \mathcal{P}_{k-1}} \| I - Ap(A) \| .$$

− doest not take into account the influence of b

− it can happen [Toh '97]

$$\|r_k\| \ll \min_{p \in \mathcal{P}_{k-1}} \| I - Ap(A) \| \qquad \forall \, \|b\| = 1$$

+ usually characterizes the GMRES worst-case behaviour

A general matrix approximation problem

- $A \in \mathbb{R}^{n \times n}$
- f and $\varphi_1, \ldots, \varphi_k$ are given (scalar) functions,
- $\mathcal{V}_k = \text{span}\{\varphi_1, \ldots, \varphi_k\}$,

$$\min_{s \in \mathcal{V}_k} \| f(A) - s(A) \|$$

Ideal GMRES: $f \equiv 1$, $\mathcal{V}_k = \text{span}\{z, \ldots, z^k\}$

$$\min_{p \in \mathcal{P}_{k-1}} \| I - Ap(A) \|$$

A new kind of problems: uniqueness, computation, convergence?

Uniqueness

Uniqueness

Uniqueness of ideal GMRES $\rightarrow$ [Greenbaum, Trefethen '94].

Consider

$$\min_{s \in \mathcal{V}_k} \| f(A) - s(A) \|$$

for $\mathcal{V}_k = \text{span}\{\varphi_1, \ldots, \varphi_k\}$, $\varphi_j = z^m z^{j-1}$, $m \geq 0$ given.

Core of the problem

$$\min \| \gamma_0 I + \cdots + \gamma_{k-1} A^{k-1} + \gamma_k A^k + \cdots + \gamma_\ell A^\ell \| > 0 \,,$$

This problem has a **unique** solution. [Liesen, T. '09]

Consider

$$\min \| \gamma_0 I + \cdots + \gamma_{k-1} A^{k-1} + \gamma_k A^k + \cdots + \gamma_\ell A^\ell \| > 0 \,,$$

with **some** coefficients **fixed**. Does it have a unique solution?

Uniqueness of the solution of

$$\min_{s \in \mathcal{V}_k} \| f(A) - s(A) \|$$

where φ_j satisfy the Haar condition?

What about **rational** approximations?

Computation

A semidefinite program

A semidefinite program

Given $c \in \mathbb{R}^m$ and symmetric matrices $F_0, \ldots, F_m \in \mathbb{R}^{n \times n}$,

$$\text{minimize} \quad c^T x$$

subject to

$$F(x) \geq 0$$

where

$$F(x) \equiv F_0 + \sum_{k=1}^{m} x_i F_i \,.$$

Matlab software **SDPT3** (Toh, Todd, Tutuncu).

Now a part of **CVX** (Boyd, Grant - Stanford university).

The matrix approximation problems

as a semidefinite program

- Given $A \in \mathbb{R}^{n \times n}$, $\|A\|$ = the maximal eigenvalue of

$$\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}.$$

- We want to minimize the norm of

$$G(\alpha) \equiv f(A) - \sum_{j=1}^{k} \alpha_j \varphi_j(A),$$

i.e the maximal eigenvalue of

$$\begin{bmatrix} 0 & G(\alpha) \\ G(\alpha)^T & 0 \end{bmatrix}.$$

The matrix approximation problems

as a semidefinite program

Equivalently, find minimal λ such that $\exists\ \alpha \in \mathbb{R}^k$ with

$$\lambda I - \begin{bmatrix} 0 & G(\alpha) \\ G(\alpha)^T & 0 \end{bmatrix} \geq 0,$$

i.e.,

$$\underbrace{-\begin{bmatrix} 0 & f(A) \\ f(A)^T & 0 \end{bmatrix}}_{F_0} + \sum_{j=1}^{k} \alpha_j \underbrace{\begin{bmatrix} 0 & \varphi_j(A) \\ \varphi_j(A)^T & 0 \end{bmatrix}}_{F_j} + \lambda \underbrace{I}_{F_{k+1}} \geq 0$$

Defining $x \equiv [\alpha_1, \ldots, \alpha_k, \lambda]^T$, $c \equiv [0, \ldots, 0, 1]^T$ we want to

$$\text{minimize} \quad c^T x \quad \text{subject to} \quad F(x) \geq 0\,.$$

Matrix approximation problems

- $A \in \mathbb{R}^{n \times n}$
- f and $\varphi_1, \ldots, \varphi_k$ are given (scalar) functions,
- $\mathcal{V}_k = \text{span}\{\varphi_1, \ldots, \varphi_k\}$,

$$\min_{s \in \mathcal{V}_k} \| f(A) - s(A) \|$$

A new kind of problems:

