Matrix functions and their approximation using Krylov subspaces

Matrixfunktionen und ihre Approximation in Krylov-Unterräumen

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Overview

What is a matrix function?

In general...

$f : D \rightarrow R$, from a domain $D \subseteq \mathbb{C}^{k \times l}$ to some range area $R \subseteq \mathbb{C}^{m \times n}$.

$f : D \rightarrow R$	$m = n = 1$	$m = 1$ or $n = 1$	m, n arbitrary
$k = l = 1$	scalar function of a single variable	vector function of a single variable	matrix-valued f. of a single variable
$k = 1$ or $l = 1$	scalar function of a vector	vector field	matrix function of a vector
k, l arbitrary	scalar function	vector function	matrix function

Tabelle: Classification of matrix functions

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Definition 1
Polynomial matrix functions

Given $A \in \mathbb{C}^{N\times N}$ and $p(z)$ of degree m with complex coefficients, i.e. $p(z) = \alpha_m z^m + \alpha_{m-1} z^{m-1} + \cdots + \alpha_0$. Notation: $p \in \mathcal{P}_m(z)$.
Since the powers $I, A, A^2, \ldots$ exist we may give the following

Definition

$$p(A) := \alpha_m A^m + \alpha_{m-1} A^{m-1} + \cdots + \alpha_0 I \in \mathbb{C}^{N\times N}. \qquad \text{(D1)}$$

p is a polynomial matrix function.

We no longer have to distinguish between $\mathcal{P}_m(z)$ and the set of polynomials in A of degree $\leq m$. We simply write $\mathcal{P}_m$.

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Properties of polynomials in matrices

Lemma

Let $p \in \mathcal{P}_m$ *be a polynomial,* $A \in \mathbb{C}^{N \times N}$ *and* $A = TJT^{-1}$ *where* $J = \mathrm{diag}(J_1, J_2, \ldots, J_k)$ *is block-diagonal. Then*

1. $p(A) = Tp(J)T^{-1}$,
2. $p(J) = \mathrm{diag}\left(p(J_1), p(J_2), \ldots, p(J_k)\right)$,
3. *If* $A\mathbf{v} = \lambda\mathbf{v}$ *then* $p(A)\mathbf{v} = p(\lambda)\mathbf{v}$,
4. *Given another polynomial* $\tilde{p} \in \mathcal{P}_{\tilde{m}}$, *then* $p(A)\tilde{p}(A) = \tilde{p}(A)p(A)$.

The Jordan canonical form

Every square matrix A is similar to a block-diagonal *Jordan matrix* $J = \text{diag}(J_1, J_2, \ldots, J_k)$, where each *Jordan block* $J_j = J_j(\lambda_j) \in \mathbb{C}^{n_j \times n_j}$ has entries λ_j on the main diagonal and 'ones' on the first upper diagonal ($j = 1, 2, \ldots, k$):

$$J_j(\lambda_j) := \text{toep}(\underline{\lambda_j}, 1) = \begin{bmatrix} \lambda_j & 1 & & & \\ & \lambda_j & 1 & & \\ & & \ddots & \ddots & \\ & & & \lambda_j & 1 \\ & & & & \lambda_j \end{bmatrix}.$$

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Let $f(z) := z^m$ be the *monomial of degree m*.

Then

$$\begin{aligned} f(J) &= \text{toep}\left(\underline{\lambda^m}, m\lambda^{m-1}, \ldots, \binom{m}{i}\lambda^{m-i}, \ldots, \binom{m}{\min\{m, n-1\}}\lambda^{m-\min\{m,n-1\}}\right) \\ &= \text{toep}\left(\underline{f(\lambda)}, f'(\lambda), \ldots, \frac{f^{(i)}(\lambda)}{i!}, \ldots, \frac{f^{(\min\{m,n-1\})}(\lambda)}{\min\{m, n-1\}!}\right) \\ &= \text{toep}\left(\underline{f(\lambda)}, f'(\lambda), \ldots, \frac{f^{(i)}(\lambda)}{i!}, \ldots, \frac{f^{(n-1)}(\lambda)}{(n-1)!}\right). \end{aligned}$$

$f(J)$ is already defined if $f, f', \ldots, f^{(n-1)}$ exist in an open subset of $\mathbb{C}$ containing λ.

