On matrix approximation theory

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based on joint work with

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Introduction

- A classical problem of approximation theory:

  Best approximation by polynomials

  $$\min_{p \in \mathcal{P}_m} \|f - p\|_K \,, \quad \|g\|_K \equiv \max_{z \in K} |g(z)|$$

- f is a given (nice) function, $K \subset \mathbb{C}$ is compact, $\mathcal{P}_m$ is the set of polynomials of degree at most m

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

- Best approximation results can be used for bounding and/or estimating "almost best" approximations

Introduction

- Classical example:
  Bound for the error of the Faber expansion of f
  (Kövari & Pommerenke, Math. Zeitschr. 1967)

4. Faber Expansion and the Best Polynomial Approximation

It is known that if K is any continuum, and that if $f(z)$ is any function continuous on K and analytic in the interior of K, there exists a polynomial $\pi_n(z)$ of degree n (the polynomial of best uniform approximation) such that for every polynomial $P_n(z)$ of degree n

$$\max_{z\in K} |f(z)-P_n(z)| \geqq \max_{z\in K} |f(z)-\pi_n(z)| = \rho_n(f, K),$$

and $\rho_n(f, K)$ is the best (uniform) polynomial approximation of the function $f(z)$ on K.

Theorem 3. *If*

$$S_n(z) = \sum_{k=0}^{n} c_k F_k(z)$$

then for any continuum K whose complement is connected and for any function $f(z)$ analytic in the interior of K and continuous on K we have

$$|f(z)-S_n(z)| \leqq A\, n^{\alpha} \cdot \rho_n(f, K) \tag{4.1}$$

where A and $\alpha < \frac{1}{2}$ are absolute constants.

Introduction

- Instead of the well studied scalar approximation problem

  $$\min_{p \in \mathcal{P}_m} \|f - p\|_K \,, \quad \|g\|_K \equiv \max_{z \in K} |g(z)|$$

  we here consider the matrix approximation problem

  $$\min_{p \in \mathcal{P}_m} \|f(A) - p(A)\| \,, \quad \|\cdot\| = \text{given matrix norm}$$

- $A \in \mathbb{C}^{n \times n}$, f is analytic in neighborhood of A's spectrum

- Does this problem have a unique solution $p_* \in \mathcal{P}_m$?

- Yes, if the matrix norm is strictly convex

Introduction

- Definition of strict convexity: For all A_1, A_2,

  if $\|A_1\| = \|A_2\| = \frac{1}{2}\|A_1 + A_2\|$ then $\|A_1\| = \|A_2\|$

- Geometrically: Unit sphere does not contain line segments

- Strictly convex matrix norm: Frobenius norm,

  $$\|A\|_F^2 \overset{(1)}{=} \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2 \overset{(2)}{=} \text{trace}(A^*A) \overset{(3)}{=} \sum_{i=1}^n \sigma_i(A)^2$$

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- Remarks:

  (1) Matrix Frobenius norm = Vector 2-norm in $\mathbb{C}^{n^2}$

  (2) $\mathbb{C}^{n\times n}$ and $\langle A, B\rangle \equiv \operatorname{trace}(A^*B)$ make a Hilbert space; associated norms are always strictly convex

  (3) Sum of *all* singular values

Introduction

- A useful matrix norm in many applications:

  Matrix 2-norm defined by $\|A\| \equiv \sigma_1(A)$

- This norm is not strictly convex

- Example:

$$A_1 = \begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix}, \quad A_2 = \begin{bmatrix} B & 0 \\ 0 & D \end{bmatrix},$$

  where $\|A_1\| = \|A_2\| = \sigma_1(B) \geq \frac{1}{2}\|C + D\|$.

  Then $\frac{1}{2}\|A_1 + A_2\| = \sigma_1(B)$. But if $C \neq D$ then $A_1 \neq A_2$.

