Projection methods for approximating the matrix exponential, with applications

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Approximation problem

Given $v \in \mathbb{R}^n$ and A symmetric and negative semidefinite, approximate

$$x = \exp(A)v$$

- Focus: A large dimension
- General approach: $x_m \in \mathcal{K}_m$ Krylov subspace

Problem in context

Wide range of applications. Here we focus on

- Numerical solution of Time-dependent PDEs
- (Analysis of) Low dimensional models of dynamical systems: approximate solution to Lyapunov equation

$$AX + XA^T + BB^T = 0$$

- Flows on constraint manifolds, e.g.,

$$Q_t = H(Q,t)Q, \quad Q(t)|_{t=0} = Q_0 \in V_k(\mathbb{R}^n)$$

V_k Stiefel manifold

Approximation using Krylov subspace

$$\mathcal{K}_m \equiv \mathcal{K}_m(A, v) = \mathrm{span}\{v, Av, \ldots, A^{m-1}v\}$$

V_m s.t. range(V_m) $= \mathcal{K}_m(A, v)$ and $V_m^* V_m = I$

Arnoldi relation

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^*$$

A common approach

$$\exp(A)v \approx x_m = V_m \exp(H_m) e_1, \qquad \|v\| = 1$$

x_m derived from interpolation problem in Hermite sense (Saad '92)

Structure preserving approaches

Motivational problem:

Approximate k largest Lyapunov exponents of

$$x'(t) = \mathcal{A}(t)x, \quad x \in \mathbb{R}^n,$$

This can be accomplished by using the associated system

$$Q_t = A(Q,t)Q, \quad Q \in \mathbb{R}^{n\times k} \qquad A \text{ skew-sym}$$

Q orthonormal columns (Stiefel manifold)

Goal:

numerical method that preserves orthogonality for long time intervals

⋆ $A_n = A(Q_n, t_n)$ skew-sym. $\Rightarrow$ $\exp(A_n)$ unitary and

$$Q_{n+1} = \exp(hA_n)Q_n \text{ orthogonal}$$

Preserving orthogonality in Krylov subspace

Let $Q^{(0)} = [q_1^{(0)}, \ldots, q_k^{(0)}]$

Regular Krylov subspaces $\mathcal{K}_m(A, q_i^{(0)})$, $i = 1, \ldots, k$

$$A \text{ skew-sym} \quad \Rightarrow \quad H_{m,i} \text{ skew-sym} \quad \Rightarrow \exp(tH_{m,i}) \text{ unitary}$$

This is not enough:

$$\exp(tA)q_i^{(0)} \quad \approx \quad q_i = V_{m,i} \exp(tH_{m,i})e_1$$

$\{q_1, \ldots, q_k\}$ not orthogonal (though unit norm)

Block Krylov methods come to rescue

Block Krylov subspace $\mathcal{K}_m(A, Q^{(0)})$ $\qquad Q^{(0)} = [q_1^{(0)}, \ldots, q_k^{(0)}]$

$$\mathcal{K}_m(A, Q^{(0)}) = \mathrm{span}\{Q^{(0)}, AQ^{(0)}, \ldots, A^{m-1}Q^{(0)}\}$$

- $\mathcal{V}_m$ orthonormal columns,

  $\mathcal{H}_m = \mathcal{V}_m^T A \mathcal{V}_m$ skew-sym

- $\mathcal{V}_m \exp(t\mathcal{H}_m)E_1$ orthonormal columns

- $\mathcal{V}_m \mathcal{R}_\nu(t\mathcal{H}_m)E_1$ orthonormal columns (Padé approx)

Further generalizations: A skew-symmetric and Hamiltonian

- $\exp(tA)$ ortho-symplectic - w.r.to $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$

- $Q^{(0)}$ ortho-symplectic then $\exp(tA)Q^{(0)}$ ortho-symplectic

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Block Krylov approximation:

- Choose *some* of the columns $\widetilde{Q}^{(0)}$ of $Q^{(0)}$,

$$V = \begin{pmatrix} \widetilde{Q}_1^{(0)} & \widetilde{Q}_2^{(0)} \\ \widetilde{Q}_2^{(0)} & -\widetilde{Q}_1^{(0)} \end{pmatrix} \qquad \mathcal{K}_m(A, V) \qquad \mathcal{H}_m = \mathcal{V}_m^T A \mathcal{V}_m$$

- $\mathcal{V}_m \exp(t\mathcal{H}_m)E_1$ columns of an ortho-symplectic matrix

X ortho-symplectic if $X^T J X = J$ and $X^T X = I$

Further generalizations. A Hamiltonian

$Q^{(0)}$ symplectic then $\exp(A)Q^{(0)}$ symplectic

Construct symplectic basis $\mathcal{V}_m$ and (logically) Hamiltonian $\mathcal{H}_m$:

Block Lanczos procedure in the block J-inner product:

$$[X, Y]_J = J_2^T X J Y \qquad X, Y \in \mathbb{R}^{2n \times 2}$$

$$J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

single vector case: Benner & Faßbender '97-'00, Watkins '04, Salam '06

An example

Linear Hamiltonian system: $\begin{cases} q' = Aq & A = J^{-1}S \\ q(0) = q_0 \end{cases}$

with $S \in \mathbb{R}^{400\times 400}$ symmetric (eigs. in [1, 100])