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Definition 2

Definition

Given $A \in \mathbb{C}^{N\times N}$ with a Jordan canonical form $J = T^{-1}AT$, where $J = \text{diag}(J_1, J_2, \ldots, J_k)$ and $J_j = J_j(\lambda_j) \in \mathbb{C}^{n_j \times n_j}$ $(j = 1, 2, \ldots, k)$. Let U be an open subset of $\mathbb{C}$ such that $\{\lambda_1, \lambda_2, \ldots, \lambda_k\} \subseteq U$. Let f be a function $f : U \subseteq D \to \mathbb{C}$.
Then f is defined on A if $f(\lambda_j), f'(\lambda_j), \ldots, f^{(d_{\lambda_j}-1)}(\lambda_j)$ exist, $d_{\lambda_j} := \max\{n_i \ : \ i = 1, 2, \ldots, k \text{ and } \lambda_i = \lambda_j\}$.
We set

$$f(A) := T\,\text{diag}\,(f(J_1), f(J_2), \ldots, f(J_k))\,T^{-1}, \tag{D2}$$

where

$$f(J_j) := \text{toep}\left(\underline{f(\lambda_j)}, f'(\lambda_j), \ldots, \frac{f^{(i)}(\lambda_j)}{i!}, \ldots, \frac{f^{(n_j-1)}(\lambda_j)}{(n_j-1)!}\right).$$

Remarks

1. This definition is independent of the choice of J and T. Hence, $f(A)$ is uniquely determined.
2. d_λ is the size of the largest Jordan block to eigenvalue λ. By $\Lambda(A) := \{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ we denote the *set of the eigenvalues of* A. The minimal polynomial of A is defined as

$$\psi_A(z) := \prod_{\lambda \in \Lambda(A)} (z - \lambda)^{d_\lambda}.$$

3. For all the λ_j being pairwise distinct,

$$\psi_A(z) = \prod_{j=1}^{k} (z - \lambda_j)^{n_j} = \chi_A(z),$$

   where $\chi_A(z)$ is the characteristic polynomial of A. Matrices with $\psi_A = \chi_A$ are called nonderogatory.
4. For all $p \in \mathcal{P}_m$ there holds (D1) $=$ (D2).

Polynomial interpolation

Theorem

1. *There holds*
$$f(A) = p(A)$$
if and only if
$$f^{(i)}(\lambda) = p^{(i)}(\lambda), \quad \lambda \in \Lambda(A), \; i = 0, 1, \ldots, d_\lambda - 1. \qquad \text{(HIP)}$$
These are $d := \deg(\psi_A)$ *interpolation conditions to* p.
2. *There exists a uniquely determined polynomial* $\hat{p} \in \mathcal{P}_{d-1}$ *that satisfies* (HIP). $\hat{p}$ *is the Hermite interpolation polynomial.*
3. *Assumed* p *is another polynomial that satisfies* (HIP). *Then*
$$p(z) = \hat{p}(z) + \psi_A(z) h(z)$$
for some polynomial $h(z)$ *and* ψ_A *the minimal polynomial of* A.

Example (1)

Let $A = [\alpha]$. Then $\psi_A(z) = z - \alpha$ and $\deg(\psi_A) = 1$, the most. Therefore $f(A) = \hat{p}(A)$ with $\deg(\hat{p}) = 0$, namely $\hat{p}(A) = f(\alpha)I$. This is a degenerated case.

Example (2)

Calculate $\hat{p}$ for $f(z) = \exp(z)$ and

$$A = \begin{bmatrix} 1 & 6 & 4 & 0 & -8 \\ 0 & 7 & 4 & 0 & -8 \\ 2 & 0 & -1 & -1 & -2 \\ 2 & -4 & 0 & 0 & 2 \\ 2 & 6 & 3 & -1 & -9 \end{bmatrix} \Rightarrow J = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

$$\Rightarrow \psi_A(z) = (z-1)(z+1)^2 z$$

$$\begin{aligned} \Rightarrow p(\lambda_1) = p(1) &\overset{!}{=} \exp(1) = \mathrm{e}, \\ p(\lambda_2) = p(-1) &\overset{!}{=} \exp(-1) = 1/\mathrm{e}, \\ p'(\lambda_2) = p'(-1) &\overset{!}{=} \exp(-1) = 1/\mathrm{e}, \\ p(\lambda_3) = p(0) &\overset{!}{=} \exp(0) = 1. \end{aligned}$$

A solution is $p(z) = \frac{\mathrm{e}^2-4\mathrm{e}+5}{4\mathrm{e}} z^3 + \frac{(\mathrm{e}-1)^2}{2\mathrm{e}} z^2 + \frac{\mathrm{e}^2+4\mathrm{e}-7}{4\mathrm{e}} z + 1$ and there holds $p(A) = f(A) = \exp(A)$. Because of $\deg(p) < \deg(\psi_A)$, $p = \hat{p}$.

