

# On Krylov subspace approximations to the matrix exponential operator

Purple team

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# Introduction

- Approximation of  $\exp(\tau A)v$  using Krylov methods,  $A$  big matrix,  $\tau$  step size
- Error bounds for Arnoldi and Lanczos algorithms
- Faster convergence than  $(I - \tau A)^{-1}v$  for stiff ODE problems, new integration methods
- Bound  $\frac{\|\tau A\|^m}{m!}$ , superlinear convergence for  $m \gg \|\tau A\|$
- Better behaviour for matrix classes: HND, skew-Hermitian, dependent on eigenvalues distribution

# Matrix function definition

- $AV_m = V_m H_m + h_{m+1,m} v_m e_m^T, H_m = V_m^* A V_m$
- $q_{m-1}(A)v = V_m q_{m-1}(H_m)e_1 \implies (\lambda I - A)^{-1}v \approx V_m(\lambda I - H_m)^{-1}e_1$
- Numerical range  $\mathcal{F}(A) = \{x^* A x : x \in \mathbb{C}^N, \|x\| = 1\}$ ,  $\mathcal{F}(H_m) \subset \mathcal{F}(A)$
- $f(A)v = \frac{1}{i2\pi} \int_{\Gamma} f(\lambda) V_m(\lambda I - H_m)^{-1} e_1 d\lambda$ ,  $\Gamma$  is contour around  $\mathcal{F}(A)$
- $f(A)v \approx V_m f(H_m) e_1$

# Error bound lemma

- $\|f(A)v - V_m f(H_m) e_1\| \leq \frac{M}{2\pi} \int_{\Gamma} |f(\lambda) - q_{m-1}(\lambda)| |\phi(\lambda)|^{-m} |d\lambda|$
- $\phi$  conformal mapping from exterior of  $E$  to exterior of unit circle
- $\Gamma$  piecewise smooth,  $f$  analytic and continuous to boundary
- $M = l(\partial E)/[d(\partial E)d(\Gamma)]$ ,  $l(\partial E)$  length of boundary,  $d(S)$  distance between  $\mathcal{F}(A)$  and subset  $S$ ,  $E$  convex closed bounded set in complex plane
- Proof idea
- $\|(\lambda I - A)^{-1}v - V_m(\lambda I - H_m)^{-1}e_1\| \leq c \|p_m(A)\|, p_m(\lambda) = 1$
- $p_m(A) = \frac{1}{2\pi i} \int_{\partial E} p_m(z)(zI - A)^{-1}dz \implies \|p_m(A)\| \leq c \max_{z \in E} |p_m(z)|$
- $\max_{z \in E} |p_m(z)| \leq c |\phi(\lambda)|^{-m}$

# Error bound for Hermitian negative semidefinite matrix

- Eigenvalues in  $[-4\rho, 0]$ ,  $\varepsilon_m = \|\exp(\tau A)v - V_m \exp(\tau H_m)e_1\|$
- $\varepsilon_m \leq 10e^{-m^2/(5\rho\tau)}$  for  $\sqrt{4\rho\tau} \leq m \leq 2\rho\tau$
- $\varepsilon_m \leq 10(\rho\tau)^{-1}e^{-\rho\tau} \left(\frac{e\rho\tau}{m}\right)^m$  for  $m \geq 2\rho\tau$
- Example:  $A$  diagonal with eigenvalues in  $[-40, 0]$ ,  $v$  random vector of dimension 1001
- Figure: Convergence compared with linear decay for CG  $(I - A)^{-1}v$  and theoretical bound (theorem and Taylor remainder)

## Error bound for Hermitian negative semidefinite matrix

Add figure

Also consider Theorem 3 for eigenvalues clustering, no graph in paper, but it would be interesting.

General note, proofs are technical and only sketched in paper. Consider some figures illustrating conformal mappings in complex plane.

# Error bound for skew-Hermitian matrix

- Eigenvalues on imaginary axis in interval of length  $4\rho$
- $\varepsilon_m \leq 12e^{-(\rho\tau)^2/m} \left(\frac{e\rho\tau}{m}\right)^m$  for  $m \geq 2\rho\tau$
- Example:  $A$  diagonal with eigenvalues in  $[-20i, 20i]$ ,  $v$  random vector of dimension 1001
- Figure: Convergence compared with linear decay for BiCG  $(I - A)^{-1}v$  and theoretical bound (theorem and Taylor remainder)

## Error bound for skew-Hermitian matrix

Add figure

Also consider Theorem 5 for numerical range in disk, no graph in paper, but it would be interesting.

# Lanczos method

- Second basis  $W_m = (w_1, \dots, w_m)$  of Krylov subspace  $K_m(A^*, w_1)$
- Biorthogonality condition  $(v_i, w_j) = \delta_{ij}$ ,  $D_m = W_m^* V_m$  block diagonal
- $H_m = D_m^{-1} W_m^* A V_m$  block triangular, short recurrences
- $\mathcal{F}(H_m) \not\subset \mathcal{F}(A)$ , oblique projection
- pseudospectrum  $\Lambda_\varepsilon(A) = \{\lambda \in \mathbb{C} : \|(\lambda I - A)^{-1}\| \geq \varepsilon^{-1}\}$
- Condition number of eigenvectors matrix  $\kappa_e(A) = \|X\| \cdot \|X^{-1}\|$

# Error bounds

- $\Lambda_e(A) \subset E, \Lambda_\gamma(A) \cup \Lambda_\gamma(H_m) \subset G$
- Error bound lemma with  $M = \frac{1}{2}(1 + \|V_m\| \cdot \|D_m^{-1}W_m^*\|)I(\partial E)/(\varepsilon\gamma)$
- $A$  diagonalizable, spectrum  $\Lambda(A) \subset E, \Lambda(H_m) \subset G$ ,  
 $\|(\lambda I - H_m)^{-1}\| \leq \gamma^{-1}$
- Error bound lemma with  $M = 3\kappa_\varepsilon(A)(\delta^{-1} + \|V_m\| \cdot \|D_m^{-1}W_m^*\|\gamma^{-1})$ ,  
 $\delta$  is distance between  $\Lambda(A)$  and  $\Gamma$

# Examples

No graphs in paper, consider some examples to show bounds.

Last section about ODE schemes could be omitted, no graphs just scheme definition.