On best approximation by polynomials of matrices

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joint work with

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A classical problem of approximation theory

Best approximation by polynomials

$$\min_{p \in \mathcal{P}_k} \max_{z \in \Omega} | f(z) - p(z) |$$

where f is a given (nice) function, $\Omega \subset \mathbb{C}$ is compact, $\mathcal{P}_k$ is the set of polynomials of degree at most k.

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, Remes 1936 . . .]

Matrix function best approximation problem

A different kind of approximation problems involving matrices instead of scalars:

$$\min_{p \in \mathcal{P}_k} \| f(\mathbf{A}) - p(\mathbf{A}) \|, \qquad \mathbf{A} \in \mathbb{C}^{n \times n},$$

$\| \cdot \|$ is the spectral norm (the matrix 2-norm),

f is analytic in neighborhood of $\mathbf{A}$'s spectrum.

- *Does this problem have a unique solution $p_* \in \mathcal{P}_k$?*
- *Can we understand this problem for a particular choice of f?*

If $\mathbf{A}$ is normal, the problem reduces to the frequently studied scalar approximation problem on the spectrum of $\mathbf{A}$,

$$\min_{p \in \mathcal{P}_k} \max_{\lambda \in \Lambda} | f(\lambda) - p(\lambda) | .$$

If $\mathbf{A}$ is non-normal, the problem appears to be a difficult one. Our main interest is the case of non-normal $\mathbf{A}$.

Examples of approximation problems involving matrices

- GMRES ($\mathbf{A}x = b$):

$$\min_{\substack{p \in \mathcal{P}_k \\ p(0)=1}} \| p(\mathbf{A}) b \| \quad \leftrightarrow \quad \min_{\substack{p \in \mathcal{P}_k \\ p(0)=1}} \| p(\mathbf{A}) \| ,$$

- Arnoldi ($\mathbf{A}v = \lambda v$):

$$\min_{p \in \mathcal{M}_k} \| p(\mathbf{A}) v \| \quad \leftrightarrow \quad \min_{p \in \mathcal{M}_k} \| p(\mathbf{A}) \| ,$$

where $\| \cdot \|$ denotes the Euclidean norm (for vectors) or the spectral norm (for matrices), $\mathcal{M}_k$ is the class of monic polynomials of degree k.

[Greenbaum, Trefethen 1994]

General matrix approximation problems

Given

- k linearly independent matrices $\mathbf{A}_1, \ldots, \mathbf{A}_k \in \mathbb{C}^{n \times n}$,
- $\mathbb{A} \equiv \operatorname{span}\{\mathbf{A}_1, \ldots, \mathbf{A}_k\}$,
- $\mathbf{B} \in \mathbb{C}^{n \times n} \backslash \mathbb{A}$,
- $\|\cdot\|$ is a matrix norm.

Consider the best approximation problem

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

This problem has a unique solution if $\|\cdot\|$ is strictly convex.

[see, e.g., Cheney 1966]

The norm $\|\cdot\|$ is *strictly convex* if for all $\mathbf{X}$, $\mathbf{Y}$,

$$\| \mathbf{X} \| = \| \mathbf{Y} \| = 1 , \quad \| \mathbf{X} + \mathbf{Y} \| = 2 \quad \Rightarrow \quad \mathbf{X} = \mathbf{Y} .$$

Spectral norm (matrix 2-norm)

The spectral norm is not strictly convex:

$$\mathbf{X} = \begin{bmatrix} \mathbf{I} & \\ & \varepsilon \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} \mathbf{I} & \\ & \delta \end{bmatrix}, \qquad \varepsilon,\ \delta \in \langle 0, 1 \rangle \,.$$

Then, for each $\varepsilon,\ \delta \in \langle 0, 1 \rangle$, we have

$$\| \mathbf{X} \| = \| \mathbf{Y} \| = 1 \qquad \text{and} \qquad \| \mathbf{X} + \mathbf{Y} \| = 2$$

but if $\varepsilon \neq \delta$, then $\mathbf{X} \neq \mathbf{Y}$.

