A COMPUTABLE STRICT UPPER BOUND FOR KRYLOV SUBSPACE APPROXIMATIONS TO THE EXPONENTIAL OF SKEW-HERMITIAN MATRICES

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Problem setting & Introduction

Approximate $\boxed{E(t)v := e^{-itH}v} = \sum_{k=0}^{\infty}\frac{(-itH)^k}{k!}v$ 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 $E(t)v$ in the Krylov subspace $\mathscr{K}_m(H,v) = \mathrm{span}\{v, Hv, \dots, H^{m-1}v\} \subseteq \mathbb{C}^n$ is given by $\boxed{S_m(t)v := V_m \mathrm{e}^{-\mathrm{i}tT_m}e_1}$.
Essential prerequisites concerning Krylov subspaces:

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

Krylov identity: $HV_m = V_mT_m + \tau_{m+1,m}v_{m+1}e_m^*$

Relevant identities:

$$e_m^* T_m^k e_1 = 0, \quad k = 1, \dots, m-2$$
$$e_m^* T_m^{m-1} e_1 = \boxed{\prod_{j=1}^{m-1}(T_m)_{j+1,j} =: \gamma_m}$$
$$H^k v = V_m T_m^k e_1, \; k = 1, \dots, m-1$$
$$H^m v = V_m T_m^m e_1 + \tau_{m+1,m}\gamma_m v_{m+1}$$

We consider the error $\boxed{L_m(t)v := E(t)v - S_m(t)v}$ as a time-dependent function. The exact solution $E(t)v$ solves the linear, homogeneous system of differential equations,

$$\partial_t\psi(t) = -\mathrm{i}H\psi(t), \qquad \psi(0) = v, \tag{1}$$

over a time step t. The Krylov approximation considered as a time integrator has an error $\|L_m(t)v\|_2 = \mathscr{O}(t^m)$. Below we prove that $\|L_m(t)v\|_2$ is *strictly bounded* by its leading order term. From known a priori results we have an approximate bound for 'reasonable' values of t, i.e., $t\|H\|_2 \overset{\approx}{\leq} m$, see [4]. To keep m sufficiently small we use trivial restarting of the Krylov approximation by applying it as a time integrator with appropriately small step sizes t. An adequate choice of t can be determined based on different choices of error estimates and is discussed below.

Defect and error

The error $L_m(t)$ applied to v solves the ODE

$$L_m'(t)v = -\mathrm{i}HL_m(t)v + D_m(t)v, \quad L_m(0)v = 0. \tag{2}$$

We call $D_m(t)$ the defect of the approximation:

$$D_m(t)v = -\mathrm{i}HS_m(t)v - S_m'(t)v = \underbrace{-\mathrm{i}\tau_{m+1,m}e_m^*\mathrm{e}^{-\mathrm{i}tT_m}e_1}_{\in\mathbb{C}}\,\underbrace{v_{m+1}}_{\in\mathbb{C}^n}.$$

Variation of constants applied to (2):

$$L_m(t)v = \int_0^t \mathrm{e}^{-\mathrm{i}(t-s)H}D_m(s)v\,\mathrm{d}s = -\mathrm{i}\tau_{m+1,m}\int_0^t \mathrm{e}^{-\mathrm{i}(t-s)H}v_{m+1}e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1\,\mathrm{d}s \tag{3}$$

Leading order term of the error:

$$\boxed{L_m(t)v = \sum_{k=m}^{\infty}\frac{(-\mathrm{i}t)^k(H^kv - V_mT_m^ke_1)}{k!} = \tau_{m+1,m}\frac{\gamma_m t^m}{m!}v_{m+1} + \mathscr{O}(t^{m+1})}$$

Error approximation by Saad [1]

The following error estimate is used in practice:

$$\|L_m(t)v\|_2 = \tau_{m+1,m}\Big\|\int_0^t \mathrm{e}^{-\mathrm{i}(t-s)H}v_{m+1}e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1\,\mathrm{d}s\Big\|_2 \approx \tau_{m+1,m}\Big\|\int_0^t v_{m+1}e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1\,\mathrm{d}s\Big\|_2$$
$$= \boxed{\tau_{m+1,m}t\,|e_m^*\phi_1(-\mathrm{i}tT_m)e_1| =: \mathrm{Err}_1}, \quad \text{with}$$

$$\phi_1(z) = z^{-1}(e^z - 1) = \sum_{k=0}^{\infty}\frac{z^k}{(k+1)!}; \qquad \tau_{m+1,m}t\,|e_m^*\phi_1(-\mathrm{i}tT_m)e_1| = \tau_{m+1,m}\frac{\gamma_m t^m}{m!} + \mathscr{O}(t^{m+1}).$$

Err_1 is an upper bound for the error up to a constant depending on spectral information, see [3].

Heuristic and asymptotic step size control

Compute step sizes such that the error is expected to satisfy a given tolerance tol:

- Use Err_a, compute step size directly: $t^{[a]} := \left(\frac{\mathrm{tol}\,m!}{\tau_{m+1,m}\gamma_m}\right)^{1/m}$.
- Use Err_1, choose $t^{[1]}$ by heuristic methods. Error estimate Err_1 by Saad can not be inverted directly!

For the step sizes we show the ratios

$$\mathrm{r}_0 := \frac{t_1^{[a]}}{t_1^{[1]}} \quad \text{and} \quad \mathrm{r}_{10} := \frac{\sum_{j=2}^{11}t_j^{[a]}}{\sum_{j=2}^{11}t_j^{[1]}}.$$

tol[log]	−6	−10	−14
$m=10$			
r_0	4.53	3.88	3.70
r_{10}	1.10	1.13	1.10
$m=30$			
r_0	4.57	4.38	4.33
r_{10}	1.05	1.10	1.11

Ratio of the initial and following step sizes for the free Schrödinger equation.