- uniqueness
- computation
- convergence

Convergence

Estimating the ideal GMRES approximation

How to estimate

$$\min_{q \in \mathcal{P}_{k-1}} \| \underbrace{I - Aq(A)}_{p(A)} \| = \min_{p \in \pi_k} \| p(A) \| \,?$$

Try to determine sets $\Omega \subset \mathbb{C}$ associated with A such that

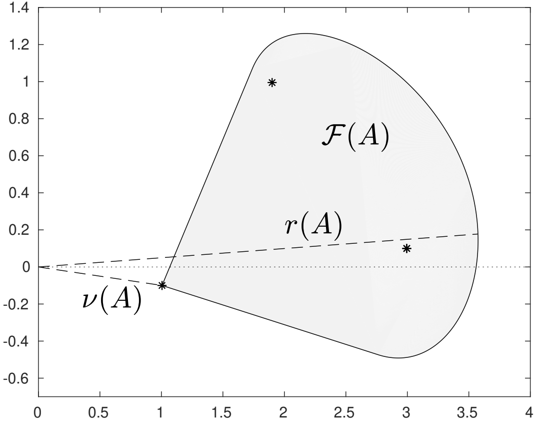
$$\| p(A) \| \sim \| p(z) \|_{\Omega}.$$

Where in the complex plane does a matrix live? [Nick Trefethen]

Candidates

- $\Omega =$ field of values $\mathcal{F}(A)$
- $\Omega = \varepsilon$-pseudospectrum of A [Trefethen '90]
- $\Omega =$ polynomial num. hull of A [Nevanlinna '93; Greenbaum '02]

Field of values of A



$$\mathcal{F}(A) \equiv \{\langle Av, v\rangle : v \in \mathbb{C}^n,\ \|v\| = 1\}$$

Crouzeix's conjecture

For any A and any polynomial p it holds that

$$\| p(A) \| \leq c \, \| p(z) \|_{\Omega}, \quad \Omega = \mathcal{F}(A).$$

- **conjecture** $c = 2$ [Crouzeix '04]
- proof $c = 11.08$ [Crouzeix '07]
- proof $c = 1 + \sqrt{2}$ [Crouzeix, Palencia '17]

" When eigenvalues do not tell the whole story,
the field of values may give more info." [Anne Greenbaum]

Crouzeix's inequality

holds in some cases

$$\| p(A) \| \leq 2 \| p(z) \|_{\Omega}, \quad \Omega = \mathcal{F}(A)$$

- if A is normal (2 can be improved to 1)
- $n = 2$ [Crouzeix '04]
- $p(z) = z^k$ [Berger, Pearcy '66]
- if $\mathcal{F}(A)$ is a disk [Badea '04, Okubo, Ando '75, von Neumann '51]
- $$A = \begin{bmatrix} \lambda & \alpha_1 & & \\ & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} \\ \alpha_n & & & \lambda \end{bmatrix}$$

[Choi, Greenbaum '12], [Choi '13]

Crouzeix ratio

$$f(p, A) = \frac{\| p(z) \|_{\mathcal{F}(A)}}{\| p(A) \|} \geq \frac{1}{2} \,?$$

[Greenbaum, Overton '18]

- optimization problem $\rightarrow$ **properties**
- use **BFGS** method, Matlab and Chebfun
- fix p or A or none
- **conjecture**: $\frac{1}{2}$ can be attained only for z^k
- **conjecture**: only for the **Crabb-Choi-Crouzeix** matrix

Crabb-Choi-Crouzeix matrix

Independently used by [Choi '13], [Crouzeix '15], [Crabb '71],

$$C_1 = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}, \quad C_n = \begin{bmatrix} 0 & \sqrt{2} & & & & \\ & 0 & 1 & & & \\ & & 0 & \ddots & & \\ & & & 0 & 1 & \\ & & & & 0 & \sqrt{2} \\ & & & & & 0 \end{bmatrix}.$$

Recall $\|A\| \leq 2r(A)$ for any square matrix. C_n^n reaches this bound.

$$\| C_n^n \| \;=\; 2r(C_n^n)\,, \qquad r(C_n^n) = r(C_n)^n\,.$$

Crouzeix's conjecture

Theorem [Hnětynková, T. '18]

$A \in \mathbb{C}^{(n+1)\times(n+1)}$, it holds that

$$\| p(A) \| = 2\| p(z) \|_{\mathcal{F}(A)}$$

for $p = z^k$ and $1 \leq k \leq n \iff A$ is unitarily similar to

$$r(A) \begin{bmatrix} C_k & \\ & B \end{bmatrix},$$

where B is of the size $n-k$, $r(B) \leq 1$ and $\|B^k\| \leq 2$.