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Remarks

1. Every function $f(\cdot)$ that is defined on the spectrum of $A \in \mathbb{C}^{N\times N}$ can be represented pointwise (i.e., for a concrete A) as a polynomial $p(A) \in \mathcal{P}_{d-1}$, $d = \deg(\psi_A)$. Or we might say, f is a field of polynomials.
2. $f(A)$ depends only on the values of $f, f', \dots$ on $\Lambda(A)$. Thus $f(A)$ and $f(B)$ have the same polynomial representation for A and B having the same minimal polynomial (e.g. similar matrices).
3. If all Jordan blocks have size 1×1 and thus J is a diagonal matrix (e.g. for normal A) then (HIP) reduces to a Lagrange interpolation problem:

$$f(\lambda) = p(\lambda), \quad \lambda \in \Lambda(A). \tag{LIP}$$

The components of A

Let again $\psi_A(z) = \prod_{\lambda \in \Lambda(A)} (z - \lambda)^{d_\lambda}$ denote the minimal polynomial of A, $d = \deg(\psi_A)$.

Definition

Define $\mathcal{H} := \{\varphi_{\lambda,i}(z) \in \mathcal{P}_{d-1} \;:\; \lambda \in \Lambda(A),\ i = 0, 1, \ldots, d_\lambda - 1\}$ such that

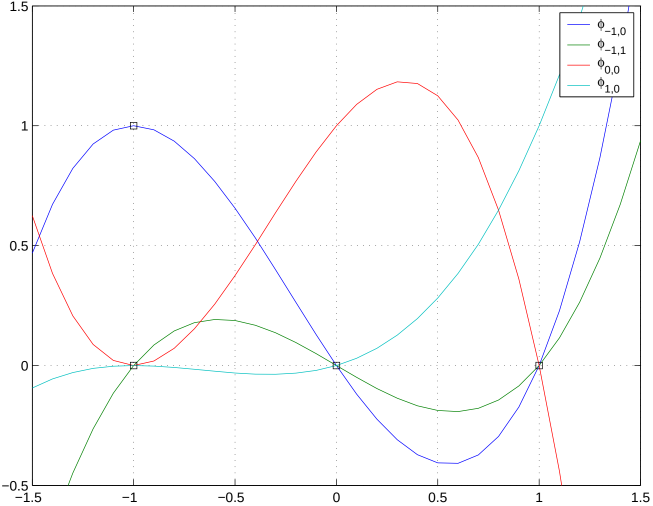
$$\varphi_{\lambda,i}^{(\nu)}(z) = \begin{cases} 1, & z = \lambda,\ i = \nu; \\ 0, & \text{otherwise}, \end{cases}$$

for all $z \in \Lambda(A)$. $\mathcal{H}$ is the Hermite basis of $\mathcal{P}_{d-1}$ with respect to ψ_A.

(It has to be shown that all the $\varphi_{\lambda,i}$ are linearly independent.)

The components of A

Hermite basis for example **(2)**



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The components $C_{\lambda,i}$ of A are defined as

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Lemma

1. $\{C_{\lambda,i} \ : \ \lambda \in \Lambda(A); \ i = 0, 1, \ldots, d_\lambda - 1\}$ *is a set of linearly independent matrices.*
2. *spectral resolution of A for f:*

$$f(A) = \sum_{\lambda \in \Lambda(A)} \sum_{i=0}^{d_\lambda - 1} f^{(i)}(\lambda) C_{\lambda,i} \ , \qquad \text{(SR)}$$

3. $\sum_{\lambda \in \Lambda(A)} C_{\lambda,0} = I$ *and* $\sum_{\lambda \in \Lambda(A)} \lambda C_{\lambda,0} + C_{\lambda,1} = A$,
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Cauchy integral formula