- Consequently: Best approximation problems in the spectral norm are not guaranteed to have a unique solution.
- Hence, in addition to non-normality of $\mathbf{A}$, we have to deal with a norm that is not strictly convex.

Uniqueness of the solution

$$\min_{p \in \mathcal{P}_k} \| f(\mathbf{A}) - p(\mathbf{A}) \|$$

Reformulation of the problem

Since $f(\mathbf{A}) = p_f(\mathbf{A})$ for a polynomial p_f, we assume that $f(z)$ is a polynomial of degree $k + \ell + 1$ $(k \geq 0,\ \ell \geq 0)$.Then we can write

$$\begin{aligned} f(z) &= z^{k+1}\, g(z) + f_k\, z^k + \ldots + f_1\, z + f_0\,, \\ p(z) &= p_k\, z^k + \ldots + p_1\, z + p_0\,, \end{aligned}$$

where g is a polynomial of degree ℓ, and

$$f(z) - p(z) = z^{k+1}\, g(z) - h_k\, z^k - \ldots - h_1\, z - h_0$$

where $h_j = p_j - f_j$, $j = 0, \ldots, k$. Therefore,

$$f(\mathbf{A}) - p(\mathbf{A}) = \mathbf{A}^{k+1} g(\mathbf{A}) - h(\mathbf{A})\,,$$

where g is a given polynomial of degree ℓ.

Matrix polynomial approximation problems

We consider two matrix approximation problems:

1. $$\min_{h \in \mathcal{P}_k} \| \mathbf{A}^{k+1} g(\mathbf{A}) - h(\mathbf{A}) \|,$$

   where g is a given polynomial of degree ℓ, and

2. $$\min_{g \in \mathcal{P}_\ell} \| \mathbf{A}^{k+1} g(\mathbf{A}) - h(\mathbf{A}) \|,$$

   where h is a given polynomial of degree $\leq k$.

They generalize two particular approximation problems

$$\min_{p \in \mathcal{P}_k} \| \mathbf{A}^{k+1} - p(\mathbf{A}) \|, \qquad \min_{p \in \mathcal{P}_k} \| \mathbf{I} - \mathbf{A}\, p(\mathbf{A}) \|,$$

called ideal Arnoldi and ideal GMRES approximation problems.
[Greenbaum, Trefethen 1994] proved uniqueness of the solution.

Uniqueness results

Theorem [Liesen, T. 2009]

1. Given $g \in \mathcal{P}_\ell$. If the value

$$\min_{h \in \mathcal{P}_k} \| \mathbf{A}^{k+1} g(\mathbf{A}) - h(\mathbf{A}) \| \neq 0\,,$$

the problem has a **unique** minimizer.

2. Let $\mathbf{A}$ be nonsingular and $h \in \mathcal{P}_k$ given. If the value

$$\min_{g \in \mathcal{P}_\ell} \| \mathbf{A}^{k+1} g(\mathbf{A}) - h(\mathbf{A}) \| \neq 0\,,$$

the problem has a **unique** minimizer.
(The nonsingularity assumption cannot be omitted in general [Special thanks to Krystyna Ziętak].)

Idea of the proof

Inspired by [Greenbaum, Trefethen 1994], proof by contradiction.

- $$\mathcal{G} \;\equiv\; \left\{ z^{k+1} g + h \;:\; g \in \mathcal{P}_\ell \text{ is given, } h \in \mathcal{P}_k \right\}.$$
  Let $q_1, q_2 \in \mathcal{G}$ be two different solutions,
  $\| \, q_1(\mathbf{A}) \, \| \;=\; \| \, q_2(\mathbf{A}) \, \| \;=\; C \, .$

- Define the polynomials
  $$q \;\equiv\; \frac{1}{2} \, (q_1 + q_2) \, , \qquad z^{k+1} g \;=\; \overbrace{(q_2 - q_1) \cdot s}^{\widetilde{q}} + r \, ,$$
  $$q_\epsilon \;\equiv\; (1 - \epsilon) \, q + \epsilon \, \widetilde{q}$$
  so that $q_\epsilon \in \mathcal{G} \; \forall \epsilon$.

