Linear algebra for exponential integrators

Antti Koskela

KTH Royal Institute of Technology

Beräkningsmatematikcirkus, 28 May 2014

The problem

Considered: time integration of stiff semilinear initial value problems

$$u'(t) = Au(t) + g(t, u(t)), \quad u(t_0) = u_0,$$

where $u(t) \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$ (n large), g a nonlinear function with a moderate Lipschitz constant.

Specifically considered: problems arising from the spatial semidiscretization of partial differential equations.

E.g.: A comes from the discretization of the linear part of a PDE, using finite elements or finite differences.

Example

Consider the Brusselator problem in 2D,

$$\frac{\partial u}{\partial t} = \nu \Delta u + \mu U \cdot \nabla u + av - (b+1)u + u^2 v,$$
$$\frac{\partial v}{\partial t} = \nu \Delta v + \mu V \cdot \nabla v + bu - u^2 v,$$

where A and B constants. Write as

$$\frac{\partial w}{\partial t} = Aw + g(w),$$

where

$$A = \begin{bmatrix} \nu\Delta + \mu U \cdot \nabla + (b+1) & a \\ b & \nu\Delta + \mu V \cdot \nabla \end{bmatrix}, \qquad w = \begin{bmatrix} u \\ v \end{bmatrix}.$$

Example

Consider the advection-diffusion equation

$$\partial_t y(t,x) = \epsilon \partial_{xx} y(t,x) + \alpha \partial_x y(t,x),$$
$$y(0,x) = 16(x(1-x))^2,\ x \in [0,1]$$

subject to homogenous Dirichlet boundary conditions.

Perform spatial discretization using the central differences $\rightarrow$

$$\text{ODE:} \quad u'(t) = Au(t),\ u(0) = u_0.$$

Compute the Krylov approximation of:

$$1)\ \exp(hA)u_0$$
$$2)\ (I + \tfrac{h}{2}A)(I - \tfrac{h}{2}A)^{-1}u_0$$

Krylov subspace

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 $H_k = Q_k^\top A Q_k \in \mathbb{R}^{k \times k}$.

Approximation of matrix functions

Cauchy's integral formula: for any analytic function f defined on $D \subset \mathbb{C}$, it holds

$$f(A) = \frac{1}{2\pi \mathrm{i}} \int_C f(\lambda)(\lambda I - A)^{-1} \, \mathrm{d}\lambda,$$

where C is a closed curve inside the domain D enclosing $\sigma(A)$. By using the approximation

$$(\lambda I - A)^{-1} b \approx Q_k (\lambda I - H_k)^{-1} Q_k^{\mathsf{T}} b,$$

and letting C enclose the field of values $\mathcal{F}(A)$, the approximation

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

is obtained.

Example

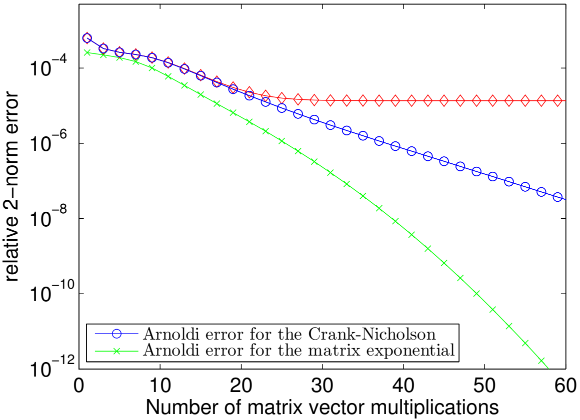

Figure: Convergence of different Krylov approximations.
Here: $h = 5 \cdot 10^{-5}$, $\|hA\| \approx 199$.

Exponential integrators

Exponential integrators are based on the variation-of-constants formula

$$u(t) = \mathrm{e}^{(t-t_0)A} u_0 + \int_{t_0}^{t} \mathrm{e}^{(t-\tau)A} g(\tau, u(\tau))\, \mathrm{d}\tau.$$

which gives the the exact solution at time t.

Example: exponential Euler method

$$u_1 = \mathrm{e}^{hA} u_0 + h\varphi_1(hA) g(t_0, u_0)$$

where h denotes the step size and φ_1 is the entire function

$$\varphi_1(z) = \frac{\mathrm{e}^{z} - 1}{z}.$$

Fast computation of series of φ - functions

Computation of one time step can be done using the following lemma (Al-Mohy and Higham 2010).

Lemma

Let $A \in \mathbb{R}^{d\times d}$*,* $W = [w_1, w_2, \dots, w_p] \in \mathbb{R}^{d\times p}, h \in \mathbb{R}$ *and*

$$\widetilde{A} = \begin{bmatrix} A & W \\ 0 & J \end{bmatrix} \in \mathbb{R}^{(d+p)\times(d+p)}, \quad J = \begin{bmatrix} 0 & 0 \\ I_{p-1} & 0 \end{bmatrix}, \quad v_0 = \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} \in \mathbb{R}^{d+p}$$

with $e_1 = [1, 0, \dots, 0]^\mathsf{T}$*. Then it holds*

$$\mathrm{e}^{hA} u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k = \begin{bmatrix} I_d & 0 \end{bmatrix} \mathrm{e}^{h\widetilde{A}} v_0.$$

References

A. Koskela and A. Ostermann. *Exponential Taylor methods: analysis and implementation.* Computers and Mathematics with Applications (2013).

A. Koskela and A. Ostermann. *A moment-matching Arnoldi iteration for linear combinations of φ-functions.* (submitted for publication).

A. Koksela. *Approximating the matrix exponential of an advection-diffusion operator using the incomplete orthogonalization method.* To appear in ENUMATH proceedings.