Let $f(z)$ be analytic in a domain G and let γ be a closed path contained in G. Then the Cauchy theorem asserts

$$f^{(i)}(z) = \frac{i!}{2\pi \mathbb{i}} \int_{\gamma} \frac{f(\zeta)}{(\zeta - z)^{i+1}} d\zeta \qquad \text{(CIF)}$$

for any $z \in G$, $\text{wind}_z(\gamma) = 1$ and $i = 0, 1, \ldots$

The resolvent of A

Lemma

Let $A \in \mathbb{C}^{N\times N}$ and $\zeta \notin \Lambda(A)$, $C_{\lambda,i}$ the components of A. There holds

$$R_\zeta(A) := (\zeta I - A)^{-1} = \sum_{\lambda\in\Lambda(A)} \sum_{i=0}^{d_\lambda - 1} \frac{i!}{(\zeta-\lambda)^{i+1}} C_{\lambda,i}.$$

$R_\zeta(A)$ is the resolvent of A to ζ.

Beweis.

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The resolvent of A

Lemma

Let $A \in \mathbb{C}^{N \times N}$ and $\zeta \notin \Lambda(A)$, $C_{\lambda,i}$ the components of A. There holds

$$R_\zeta(A) := (\zeta I - A)^{-1} = \sum_{\lambda \in \Lambda(A)} \sum_{i=0}^{d_\lambda - 1} \frac{i!}{(\zeta - \lambda)^{i+1}} C_{\lambda,i}.$$

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Theorem

Let $A \in \mathbb{C}^{N\times N}$, γ *be a closed path surrounding all* $\lambda \in \Lambda(A)$ *once, f analytic in* $\mathrm{int}(\gamma)$ *and extending continuously to it, then*

$$f(A) = \frac{1}{2\pi\mathbb{i}}\int_\gamma f(\zeta)(\zeta I - A)^{-1} d\zeta = \frac{1}{2\pi\mathbb{i}}\int_\gamma f(\zeta) R_\zeta(A) d\zeta. \tag{D3}$$

Beweis.

By multiplying both sides of $R_\zeta(A)$ by $f(\zeta)/(2\pi\mathbb{i})$ and integrating along γ we get

$$\begin{aligned}
\frac{1}{2\pi\mathbb{i}}\int_\gamma f(\zeta)(\zeta I - A)^{-1} d\zeta &= \int_\gamma \frac{f(\zeta)}{2\pi\mathbb{i}} \sum_{\lambda\in\Lambda(A)} \sum_{i=0}^{d_\lambda - 1} \frac{i!}{(\zeta-\lambda)^{(i+1)}} C_{\lambda,i}\, d\zeta \\
&= \sum_{\lambda\in\Lambda(A)} \sum_{i=0}^{d_\lambda - 1} \left(\frac{i!}{2\pi\mathbb{i}} \int_\gamma \frac{f(\zeta)}{(\zeta-\lambda)^{i+1}} d\zeta \right) C_{\lambda,i} \\
&\stackrel{\text{(CIF)}}{=} \sum_{\lambda\in\Lambda(A)} \sum_{i=0}^{d_\lambda - 1} f^{(i)}(\lambda) C_{\lambda,i} \\
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Power series

Definition

Let f be analytic in an open set $U \ni 0$ and let $f(z) = \sum_{j=0}^{\infty} \alpha_j z^j$ be the Taylor expansion of f in 0 with convergence radius $\tau \in (0, \infty]$. Then $f(A)$ is defined for every A with $\sigma(A) < \tau$ and there holds

$$f(A) = \sum_{j=0}^{\infty} \alpha_j A^j = \lim_{m\to\infty} \sum_{j=0}^{m} \alpha_j A^j. \qquad \text{(D4)}$$

$\sum_{j=0}^{\infty} \alpha_j A^j$ converges $\Leftrightarrow \forall \varepsilon > 0\ \exists n_\varepsilon \in \mathbb{N}_0 : \left\| \sum_{j=n_\varepsilon}^{\infty} \alpha_j A^j \right\| < \varepsilon$.
Assumed f has convergence radius τ (i.e., $f(z) < \infty$ for $|z| < \tau$).
Then $\left\| \sum_{j=n_\varepsilon}^{\infty} \alpha_j A^j \right\| \leq \sum_{j=n_\varepsilon}^{\infty} |\alpha_j| \|A\|^j$, thus $\sigma(A) \leq \|A\| < \tau$ is a sufficient criteria for convergence of $\sum_{j=0}^{\infty} \alpha_j A^j$ (Taylor series converge absolutely!).

