A COMPUTABLE STRICT UPPER BOUND FOR KRYLOW SUBSPACE APPROXIMATIONS TO THE EXPONENTIAL OF SKEW-HERMITIAN MATRICES
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Problem setting & Introduction
Approximate \( e^{tA} = \sum_{k=0}^{\infty} \frac{t^kA^k}{k!} \) by a Krylov subspace method. Assume the case of a large and sparse Hermitian matrix \( H \in \mathbb{C}^{n \times n} \) and \( v \in \mathbb{C}^n \). An approximation to \( e^{tA} v \) in the Krylov subspace \( K_n(H, v) = \text{span} \{ v, Hv, \ldots, H^{n-1}v \} \subseteq \mathbb{C}^n \) is given by \( \sum_{k=0}^{m} \frac{t^kA^k v}{k!} \).

The Krylov subspace of an Hermitian matrix \( H \) is computed by the Lanczos method. This results in an orthonormal basis \( V_n \in \mathbb{C}^{n \times n} \) and a real symmetric tridiagonal matrix \( T_n \in \mathbb{C}^{n \times n} \) with positive secondary diagonal.

Krylov identity: \( H V_n = V_n T_n + v_n e_n v_n^* \).

We consider the error \( \| e^{tA}v - \sum_{k=0}^{m} \frac{t^kA^k v}{k!} \| \) as a time-dependent function. The exact solution \( e^{tA} v \) can be determined based on different choices of error estimates and is discussed below.

Defect and error
The error \( L_n(t) \) applied to \( v \) solves the ODE
\[
L_n(t)v = -iH L_n(t)v + D_n(t) v, \quad L_0(t)v = 0.
\]
We call \( D_n(t) \) the defect of the approximation:
\[
D_n(t)v = -iH S_n(t)v - S_n(t)v = -iT_m A_1 e_1 + S_n(t) v - i T_m A_1 e_1.
\]
Variation of constants applied to (2):
\[
L_n(t)v = \int e^{-i(t-s)H} D_n(s)v ds = -i T_m A_1 \int e^{-i(t-s)H} v e_1 ds.
\]

Error approximation by Saad [1]
The following error estimate is used in practice:
\[
\| L_n(t)v \| \leq \sum_{k=0}^{m} \| \frac{t^kA^k v}{k!} \| \approx \sum_{k=0}^{m} \| \frac{t^kA^k v}{k!} \| \leq \sum_{k=0}^{m} \| \frac{t^kA^k v}{k!} \|.
\]

Heuristic and asymptotic step size control
Compute step sizes such that the error is expected to satisfy a given tolerance tol. Use
\[
t^{(h)} := \frac{\text{tol}}{\text{Error}(t^{(h)})}.
\]
Use \( t^{(h)} \) or \( t^{(p)} \) by heuristic methods. Error estimate \( \text{Error} \) by Saad can not be inverted directly.

For the step sizes we show the ratios
\[
t^{(h)} = \frac{t^{(h)}}{t^{(p)}} \quad \text{and} \quad t^{(p)} = \frac{t^{(p)}}{t^{(h)}}.
\]

Computable strict upper bound
Our analysis is related to [2],[3].

Use \( \| e^{tA}v \| \leq 1 \) and \( \| \frac{t^kA^k v}{k!} \| \approx 1 \) in (3):
\[
\| L_n(t)v \| \leq \sum_{k=0}^{m} \| \frac{t^kA^k v}{k!} \| e^{\| \frac{t^kA^k}{k!} \|} \leq \sum_{k=0}^{m} \| \frac{t^kA^k v}{k!} \| e^{\| \frac{t^kA^k}{k!} \|}
\]
with\( \| \frac{t^kA^k}{k!} \| = \| \frac{t^kA^k}{k!} \| \)

Derivation of an upper bound for \( \int e^{\| \frac{t^kA^k}{k!} \|} ds \): We use the representation of \( e^{\| \frac{t^kA^k}{k!} \|} \) via a Newton interpolant (see [5]),
\[
e^{\| \frac{t^kA^k}{k!} \|} = p(\lambda_1) \cdots p(\lambda_n) \lambda^m e_{\lambda_1}\cdots e_{\lambda_n}.
\]

Apply Gencoch-Hermite formula with \( e^{\| \frac{t^kA^k}{k!} \|} = \sum_{i=0}^{n} \lambda^i \prod_{j \neq i} p(\lambda_j) \lambda^m e_{\lambda_1}\cdots e_{\lambda_n} \)
\[
\sum_{i=0}^{n} \lambda^i \prod_{j \neq i} p(\lambda_j) \lambda^m e_{\lambda_1}\cdots e_{\lambda_n} \]

Numerical results
Error \( \| L_n(t)v \| \) and the error estimates \( \text{Err} \) and \( \text{Err}(t) \) for the free Schrödinger problem and Krylov subspace dimensions \( m = 10 \) and \( m = 30 \). Both error estimates are asymptotically correct for \( t \to 0 \).

For larger choices of \( m \) we observe a loss of local order for a range of practically relevant values \( t \) (topic of further investigations).

References

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