Numerical methods for matrix functions

SF2524 - Matrix Computations for Large-scale Systems

Lecture 15: Krylov methods for matrix functions

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$$(A-zI)^{-1}b \qquad (\star)$$

Note: $(\star)$ is a shifted linear system of equations:

$$(A-zI)x = b.$$

We will solve the shifted linear system using an Arnoldi method.

The rest of this lecture

1. Arnoldi's method for shifted systems
2. GMRES-variant (FOM) for shifted systems
3. Use Cauchy definition $\Rightarrow$ Krylov method for matrix functions
4. Application to exponential integrators

Shift invariance of Krylov subspaces

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Recall: $W = VR$ and R non-singular and $w_1, \ldots, w_m$ linear independent
$\Rightarrow \text{span}(w_1, \ldots, w_m) = \text{span}(v_1, \ldots, v_m)$ * Sketch on board *

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Lemma

Suppose $Q_m \in \mathbb{C}^{n\times m}$, $\underline{H}_m \in \mathbb{C}^{(m+1)\times m}$ is an Arnoldi factorization ($\star$) associated with $\mathcal{K}_m(A, b)$. Then, for any $\sigma \in \mathbb{C}$, $Q_m \in \mathbb{C}^{n\times m}$ and $\underline{H}_m - \sigma I_{m+1,m}$ is an Arnoldi factorization associated with $\mathcal{K}_m(A - \sigma I, b)$,

$$(A - \sigma I)Q_m = Q_{m+1}(\underline{H}_m - \sigma I_{m+1,m}). \tag{$\star\star$}$$

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where

$$I_{m+1,m} = \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{(m+1)\times m}.$$

FOM - almost GMRES for linear system

We now wish to solve linear systems:

$$Cx = b$$

(where we later set $C = A - \sigma I$.)

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Full Orthogonalization Method (FOM)

- Compute an Arnoldi factorization $AQ_n = Q_{n+1}\underline{H}_n$
- Compute `z=H(1:n,1:n)\e1` $\Leftrightarrow z = H_n^{-1}e_1$
- Compute approximation $\tilde{x} = Q_n z \|b\|$

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Relationship with GMRES

- GMRES corresponds to $(AQ_n)^T(A\tilde{x} - b) = 0$ (lecture 8)
- FOM corresponds to $Q_n^T(A\tilde{x} - b) = 0$

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FOM for shifted systems

1. Compute an Arnoldi factorization $AQ_n = Q_{n+1}\underline{H}_n$ from (A, b)
2. Compute `zs=(H(1:n,1:n)-`σ`I)\e1` $\Leftrightarrow z_\sigma = (H_n - \sigma I)^{-1}e_1$
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3. Compute approximation $\tilde{x}_{\sigma} = Q_n z_{\sigma}\|b\|$

Note: Step 1 is independent of σ and the Step 2-3 can be done for many σ without carrying out Arnoldi method:

$$x_{\sigma} \approx \tilde{x}_{\sigma} = Q_n(H_n - \sigma I)^{-1}e_1\|b\|.$$

* On black board *

Cauchy integral definition and use FOM-approximation:

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* Video [link] *

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Theorem

Suppose $A \in \mathbb{C}^{n\times n}$ is a normal matrix and suppose $\Omega \subset \mathbb{C}$ is a convex compact set such that $\lambda(A) \subset \Omega$. Let f_m be the Krylov approximation of $f(A)b$. Then,

$$\|f(A)b - f_m\| \leq 2\|b\| \min_{p \in P_{m-1}} \max_{z\in\Omega} |f(z) - p(z)|.$$

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* Examples *

Application to exponential integrators
PDF lecture notes 4.4.3

We already know that the initial value problem

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has the solution

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- Look at linear inhomogeneous ODE
- Use to approximate nonlinear ODE

Lemma (Explicit solution linear inhomogeneous ODE)

In the special case of a linear inhomogeneous ODE with right-hand side $g(y) = g_1(y) := Ay + b$, *and*

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The matrix function φ is called a φ-function

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* Julia: plot phi-function *
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* Proof (if time) *

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Let $0 = t_0 < t_1 < \cdots < t_N$. The *forward Euler exponential integrator* generate the approximations $y_k \approx y(t_k)$, $k =, \ldots, N$ defined as

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Properties:

- Exact for the linear inhomogeneous case (1), and one step can be proven to be second order in h in the general case.
- Requires the computation of $\varphi(h_k A_k) g(y_k)$ in every step. Suitable to be used with matrix functions.

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Trade-off of time-step h

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More elaborate example in Lecture notes PDF.

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SF2526 *"Numerics for data science"* [link]

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  ⇒ Solve many problems as preparation:
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Good luck on the exam

Please fill out the course evaluation (later)