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Power series

Example

Let $f(z) = \exp(z)$. f has convergence radius $\tau = \infty$. Thus $f(A)$ is defined for every $A \in \mathbb{C}^{N\times N}$ and there holds

$$f(A) = \exp(A) = \sum_{j=0}^{\infty} \frac{A^j}{j!}.$$

Some facts

Because of

$$\begin{aligned} f(z) = \alpha \in \mathbb{C} \quad &\Rightarrow \quad f(A) = \alpha I, \\ f(z) = z \quad &\Rightarrow \quad f(A) = A, \\ f(z) = g(z) + h(z) \quad &\Rightarrow \quad f(A) = g(A) + h(A) \\ f(z) = g(z)h(z) \quad &\Rightarrow \quad f(A) = g(A)h(A), \end{aligned}$$

any rational identity in scalar functions of a complex variable will be fulfilled by the corresponding matrix function.

Examples

- $\sin^2(A) + \cos^2(A) = I$,
- $\exp(\mathrm{i}A) = \cos(A) + \mathrm{i}\sin(A)$,
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Krylov subspaces

Definition

Problem

Given $A \in \mathbb{C}^{N \times N}$, $\mathbf{b} \in \mathbb{C}^N$, f defined on A.
Calculate $f(A)\mathbf{b}$!

Definition

The m-th Krylov (sub)space of A and $\mathbf{b}$ is defined by

$$\mathcal{K}_m(A, \mathbf{b}) = \mathcal{K}_m := \operatorname{span}\{\mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \ldots, A^{m-1}\mathbf{b}\}.$$

Lemma

There exists an index $L = L(A, \mathbf{b}) \le \deg(\psi_A)$ *such that*

$$\mathcal{K}_1(A, \mathbf{b}) \subsetneq \mathcal{K}_2(A, \mathbf{b}) \subsetneq \ldots \subsetneq \mathcal{K}_L(A, \mathbf{b}) = \mathcal{K}_{L+1}(A, \mathbf{b}) = \ldots$$

Moreover $f(A)\mathbf{b} \in \mathcal{K}_L$.

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The Arnoldi process

Task: Generate an orthonormal basis of $\mathcal{K}_m$, $m \leq L$.

Algorithm

$\mathbf{v}_1 := \mathbf{b}/\|\mathbf{b}\|$
`for` $j = 2, 3, \ldots, m$
$\quad \mathbf{w}_j := A\mathbf{v}_{j-1}$
$\quad \tilde{\mathbf{v}}_j := \mathbf{w}_j - \sum_{i=1}^{j-1} (\mathbf{w}_j, \mathbf{v}_i)\mathbf{v}_i$
$\quad \mathbf{v}_j := \tilde{\mathbf{v}}_j / \|\tilde{\mathbf{v}}_j\|$
`end`

Output: A matrix $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m] \in \mathbb{C}^{N \times m}$. An unreduced upper Hessenberg matrix $H_m \in \mathbb{C}^{m \times m}$.

Arnoldi decomposition

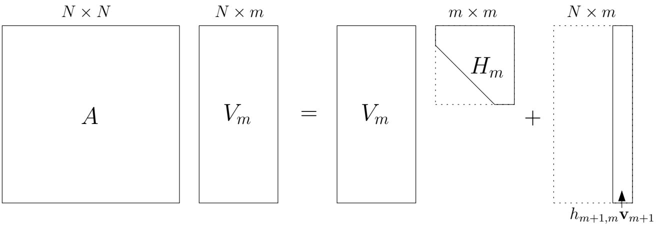
Theorem

Let $m < L$. There exist orthonormal vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m, \mathbf{v}_{m+1} \in \mathbb{C}^N$ and an unreduced upper Hessenberg matrix $H_m \in \mathbb{C}^{m\times m}$, such that

$$AV_m = V_m H_m + h_{m+1,m}\mathbf{v}_{m+1}\mathbf{e}_m^T,$$

where $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]$ and $h_{m+1,m} \in \mathbb{C}$. For $m = L$ there holds

$$AV_m = V_m H_m.$$



Arnoldi approximation

Lemma

Let $p(z) = \alpha_m z^m + \cdots + \alpha_1 z + \alpha_0 \in \mathcal{P}_m$ *be a polynomial,* $1 \leq m < L$. *Then there holds*