- Consequently: Best approximation problems in the matrix 2-norm are not guaranteed to have a unique solution

Uniqueness results

- We here consider the matrix approximation problem

$$\min_{p \in \mathcal{P}_m} \|f(A) - p(A)\|\,, \quad \|\cdot\| = \text{matrix 2-norm}$$

- Well known: $f(A) = p_f(A)$ for a polynomial p_f depending on values and possibly derivatives of f on A's spectrum

- We therefore ask:
Given a polynomial b and a nonnegative integer $m < \deg b$.
Does the best matrix approximation problem

$$\min_{p \in \mathcal{P}_m} \|b(A) - p(A)\|$$

have a unique solution ?

- Not much known about such problems so far

Uniqueness results

- Our problem: $\min_{p \in \mathcal{P}_m} \|b(A) - p(A)\|$
- The special case $b(A) = A^{m+1}$ is called the $(m+1)$st ideal Arnoldi approximation problem
- Introduced in (Greenbaum & Trefethen, SISC 1994), paper contains uniquness result ($\rightarrow$ story of the proof)

Uniqueness results

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- Introduced in (Greenbaum & Trefethen, SISC 1994), paper contains uniquness result ($\rightarrow$ story of the proof)
- $(m+1)$st ideal Arnoldi polynomial of A later named $(m+1)$st Chebyshev polynomial of A
- Reason: For normal A we have

  $\min_{p \in \mathcal{P}_m} \|A^{m+1} - p(A)\| = \min_{p \in \mathcal{P}_m} \|z^{m+1} - p(z)\|_K$

  with $K =$ spectrum of A (*scalar* approximation problem)
- Some work on these polynomials in (Toh PhD thesis, 1996), (Toh & Trefethen, SIMAX 1998), (Trefethen & Embree, Book, 2005)

Uniqueness results

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- $\ell \geq 0$ and $m \geq 0$ given, polynomial b given by

$$b = \sum_{j=0}^{\ell+m+1} \beta_j z^j \in \mathcal{P}_{\ell+m+1}$$

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- We rewrite the problem for convenience:

$$\min_{p\in\mathcal{P}_m} \|b(A) - p(A)\| = \min_{p\in\mathcal{P}_m} \| b(A) - \Big(p(A) + \sum_{j=0}^{m} \beta_j A^j\Big) \|$$

$$= \min_{p\in\mathcal{P}_m} \| \sum_{j=m+1}^{\ell+m+1} \beta_j A^j - p(A) \|$$

$$= \min_{p\in\mathcal{P}_m} \| A^{m+1} \sum_{j=0}^{\ell} \beta_{j+m+1} A^j - p(A) \|$$

Uniqueness results

- We have rewritten the problem as

$$\min_{p \in \mathcal{P}_m} \| A^{m+1} \sum_{j=0}^{\ell} \beta_{j+m+1} A^j - p(A) \|$$

- The polynomials are of the form $z^{m+1} g + h$, where $g \in \mathcal{P}_\ell$ is *given*, and $h \in \mathcal{P}_m$ is *sought*

- Our problem therefore is:

$$\min_{p \in \mathcal{G}_{\ell,m}^{(g)}} \|p(A)\|, \quad \mathcal{G}_{\ell,m}^{(g)} \equiv \left\{ z^{m+1} g + h \,:\, g \in \mathcal{P}_\ell \text{ is given}, h \in \mathcal{P}_m \right\}$$

- $\mathcal{G}_{\ell,m}^{(g)}$ = subset of $\mathcal{P}_{\ell+m+1}$, where the coefficients at $z^{m+1}, \ldots, z^{\ell+m+1}$ are fixed

Uniqueness results

$$\min_{p \in \mathcal{G}_{\ell,m}^{(g)}} \|p(A)\|, \quad \mathcal{G}_{\ell,m}^{(g)} \equiv \{ z^{m+1} g + h \,:\, g \in \mathcal{P}_\ell \text{ is given}, h \in \mathcal{P}_m \}$$

