Krylov approximation of ODEs with polynomial parameterization

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Problem

Let $A_0, A_1, \ldots, A_N \in \mathbb{C}^{n\times n}$ and consider the parameterized linear time-independent ordinary differential equation

$$\frac{\partial u}{\partial t}(t,\varepsilon) = A(\varepsilon)\, u(t,\varepsilon), \quad u(0,\varepsilon) = u_0,$$

where A is the matrix polynomial

$$A(\varepsilon) := A_0 + \varepsilon A_1 + \cdots + \varepsilon^N A_N.$$

Specifically considered: problems arising from spatial

semidiscretizations of partial differential equations.

Series representation

Let the coefficients of the Taylor expansion of the solution with respect to the parameter ε be denoted by $c_0(t)$, $c_1(t)$, ..., i.e.,

$$u(t, \varepsilon) = \exp(tA(\varepsilon))\, u_0 = \sum_{\ell=0}^{\infty} \varepsilon^{\ell} c_{\ell}(t). \qquad (1)$$

As $\exp\left(tA(\varepsilon)\right)$ is an entire function of a matrix polynomial, the expansion (1) exists for all $\varepsilon \in \mathbb{C}$.

Approximation

Consider the approximation stemming from the truncation of the Taylor series
and from an approximation of the Taylor coefficients:

$$u_k(t,\varepsilon) := \sum_{\ell=0}^{k-1} \varepsilon^\ell c_\ell(t) \approx \sum_{\ell=0}^{k-1} \varepsilon^\ell \widetilde{c}_\ell(t) =: \widetilde{u}_k(t,\varepsilon).$$

Our approach gives an explicit parameterization with respect to t of the approximate coefficients $\widetilde{c}_0(t),\ldots,\widetilde{c}_{k-1}(t)$.

Via (2) this gives an approximate solution with an explicit parameterization with respect to ε and t.

Main theorem

The Taylor coefficients $c_0(t), \ldots, c_{m-1}(t)$ are explicitly given by

$$\operatorname{vec}(c_0(t), \ldots, c_{m-1}(t)) = \exp(tL_m)\,\widetilde{u}_0,$$

where

$$L_m := \begin{bmatrix} A_0 & & & & & \\ A_1 & \ddots & & & & \\ \vdots & \ddots & \ddots & & & \\ A_{\widehat{N}} & \ddots & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & A_{\widehat{N}} & \ldots & A_1 & A_0 \end{bmatrix} \in \mathbb{C}^{mn \times mn}, \quad \widetilde{u}_0 = \begin{bmatrix} u_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

and $\widehat{N} = \min(m-1, N)$.

- I.Najfeld and T.F. Havel. *Derivatives of the matrix exponential and their computation.* Advances in Applied Mathematics 16.3 (1995): 321-375.

Krylov approximation of matrix functions

The Arnoldi iteration gives an orthogonal basis $Q_k \in \mathbb{R}^{n\times k}$ for the Krylov subspace

$$\mathcal{K}_k(A, b) = \mathrm{span}\{b, Ab, A^2 b, ..., A^{k-1} b\},$$

and the Hessenberg matrix $H_k = Q_k^{\mathsf{T}} A Q_k \in \mathbb{R}^{k\times k}$.

For any polynomial p_n of degree $n \leq k-1$ it holds

$$p_n(A)b = Q_k p_n(H_k) Q_k^* b = Q_k p_n(H_k) e_1.$$

We use the approximation

$$\exp(A)b \approx Q_k \exp(H_k) Q_k^{\mathsf{T}} b.$$

Matvecs for the Arnoldi iteration

Lemma. Suppose $x = \mathrm{vec}(x_1, \ldots, x_j, 0, \ldots, 0) = \mathrm{vec}(X) \in \mathbb{C}^{nm}$, where $x_1, \ldots, x_j \in \mathbb{C}^n$ and $m > j + N$. Then,

$$L_m x = \mathrm{vec}(y_1, \ldots, y_{j+N}, 0, \ldots, 0),$$

where

$$y_\ell = \sum_{i=\max(0,\ell-k)}^{\min(N,\ell-1)} A_i x_{\ell-i}, \quad \ell = 1, \ldots, j + N.$$