- Show that, for sufficiently small ϵ,
  $$\| \, q_\epsilon(\mathbf{A}) \, \| \;<\; C \, .$$

Chebyshev polynomials of matrices

$$\min_{p \in \mathcal{M}_k} \| \, p(\mathbf{A}) \, \|$$

Chebyshev polynomials of a compact set

- Chebyshev polynomials on the interval $[-1;1]$ [Chebyshev 1859].
- Generalized by [G. Faber 1920] to the idea of Chebyshev polynomials of Ω, where Ω is a compact set in the complex plane $\mathbb{C}$: These polynomials $T_k^{\Omega}(z)$ solve the problem

$$\min_{p \in \mathcal{M}_k} \max_{z \in \Omega} |\, p(z) \,| \, .$$

Examples:

Ω is an interval, a set of discrete points, the unit disk, etc.

Chebyshev polynomials of matrices

Let $\mathbf{A} \in \mathbb{C}^{n \times n}$ be a general matrix. We consider the problem

$$\min_{p \in \mathcal{M}_k} \| p(\mathbf{A}) \| = \min_{p \in \mathcal{P}_{k-1}} \| \mathbf{A}^k - p(\mathbf{A}) \|,$$

i.e. a matrix function approximation problem for $f(\mathbf{A}) \equiv \mathbf{A}^k$.

- Introduced in [Greenbaum, Trefethen 1994], studied in [Toh PhD thesis 1996], [Toh, Trefethen 1998], [Trefethen, Embree 2005] .
- The unique solution $T_k^{\mathbf{A}}(z) \in \mathcal{M}_k$ is called the kth Chebyshev polynomial of $\mathbf{A}$.
- If $\mathbf{A}$ is normal and $\Omega = \{\lambda_1, \dots, \lambda_n\}$, the problem is solved by Chebyshev polynomials of Ω, $T_k^{\mathbf{A}}(z) = T_k^{\Omega}(z)$.
- If $\mathbf{A}$ is non-normal, it is unclear whether some known scalar approximation problem is solved or not.

Motivation

Example: Let $\lambda \in \mathbb{C}$. Consider an n by n Jordan block $\mathbf{J}_\lambda$. Chebyshev polynomials of $\mathbf{J}_\lambda$ are given by

$$T_k^{\mathbf{J}_\lambda}(z) = (z - \lambda)^k .$$

[Liesen, T. 2009]

- Observation: $T_k^{\mathbf{J}_\lambda}(z) = T_k^{\Omega}(z)$, where Ω is any disk in the complex plane centered at λ. In this example, the Chebyshev polynomial of a matrix (here: $\mathbf{J}_\lambda$) coincides with the Chebyshev polynomial of a compact set (here: disk centered at λ).
- Further such examples would be desirable as well as better understanding general properties of Chebyshev polynomials of matrices.

Shifts and scaling

Theorem [Faber, Liesen, T. 2010]

For $\mathbf{A} \in \mathbb{C}^{n\times n}$ and $\alpha \in \mathbb{C}$ the following hold:

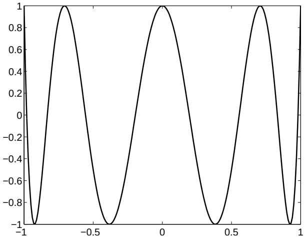
$$\min_{p\in\mathcal{M}_k} \|p(\,\mathbf{A} \,+\, \alpha\,\mathbf{I}\,)\| \;=\; \min_{p\in\mathcal{M}_k} \|p(\mathbf{A})\|\,,$$

$$\min_{p\in\mathcal{M}_k} \|p(\,\alpha\,\mathbf{A}\,)\| \;=\; |\alpha|^k \min_{p\in\mathcal{M}_k} \|p(\mathbf{A})\|\,.$$

- Shift invariance: Not surprising, because the polynomials are normalized at infinity.
- Paper contains explicit relations between the coefficients of $T_k^{\mathbf{A}}(z)$, $T_k^{\mathbf{A}+\alpha\mathbf{I}}(z)$, and $T_k^{\alpha\mathbf{A}}(z)$.