- Here the $\ell + 1$ largest coefficients are fixed
- Related problem: Fix the $m + 1$ smallest coefficients, i.e. those at $1, \ldots, z^m$
- This is the following approximation problem:

$$\min_{p \in \mathcal{H}_{\ell,m}^{(h)}} \|p(A)\|, \quad \mathcal{H}_{\ell,m}^{(h)} \equiv \{ z^{m+1} g + h \,:\, h \in \mathcal{P}_m \text{ is given}, \ g \in \mathcal{P}_\ell \}$$

- The special case $m = 0$ and $h = 1$ is called the $(\ell + 1)$st ideal GMRES approximation problem

Uniqueness results

$$(1)\quad \min_{p\in\mathcal{G}^{(g)}_{\ell,m}} \|p(A)\|, \quad \mathcal{G}^{(g)}_{\ell,m} \equiv \left\{ z^{m+1}g + h \,:\, g \in \mathcal{P}_\ell \text{ is given}, \, h \in \mathcal{P}_m \right\}$$

$$(2)\quad \min_{p\in\mathcal{H}^{(h)}_{\ell,m}} \|p(A)\|, \quad \mathcal{H}^{(h)}_{\ell,m} \equiv \left\{ z^{m+1}g + h \,:\, h \in \mathcal{P}_m \text{ is given}, \, g \in \mathcal{P}_\ell \right\}$$

- Uniqueness question is only of interest when value is > 0
- Lemma below gives conditions for this

Lemma (L. & Tichý, 2008)

Let $d(A)$ = degree of A's minimal polynomial.

(1) > 0 for *all* nonzero $g \in \mathcal{P}_\ell$ if and only if $\ell + m + 1 < d(A)$.

If A is nonsingular, the previous are equivalent with

(2) > 0 for *all* nonzero $h \in \mathcal{P}_m$.

Uniqueness results

$$(1) \quad \min_{p \in \mathcal{G}^{(g)}_{\ell,m}} \|p(A)\|, \quad \mathcal{G}^{(g)}_{\ell,m} \equiv \{ z^{m+1} g + h \;:\; g \in \mathcal{P}_\ell \text{ is given, } h \in \mathcal{P}_m \}$$

$$(2) \quad \min_{p \in \mathcal{H}^{(h)}_{\ell,m}} \|p(A)\|, \quad \mathcal{H}^{(h)}_{\ell,m} \equiv \{ z^{m+1} g + h \;:\; h \in \mathcal{P}_m \text{ is given, } g \in \mathcal{P}_\ell \}$$

Theorem (L. & Tichý, 2008)

(1) $A \in \mathbb{C}^{n \times n}$, $\ell \geq 0$, $m \geq 0$, nonzero $g \in \mathcal{P}_\ell$.
If (1) > 0, then the minimizer is unique.

(2) $A \in \mathbb{C}^{n \times n}$ nonsingular, $\ell \geq 0$, $m \geq 0$, nonzero $h \in \mathcal{P}_m$.
If (2) > 0, then the minimizer is unique.

- Recall: $\ell + m + 1 < d(A)$ is sufficient for (1), (2) > 0
- We don't know whether nonsingularity in (2) is necessary

General characterizations

- A more general matrix approximation problem is

  $$\min_{M \in \mathbb{A}} \|B - M\|,$$

  where $\mathbb{A} \equiv \text{span}\{A_1, \ldots, A_m\}$,
  $A_1, \ldots, A_m \in \mathbb{R}^{n \times n}$ lin. indep., $B \in \mathbb{R}^{n \times n} \backslash \mathbb{A}$

- $A_* \in \mathbb{A}$ achieving the minimum is called a
  spectral approximation of B from the subspace $\mathbb{A}$

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Theorem (Ziętak, LAA 1993)

If $R(A_*) = B - A_*$ has an n-fold maximal singular value, then the spectral approximation A_* of B is unique.