$$p(A)\mathbf{b} = \|\mathbf{b}\| V_m p(H_m)\mathbf{e}_1 + \|\mathbf{b}\| \alpha_m \gamma_m \mathbf{v}_{m+1},$$

where $\gamma_m = \prod_{j=1}^{m} h_{j+1,j}$. *In particular, for* $p \in \mathcal{P}_{m-1}$*, there holds*

$$p(A)\mathbf{b} = \|\mathbf{b}\| V_m p(H_m)\mathbf{e}_1.$$

Definition

We define the Arnoldi approximation from $\mathcal{K}_m(A, \mathbf{b})$ to $f(A)\mathbf{b}$ as $\mathbf{f}_m := \|\mathbf{b}\| V_m f(H_m)\mathbf{e}_1$.

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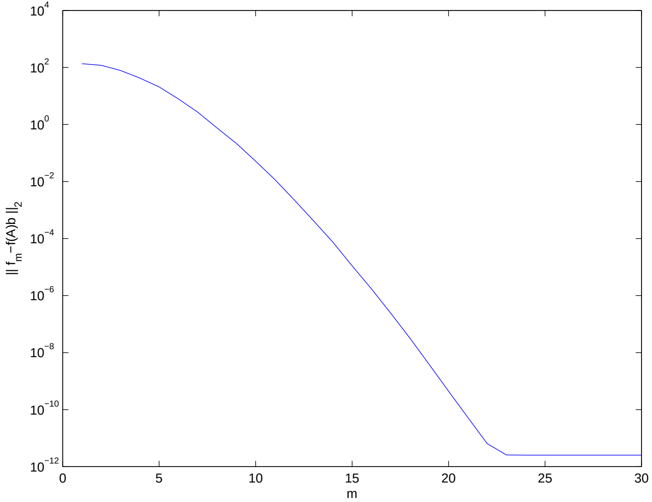
$f(z) = exp(z)$, $N = 500$, A sparse with $nz = 3106$ (1.25 percent) and $(0, 1)$-normal-distributed entries. b full with $(0, 1)$-normal-distributed entries.



Execution speed: `expm(A)*b` $\approx 2.2840s$, $\mathbf{f}_{25} \approx 0.0900s$.

Krylov subspace methods?

Why to use them?

- `expm(A), logm(A), funm(A,@sin), etc.` operate only on full matrices,
- Arnoldi methods involve only matrix-vector-products $A\mathbf{b}$,
- speed and storage matters.

Why to seek for convergence estimates?

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How good are Krylov approximations?

Remember: $\mathbf{f}_m = \|\mathbf{b}\| V_m f(H_m)\mathbf{e}_1$.

The best approximation (for the $\|\cdot\|_2$-norm) $\mathbf{f}_m^*$ to $f(A)\mathbf{b}$ from $\mathcal{K}_m(A,\mathbf{b})$ is its orthogonal projection, i.e.

$$\mathbf{f}_m^* = V_m V_m^H f(A)\mathbf{b} = \|\mathbf{b}\| V_m [V_m^H f(A) V_m]\mathbf{e}_1$$

which is computationally unfeasible. Another representation of $\mathbf{f}_m^*$ is

$$\begin{aligned}\mathbf{f}_m^* &= \|\mathbf{b}\| V_m [V_m^H f(V_L H_L V_L^H) V_m]\mathbf{e}_1 = \|\mathbf{b}\| V_m [V_m^H V_L f(H_L) V_L^H V_m]\mathbf{e}_1 \\ &= \|\mathbf{b}\| V_m [I_m\ O] f(H_L) [I_m\ O]^T \mathbf{e}_1 = \|\mathbf{b}\| [V_m\ O] f(H_L)\mathbf{e}_1.\end{aligned}$$

Furthermore

$$\mathbf{f}_m = \|\mathbf{b}\| V_m f(V_m^H A V_m)\mathbf{e}_1 = \|\mathbf{b}\| V_m f([I_m\ O] H_L)\mathbf{e}_1.$$

How good are Krylov approximations?

Lemma

Let A be normal and Ω a compact set, $\Lambda(A) \cup \Lambda(H_m) \subseteq \Omega$. Then

$$\|f(A)\mathbf{b} - \mathbf{f}_m\|_2 \leq 2\|\mathbf{b}\| \min_{p \in \mathcal{P}_{m-1}} \max_{\lambda \in \Omega} |f(\lambda) - p(\lambda)|.$$

To be continued...

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To be continued...

Weiterführende Literatur I

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