Alternation properties?

- Chebyshev polynomials of compact sets are characterized by alternation properties.
- E.g., $T_k^\Omega(z)$ for $\Omega = [a, b] \subset \mathbb{R}$ has $k+1$ alternations, the maximum absolute value is attained at $k+1$ points.



- It works also for Chebyshev polynomials of diagonal matrices.
- Is there an analogy, e.g., for block diagonal matrices?

Chebyshev polynomials of block diagonal matrices

$$\mathbf{A} \;=\; \mathrm{diag}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4)\,,$$

$$p(\mathbf{A}) \;=\; \begin{bmatrix} p(\mathbf{A}_1) & & & \\ & p(\mathbf{A}_2) & & \\ & & p(\mathbf{A}_3) & \\ & & & p(\mathbf{A}_4) \end{bmatrix},$$

$$\|\, p(\mathbf{A})\,\| \;=\; \max\left(\|\, p(\mathbf{A}_1)\,\|, \ldots, \|\, p(\mathbf{A}_4)\,\|\right)\;.$$

Is the norm $\|\, T_k^{\mathbf{A}}(\mathbf{A})\,\|$ attained on several blocks for $p = T_k^{\mathbf{A}}$?

An alternation theorem for block diagonal matrices

Theorem [Faber, Liesen, T. 2010]

Consider a block-diagonal matrix $\mathbf{A} = \mathrm{diag}(\mathbf{A}_1, \ldots, \mathbf{A}_h)$ where $d(\mathbf{A}_j) \le m$, $j = 1, \ldots, h$. Then the matrix

$$T_k^{\mathbf{A}}(\mathbf{A}) = \mathrm{diag}(\mathbf{B}_1, \ldots, \mathbf{B}_h)\,, \qquad k < d(\mathbf{A})\,,$$

has at least $\lfloor k/m + 1 \rfloor$ diagonal blocks $\mathbf{B}_j$ such that

$$\| \, \mathbf{B}_j \, \| \; = \; \| \, T_k^{\mathbf{A}}(\mathbf{A}) \, \| \, .$$

Example: If $\mathbf{A} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n) \in \mathbb{C}^{n \times n}$, then $T_k^{\mathbf{A}}(\mathbf{A})$ has at least $k+1$ diagonal entries with the same maximal absolute value.

Experiment

Consider a block diagonal matrix

$$\mathbf{A} \;=\; \mathrm{diag}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4)$$

where each $\mathbf{A}_j = \mathbf{J}_{\lambda_j}$ is a 3×3 Jordan block. The four eigenvalues are $-3, -0.5, 0.5, 0.75$, and $m = d(\mathbf{A}_j) = 3$.

k	$\|T_k^{\mathbf{A}}(\mathbf{A}_1)\|$	$\|T_k^{\mathbf{A}}(\mathbf{A}_2)\|$	$\|T_k^{\mathbf{A}}(\mathbf{A}_3)\|$	$\|T_k^{\mathbf{A}}(\mathbf{A}_4)\|$
1	2.6396	1.4620	2.3970	2.6396
2	4.1555	4.1555	3.6828	4.1555
3	9.0629	5.6303	7.6858	9.0629
4	14.0251	14.0251	11.8397	14.0251
5	22.3872	20.7801	17.6382	22.3872
6	22.6857	22.6857	20.3948	22.6857
7	26.3190	26.3190	26.3190	26.3190

Chebyshev polynomials of particular matrices

$$\mathbf{A} = \begin{bmatrix} \mathbf{D} & & & \\ & \mathbf{D} & & \\ & & \ddots & \\ & & & \mathbf{D} \end{bmatrix} + \begin{bmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix},$$

where $\mathbf{D} = \mathrm{diag}(\lambda_1, \ldots, \lambda_\ell)$, and $\lambda_1, \ldots, \lambda_\ell \in \mathbb{C}$ are given.