A priori error bound

After p steps, the error

$$\mathrm{err}_p(t,\varepsilon) := \|u(t,\varepsilon) - \widetilde{u}_p(t,\varepsilon)\|$$

is bounded as

$$\mathrm{err}_p(t,\varepsilon) \leq C_1(t,\varepsilon) \sum_{\ell=0}^{N-1} \frac{C_2(t,\varepsilon)^{p+\ell-1} \mathrm{e}^{C_2(t,\varepsilon)}}{(p+\ell-2)!} \|u_0\| + 2\sqrt{\frac{1-|\varepsilon|^{2N(p-1)}}{1-|\varepsilon|^2}} \frac{(t\alpha)^p \mathrm{e}^{t\gamma}}{p!} \|u_0\|, \qquad (2)$$

where $C_1(t,\varepsilon)$ and $C_2(t,\varepsilon)$ depend only on t and ε, and

$$\alpha = \sum_{\ell=0}^{N} \|A_\ell\| \qquad \text{and} \qquad \gamma = \mu(A_0) + \sum_{\ell=1}^{N} \|A_\ell\|,$$

and $\mu(B)$ denotes the logarithmic 2-norm.

The first term in (2) corresponds to the truncation of the Taylor series,
the second to the error given by the Arnoldi approximation.

Integral representation of the coefficients

Fromo the main theorem it follows that

$$c_j'(t) = \sum_{i=0}^{\min(N,j)} A_i c_{j-i}(t).$$

Using the variation-of-constants formula

$$u(t) = \mathrm{e}^{tA_0} u_0 + \int_0^t \mathrm{e}^{tA} g(u(\tau))\,\mathrm{d}\tau,$$

which gives the the exact solution at time t for the semilinear ODE

$$u'(t) = A_0 u(t) + g(u(t)), \quad u(0) = u_0,$$

we get an integral formula for the coefficients $c_\ell(t)$.

Integral representation of the coefficients

Let ℓ and N be positive integers such that $N \leq \ell$. Denote by C_ℓ the set of compositions of ℓ, i.e.,

$$C_\ell = \{(i_1, \ldots, i_r) \in \mathbb{N}_+^r \, : \, i_1 + \cdots + i_r = \ell\},$$

and further denote

$$C_{\ell,N} := \{(i_1, \ldots, i_r) \in C_\ell \, : \, i_s \leq N \text{ for all } 1 \leq s \leq r\}.$$

Then,

$$c_0(t) = \mathrm{e}^{tA_0} u_0,$$

$$c_\ell(t) = \sum_{(i_1,\ldots,i_r)\in C_{\ell,N}} \int_0^t \mathrm{e}^{(t-t_{i_1})A_0} A_{i_1} \int_0^{t_{i_1}} \mathrm{e}^{(t_{i_1}-t_{i_2})A_0} A_{i_2} \ldots \int_0^{t_{i_{r-1}}} \mathrm{e}^{(t_{i_{r-1}}-t_{i_r})A_0} A_{i_r} c_0(t_{i_r}) \, \mathrm{d}t_{i_1} \ldots \mathrm{d}t_{i_r} \quad \text{for} \quad \ell > 0.$$

A posteriori error estimate

A posteriori error estimates obtained using techniques given in

- Y.Saad. *Analysis of some Krylov subspace approximations to the matrix exponential operator.* SIAM J. Numer. Anal., 29 (1992), pp. 209–228.

