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On the Construction of a Validated Exponential Integrator

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Outline

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2. Exponential integrators
3. Validated exponential integrators
4. To do

Introduction

Setting

- Discretization of PDE by method of lines yields dissipative system of ODEs.
- Stiff dissipative ODE:

  Traditional explicit methods require much smaller time steps than implicit methods.
- Alternative to implicit methods: Exponential integrators.

Dissipative ODE

- Dissipative ODE: $u' = f(u)$ where $f : D \to \mathbb{R}^m$ and $\exists \mu \leq 0$ s.t.

$$< f(u) - f(v), u - v > \ \leq \ \mu < u - v, u - v > \quad \forall u, v \in D.$$

- Linear case: $u' = Au$, $A \in R^{m \times m}$, $A = A^T$ is dissipative iff

$$\lambda_{\max}(A) = \sup_{v \neq 0} \frac{v^T A v}{v^T v} =: \mu \leq 0.$$

- General case:

$$f \text{ dissipative} \quad \Rightarrow \|u(t) - v(t)\| \leq e^{\mu(t - t_0)} \|u_0 - v_0\| \leq \|u_0 - v_0\| .$$

Exponential integrators

Linearized Autonomous IVP

IVP:

$$u' = f(u), \quad u(0) = u_0.$$

Linearized form:

$$u' = -Au + g(u), \quad u(0) = u_0$$

where $A \in \mathbb{R}^{n \times n}$.

Exponential Rosenbrock methods:

$$-A = \frac{\partial}{\partial u} f(u_k), \quad g(u) = f(u) - \frac{\partial}{\partial u} f(u_k) u, \quad t \in [t_k, t_{k+1}].$$

Variation of Constants

IVP:

$$u' = -Au + g(u), \quad u(0) = u_0.$$

VOC:

$$u(h) = e^{-hA}u_0 + \int_0^h e^{-(h-\tau)A} g\big(u(\tau)\big)\, d\tau$$

$$= e^{-hA}u_0 + h\int_0^1 e^{-(1-\theta)hA} g\big(u(\theta h)\big)\, d\theta$$

where $\quad e^A = \sum_{\nu=0}^{\infty} \frac{A^\nu}{\nu!}.$

Variation of Constants

Approximation: Replace $g\big(u(\theta h)\big)$ by polynomial $p(\theta h)$:

$$u(h) \approx e^{-hA}u_0 + h\int_0^1 e^{-(1-\theta)hA}p(\theta h)\,d\theta.$$

Evaluation of integral: φ-functions.

Let $\varphi_0(z) = e^z$ and for $k \geq 1$

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z}\frac{\theta^{k-1}}{(k-1)!}\,d\theta.$$

φ-functions

Recurrence relation:

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z} = \frac{\varphi_k(z) - \frac{1}{k!}}{z}.$$

Relation with e^z:

$$\varphi_k(z) = \frac{e^z - T_{k-1}(z)}{z^k} = \sum_{\nu=k}^{\infty} \frac{z^{\nu-k}}{\nu!} = \sum_{\nu=0}^{\infty} \frac{z^\nu}{(\nu+k)!}$$

where $\quad T_k(z) = \sum_{\nu=0}^{k} \frac{z^\nu}{\nu!}.$

Exponential Rosenbrock Methods

Let $\quad p(t) = \sum_{k=0}^{n} a_k t^k. \quad$ Then

$$u(h) \approx e^{-hA}u_0 + h\int_0^1 e^{-(1-\theta)hA} p(\theta h)\, d\theta$$

$$= e^{-hA}u_0 + h\int_0^1 \sum_{k=0}^{n} e^{-(1-\theta)hA} a_k \theta^k h^k \, d\theta$$

$$= e^{-hA}u_0 + h\sum_{k=0}^{n} k!h^k \varphi_{k+1}(-hA)a_k.$$

Exponential Rosenbrock-Taylor Method

Let

$$p(t) = \sum_{k=0}^{n} \frac{g^{(k)}}{k!}(u_0)t^k.$$

Then

$$u(h) \approx e^{-hA}u_0 + h\int_0^1 e^{-(1-\theta)hA}p(\theta h)\,d\theta$$

$$= e^{-hA}u_0 + \int_0^1 \sum_{k=0}^{n} h^{k+1} e^{-(1-\theta)hA}\frac{\theta^k}{k!}g^{(k)}(u_0)\,d\theta$$

$$= e^{-hA}u_0 + \sum_{k=0}^{n} h^{k+1}\varphi_{k+1}(-hA)g^{(k)}(u_0).$$

Validated exponential integrators

Validated exponential RT Method

Let

$$p(t) \in \sum_{k=0}^{n} \frac{g^{(k)}}{k!}(\boldsymbol{u}_0)t^k + \boldsymbol{i}.$$