Conjectures [Greenbaum, Overton '18]:

- $\frac{1}{2}$ can be attained only for z^k ?
- only for the **Crabb-Choi-Crouzeix** matrix $\rightarrow$ **yes**.

Crouzeix's conjecture

and the consequence for GMRES

If Crouzeix's conjecture is true, then

$$\begin{aligned} \|r_k\| &\leq \min_{p\in\pi_k} \| \, p(A) \, \| \\ &\leq 2 \min_{p\in\pi_k} \| \, p(z) \, \|_{\mathcal{F}(A)} \\ &= 2 \min_{p\in\pi_k} \max_{z\in\mathcal{F}(A)} | \, p(z) \, | \, . \end{aligned}$$

Usually a large overestimation.

Open problem: Can we find **a better set**?

Greenbaum-Trefethen problem #4

Can any matrix be simulated by a normal matrix?

GMRES $\rightarrow$ yes [Greenbaum, Strakoš '94].Ideal GMRES $\rightarrow$ **unknown** .

Is it possible to find a discrete set $\Omega = \{\mu_1, \ldots, \mu_m\} \subset \mathbb{C}$ s.t.

$$\min_{p \in \pi_k} \| \, p(A) \, \| \; = \; \min_{p \in \pi_k} \max_{\lambda \in \Omega} |p(\lambda)| \, ?$$

Given a nonincreasing positive sequence

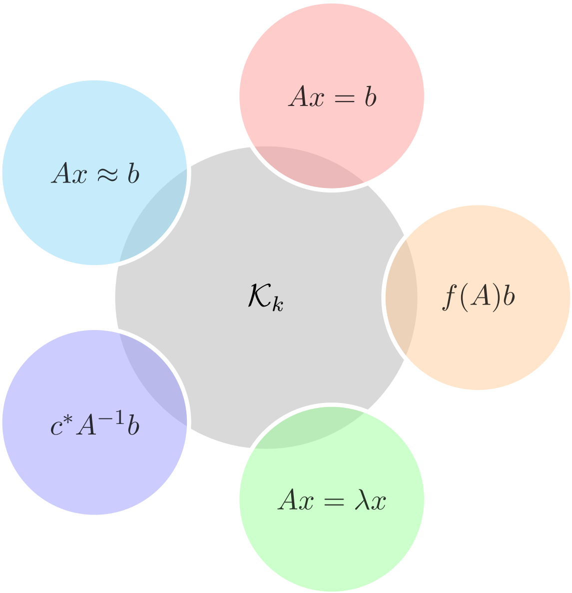
$$f_0 \geq f_1 \geq \cdots \geq f_{n-1} > 0,$$

is there a set $\Omega = \{\mu_1, \ldots, \mu_m\} \subset \mathbb{C}$ such that

$$\min_{p \in \pi_k} \max_{\lambda \in \Omega} |p(\lambda)| \; = \; f_k \, ?$$

Properties of $\Omega \longleftrightarrow A$?

Summary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Summary

- **normal** matrices $\rightarrow$ well understood, conjecture

$$\min_{s\in\mathcal{V}_k} \| f - s \|_\Omega \leq \frac{4}{\pi} \min_{s\in\mathcal{V}_k} \| f - s \|_S \,?$$

- **non-normal** matrices $\rightarrow$ not well understood

$$\min_{s\in\mathcal{V}_k} \| f(A) - s(A) \|$$

  - Uniqueness is in general open.
  - Where in the complex plane does a matrix live?

$$\| p(A) \| \sim \| p(z) \|_\Omega$$

  - Crouzeix's conjecture, for $\Omega = \mathcal{F}(A)$, constant 2.
  - Is there a better (discrete) set Ω ?

Related papers

- M. Crouzeix and C. Palencia, [The numerical range is a $(1+\sqrt{2})$-spectral set, SIMAX 38 (2017), pp. 649–655]
- A. Greenbaum and N. L. Trefethen, [GMRES/CR and Arnoldi/Lanczos as matrix approx. problems, SISC, 15 (1994), pp. 359–368]
- A. Greenbaum and M. L. Overton, [Numerical investigation of Crouzeix's conjecture, LAA 542 (2018), pp. 225–245]
- I. Hnětynková and P. Tichý, [Characterization of half-radial matrices, LAA 559 (2018), pp. 227–243]
- J. Liesen and P. Tichý, [On best approximations of polynomials in matrices in the matrix 2-norm, SIMAX, 31 (2009), pp. 853–863.]

Thank you for your attention!