Note the significant difference in the first step (r_0) caused by an a priori error estimate which is necessary to determine the initial step of the heuristic step size control.

For step sizes t out of the asymptotic scope of $\|L_m(t)v\|_2$, $t^{[a]}$ and $t^{[1]}$ both lose sharpness.

Computable strict upper bound

Our analysis is related to [2],[3].
Use $\|\mathrm{e}^{\mathrm{i}(t-s)H}\|_2 = 1$ and $\|v_{m+1}\|_2 = 1$ in (3):

$$\|L_m(t)v\|_2 = \tau_{m+1,m}\Big\|\int_0^t \mathrm{e}^{\mathrm{i}(t-s)H}v_{m+1}e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1\,\mathrm{d}s\Big\|_2 \leq \tau_{m+1,m}\int_0^t|\underbrace{e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1}_{\in\mathbb{C}}|\,\mathrm{d}s$$

Derivation of an upper bound for $\int_0^t|e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1|\,\mathrm{d}s$**:** We use the representation of $\mathrm{e}^{-\mathrm{i}tT_m}$ via a Newton interpolant (see [5]), $\quad \mathrm{e}^{-\mathrm{i}tT_m} = p_t(T_m)$,

with the interpolation polynomial p_t of $\theta_t(\lambda) := \mathrm{e}^{-\mathrm{i}t\lambda}$ at the distinct and real-valued eigenvalues $(\lambda_1, \dots, \lambda_m)$ of T_m. Thus,

$$e_m^*\mathrm{e}^{-\mathrm{i}sT_m}e_1 = e_m^*p_t(T_m)e_1 = \sum_{j=0}^{m-1}\theta_t[\lambda_1,\dots,\lambda_{j+1}]\,e_m^*\omega_j(T_m)e_1 = \theta_t[\lambda_1,\dots,\lambda_m]\,\gamma_m$$

Apply Genocchi-Hermite formula with $|\frac{\mathrm{d}^{m-1}}{\mathrm{d}\lambda^{m-1}}\theta_t(\lambda)| = |(\mathrm{i}t)^{m-1}\mathrm{e}^{\mathrm{i}t\lambda}| = t^{m-1}$:

$$|\theta_t[\lambda_1,\dots,\lambda_m]| \leq t^{m-1}\int_0^1\int_0^{\eta_1}\cdots\int_0^{\eta_{m-2}}1\,\mathrm{d}\eta_{m-1}\dots\mathrm{d}\eta_2\mathrm{d}\eta_1 = \frac{t^{m-1}}{(m-1)!}$$

We get

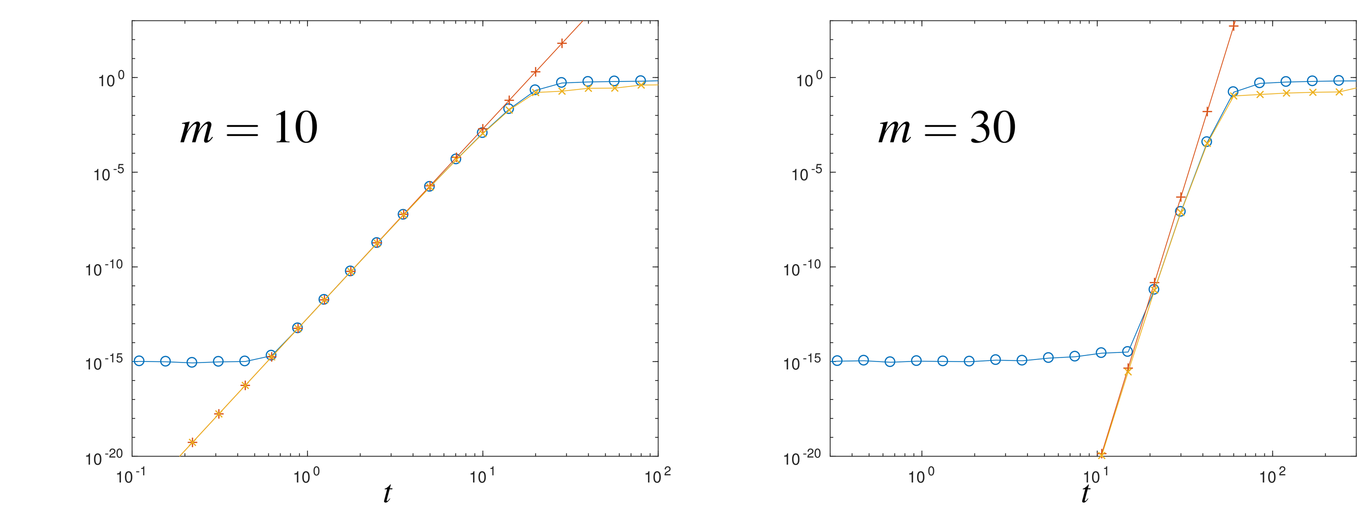
$$\|L_m(t)v\|_2 \leq \tau_{m+1,m}\gamma_m\int_0^t\frac{s^{m-1}}{(m-1)!}\mathrm{d}s = \tau_{m+1,m}\gamma_m\frac{t^m}{m!}.$$

Thus, the error estimate

$$\boxed{\mathrm{Err}_a := \tau_{m+1,m}\gamma_m\frac{t^m}{m!}}$$

is a strict upper bound. It can be proven to be asymptotically correct for $t \to 0$ and can be computed along with the construction of the Krylov subspace.

Numerical results



Error $\|L_m(t)v\|_2$ (∘) and the error estimates Err_1 (×) and Err_a (+) 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).

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