Then

$$u(h) \in e^{-h\boldsymbol{A}}\boldsymbol{u}_0 + \sum_{k=0}^{n} h^{k+1}\varphi_{k+1}(-h\boldsymbol{A})g^{(k)}(\boldsymbol{u}_0) + h^{n+2}\varphi_{n+2}(-h\boldsymbol{A})\boldsymbol{i}$$

where

$$-\boldsymbol{A} \supseteq \frac{\partial}{\partial u} f(\boldsymbol{u}_0).$$

Validated exponential RT Method

Reduced dependency I:

$$\frac{\partial}{\partial u} f(\widehat{u}_0) \in -\boldsymbol{A} \in \mathbb{IR}^{n \times n}$$

for some $\widehat{u}_0 \in \boldsymbol{u}_0$.

Computation of interval matrix exponential by scaling and squaring (Goldsztejn 2009).

Validated exponential RT Method

Reduced dependency II: Mean value form for $g^{(k)}(\boldsymbol{u}_0)$:

$$g^{(k)}(\boldsymbol{u}_0) = g^{(k)}(\widehat{u}_0) + J\big(g^{(k)}(\boldsymbol{u}_0)\big)(\boldsymbol{u}_0 - \widehat{u}_0).$$

Finally,

$$u(h) \in e^{-h\boldsymbol{A}}\boldsymbol{u}_0 + \sum_{k=0}^{n} h^{k+1}\varphi_{k+1}(-h\boldsymbol{A})g^{(k)}(\widehat{u}_0)$$

$$+ \Big(\sum_{k=0}^{n} h^{k+1}\varphi_{k+1}(-h\boldsymbol{A})J\big(g^{(k)}(\boldsymbol{u}_0)\big)\Big)(\boldsymbol{u}_0 - \widehat{u}_0) + h^{n+2}\varphi_{n+2}(-h\boldsymbol{A})\boldsymbol{i}.$$

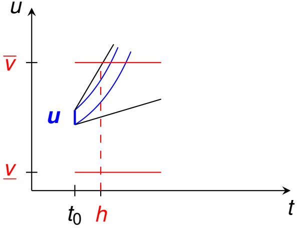
A priori Enclosure

Remainder bound of order n:

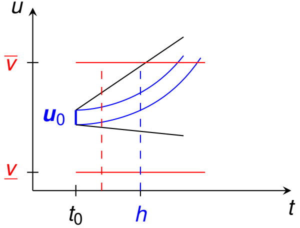
$$\sum_{k=0}^{m} g^{(k)}(\widehat{u}_0)t^k + g^{(n+1)}(\boldsymbol{v})t^{m+1}$$

Computation of $\boldsymbol{v}$ by FP iteration benefits from $g^{(1)}(\boldsymbol{u}_0) \approx 0$.

$$\boldsymbol{u}_0 + [0,h]f(\boldsymbol{v}) \subseteq \boldsymbol{v}$$



$$\boldsymbol{u}_0 + [0,h]g(\boldsymbol{v}) \subseteq \boldsymbol{v}$$



Inclusion Functions for φ-Functions

1. Scalar case:
   1. Similar approach as for elementary functions: Taylor approximation.
   2. Scaling and squaring? Argument reduction?
   3. Approximation interval is very small: $[0, h]$.
   4. Monotonicity on $\mathbb{R}$: Only point evaluations at the endpoints of an argument interval are needed.
2. Matrix case:
   1. Is Taylor approximation accurate enough?
   2. Approximation interval is very small: $[0, h]$.
   3. Hard problem: Even if h is small, $h\boldsymbol{A}$ in $\varphi_k(-h\boldsymbol{A})$ may be large.

To do

To Do

- Work out details.
- Additional considerations
  (e.g. QR factorization in the propagation of $e^{-h\mathbf{A}}\mathbf{u}_k$).
- Library of interval matrix φ-functions.