For the Arnoldi approximation of $\mathrm{e}^{A}b$ it holds that

$$\mathrm{e}^{A}b - Q_p \exp(H_p)e_1 = h_{p+1,p} \sum_{\ell=1}^{\infty} e_p^T \varphi_\ell(H_p)e_1 \, A^{\ell-1} q_{p+1},$$

where $h_{p+1,p}$ is the subdiagonal element of the Hessenberg matrix, and

$$\varphi_\ell(z) = \sum_{j=0}^{\infty} \frac{z^j}{(j+\ell)!}.$$

Numerical example

Consider the damped wave equation inside the 3D unit box. The governing $2n$-dimensional first-order ODE:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}u(t)\\u'(t)\end{bmatrix}\begin{bmatrix}0 & I\\-M^{-1}K & -M^{-1}C(\gamma)\end{bmatrix}\begin{bmatrix}u(t)\\u'(t)\end{bmatrix}, \quad \begin{bmatrix}u(0)\\u'(0)\end{bmatrix}=\begin{bmatrix}u_0\\u_0'\end{bmatrix}\in\mathbb{R}^{2n},$$

where $C(\gamma_1,\gamma_2)=\gamma_1 C_1+\gamma_2 C_2$.

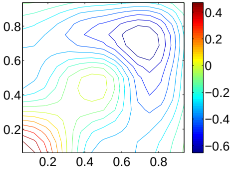
ODE obtained by finite differences with 15 discretization points in each dimension, i.e., $n=15^3$.

K denotes the discretized Laplacian, $C(\gamma_1,\gamma_2)$ the damping matrix stemming from Robin boundary conditions, and M the mass matrix.

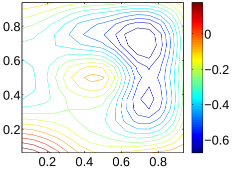
Reformulate the ODE by setting

$$A_0=\begin{bmatrix}0 & I\\-M^{-1}K & -M^{-1}\gamma_1 C_1\end{bmatrix}, \quad A_1=\begin{bmatrix}0 & 0\\0 & -M^{-1}C_2\end{bmatrix}.$$

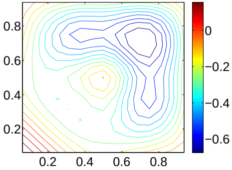
Linear example 2



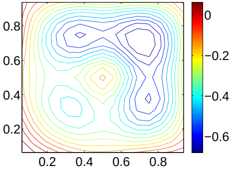
(a) $\gamma_1 = \gamma_2 = 0$



(b) $\gamma_1 = 2$, $\gamma_2 = 0$



(c) $\gamma_1 = 1$, $\gamma_2 = 1$



(d) $\gamma_1 = 2$, $\gamma_2 = 2$

Figure : The solution in the plane $z = 0.5$, for different values of (γ_1, γ_2) at $t = 1$.

Numerical example

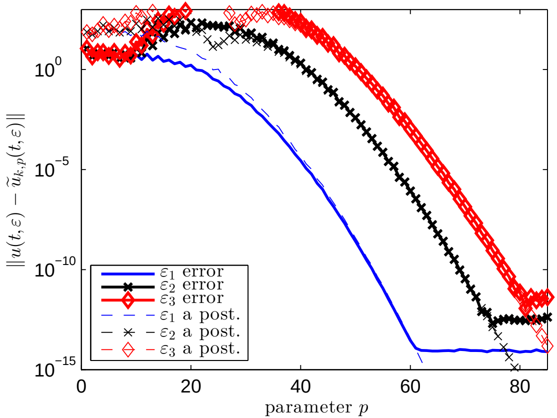


Figure : 2-norm errors of approximations $\widetilde{u}_{k,p}(t,\varepsilon)$ and the error estimates, when $\gamma_1 = 2$ and γ_2 has the values $\varepsilon_1 = 1$, $\varepsilon_2 = 1.5$ and $\varepsilon_3 = 2$.

References

A. Koskela, E. Jarlebring and M. Hochstenbach. *Krylov approximation of ODEs with polynomial parameterization.* arXiv:1507.07507 (2015).