[Reichel, Trefethen 1992]

- Let $p(z) = (z - \lambda_1) \cdot \cdots \cdot (z - \lambda_\ell)$,
- define the lemniscatic region $\mathcal{L}(p) \equiv \{z \in \mathbb{C} \,:\, |p(z)| \leq 1\}$.

Theorem [Faber, Liesen, T. 2010]

For $m = 1, 2, \ldots, h-1$ it holds that

$$T_{\ell \cdot m}^{\mathcal{L}(p)}(z) = T_{\ell \cdot m}^{\mathbf{A}}(z), \quad \max_{z \in \mathcal{L}(p)} |T_{\ell \cdot m}^{\mathcal{L}(p)}(z)| = \| T_{\ell \cdot m}^{\mathbf{A}}(\mathbf{A}) \|.$$

Idea of the proof

- Show that $T_{\ell \cdot m}^{\mathbf{A}}(z) = (z - \lambda_1)^m \cdot \cdots \cdot (z - \lambda_\ell)^m$.
- Use the result of [Kamo, Borodin 1994], [Fischer, Peherstorfer 2001].

Chebyshev polynomials of Ω and Ψ [Kamo, Borodin 1994]

Let T_k^{Ω} be the kth Chebyshev polynomial of the infinite compact set $\Omega \subset \mathbb{C}$, let $p(z)$ be a monic polynomial of degree ℓ, and let

$$\Psi \equiv p^{-1}(\Omega) = \{z \in \mathbb{C} : p(z) \in \Omega\}$$

be the pre-image of Ω under the polynomial map p. Then

$$T_{k \cdot \ell}^{\Psi}(z) = T_k^{\Omega}(p(z)).$$

Summary

- For a general (non-normal) $\mathbf{A}$, we showed uniqueness of the matrix best approximation problem in the spectral norm,

$$\min_{p \in \mathcal{P}_k} \| f(\mathbf{A}) - p(\mathbf{A}) \| .$$

- We considered Chebyshev polynomials of matrices and showed some general properties (shifts and scaling, alternation).

- We found explicit formulas of Chebyshev polynomials of certain classes of matrices and explored the connection to the Chebyshev polynomials of sets in the complex plane.

- **Open question:** Is it possible to translate the problem

$$\min_{p \in \mathcal{M}_k} \| p(\mathbf{A}) \|$$

into the language of classical approximation problems?

Related papers

- A. Greenbaum and N. L. Trefethen, [GMRES/CR and Arnoldi/Lanczos as matrix approximation problems, SISC, 15 (1994), no. 2, pp. 359–368]
- K.-C. Toh and L. N. Trefethen, [The Chebyshev polynomials of a matrix, SIMAX, 20 (1998), pp. 400–419.]
- J. Liesen and P. Tichý, [On best approximations of polynomials in matrices in the matrix 2-norm, SIMAX, 31 (2009), pp. 853–863.]
- V. Faber, J. Liesen and P. Tichý, [On Chebyshev polynomials of matrices, SIMAX, 31 (2010), pp. 2205–2221.]

Software

- S. Benson, Y. Ye, and X. Zhang, [DSDP – Software for semidefinite programming, v. 5.8, January 2006.]
  `http://www.mcs.anl.gov/hs/software/DSDP/`
- K. C. Toh, M. J. Todd, and R. H. Tütüncü, [SDPT3 4.0 – a Matlab software package for semidefinite programming, 2006.]
  `http://www.math.nus.edu.sg/~mattohkc/sdpt3.html`

Thank you for your attention!