Energy function: $E(Q(t)) = Q(t)^T S Q(t)$, constant for all $t > 0$

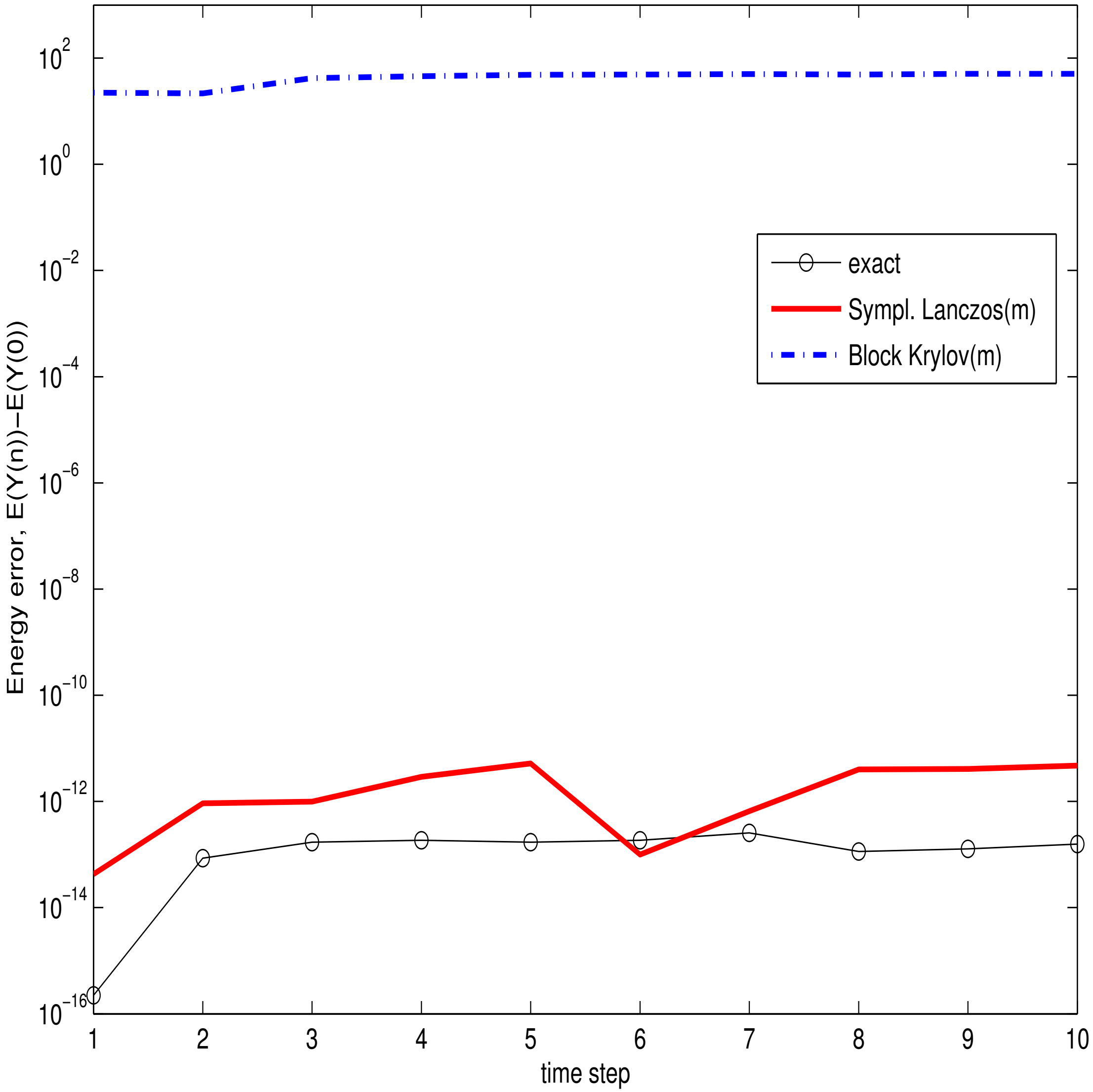
Numerical symplectic integrator: starting with $Q^{(0)} = Q_0$,

$$Q^{(r+1)} = \exp(hA)Q^{(r)}, \qquad r \geq 0 \qquad h = \frac{1}{40}$$

$\star$ $X_m = \exp(hA)Q^{(r)}$ standard Krylov subspace approximation

$\Rightarrow$ energy function is **not** constant, unless X_m is accurate

Conservation of energy. Error: $|E(Q^{(r)}) - E(Q_0)|$



Conclusions and Outlook

Implementation: For A Hamiltonian,

⋆ Stability Stability **Stability**

⋆ Robustness: (quasi) breakdown ?

Theoretical issues:

- Convergence properties
- Further generalizations

[1] L. Lopez & Simoncini, *Preserving Geometric Properties of the Exponential matrix by block Krylov subspace methods*, Dec. 2005. Submitted.

[2] A. Frommer & Simoncini, *Matrix functions*, March 2006. Submitted.