General characterizations

Theorem (Lau & Riha, LAA 1981)

A_* is a spectral approximation of B if and only if

there exist k rank-one matrices $w_1 z_1^T, \ldots, w_k z_k^T$,

with $\|w_i\| = \|z_i\| = 1$, $i = 1, \ldots, k$, where $1 \leq k \leq m+1$,

and k positive real numbers $\lambda_1, \ldots, \lambda_k$, $\sum_{i=1}^k \lambda_i = 1$,

such that

$\sum_{i=1}^k \lambda_i w_i^T M z_i = 0, \quad$ for all $M \in \mathbb{A}$ and

$w_i^T R(A_*) z_i = \|R(A_*)\|, \qquad i = 1, \ldots, k.$

General characterizations

- Using the theorem of Lau & Riha we can show:

Lemma (L. & Tichý, 2008)

Let J_λ be the $n \times n$ Jordan block with eigenvalue $\lambda \in \mathbb{R}$.

Then for $m+1 < n$ the $(m+1)$st ideal Arnoldi (or Chebyshev) polynomial of J_λ is given by $(z-\lambda)^{m+1}$.

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- Equivalently, $A_* = J_\lambda^{m+1} - (J_\lambda - \lambda I)^{m+1}$ is the spectral approximation of $B = J_\lambda^{m+1}$ from $\mathbb{A} = \text{span}\{I, J_\lambda, \ldots, J_\lambda^m\}$
- $R(A_*) = J_0^{m+1}$ has $m+1$ singular values equal to zero, and $n-m-1$ singular values equal to one
- Apparently, Ziętak's sufficient condition is not satisfied

General characterizations

- Recall:

  Ideal Arnoldi problem: $\min_{p \in \mathcal{P}_m} \|J_\lambda^{m+1} - p(J_\lambda)\|$

  Ideal GMRES problem: $\min_{p \in \mathcal{P}_m} \|I - J_\lambda p(J_\lambda)\|$

- The ideal Arnoldi polynomial is $(z - \lambda)^{m+1}$

- For $\lambda \neq 0$, we can write

  $$(z - \lambda)^{m+1} \;=\; (-\lambda)^{m+1} \cdot (1 - \lambda^{-1} z)^{m+1}$$

- Rightmost factor has value one at the origin, hence a candidate for solving ideal GMRES problem

- Is the ideal GMRES polynomial a scaled version of the ideal Arnoldi polynomial (at least for J_λ) ?

General characterizations

- **No!** Determination of ideal GMRES polynomials for J_λ is very complicated and intriguing problem
- Analysis in (Tichý, L. & Faber, ETNA 2007)
- $(m+1)$st ideal GMRES polynomial is $(1-\lambda^{-1}z)^{m+1}$

  if and only if $0 \le m+1 < n/2$ and $|\lambda| \ge \varrho_{m+1,n-m-1}^{-1}$

  $\varrho_{k,n}$ = radius of degree k polyhull of $n \times n$ Jordan block (indep. of λ)

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  $\varrho_{k,n}$ = radius of degree k polyhull of $n \times n$ Jordan block (indep. of λ)
- Among the many other cases: n even and $m+1 = n/2$

  If $|\lambda| \leq 2^{-\frac{2}{n}}$, the ideal GMRES polynomial is 1

  If $|\lambda| \geq 2^{-\frac{2}{n}}$, the ideal GMRES polynomial is

  $\frac{2}{4\lambda^n+1} + \frac{4\lambda^n-1}{4\lambda^n+1}(1-\lambda^{-1}z)^{n/2}$
- Obviously, neither 1 nor the above polynomial are scalar multiples of the corresponding ideal Arnoldi polynomial

Summary

- We showed uniqueness of best approximation of $f(A)$ by polynomials in A in the matrix 2-norm (under natural conditions)
- Nontrivial problem for nonnormal A (matrix 2-norm not strictly convex)
- Special case: Ideal Arnoldi approximation problem (aka the Chebyshev polynomials of A)
- We also showed uniqueness for a related problem, a special case of which is the ideal GMRES approximation problem
- Ideal Arnoldi and ideal GMRES only differ by scaling (highest vs. lowest coefficient), but the corresponding polynomials can vastly differ
- Ultimate goal: Fully understand convergence ... a long way to go
- More details in
  P. Tichý, J.L., V. Faber, ETNA 26 (2007), pp. 453–473
  J.L., P. Tichý, *in preparation*, check my website after Householder