Generalized mid-point and trapezoidal rules for Lipschitzian RHS

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Consider initial value problem of the form

\[ \dot{x}(t) = F(x, t), \quad x \in \mathbb{R}^n, F : \mathbb{R}^n \to \mathbb{R}^m \]

\[ x(0) = x_0 \]

- We assume **local Lipschitz continuity** of RHS
- \( F \) might be **non-smooth** (e.g. by using max, min)
- Most classical methods can drop to first order
Classical Approach

Approximation of Integral:

\[ \hat{x} - \check{x} := x(h) - x(0) = \int_{0}^{h} F(x(t)) dt \approx h F\left( \frac{\check{x} + \hat{x}}{2} \right) \]

\[ \hat{x} - \check{x} := x(h) - x(0) = \int_{0}^{h} F(x(t)) dt \approx h \frac{F(\check{x}) + F(\hat{x})}{2} \]

for midpoint rule and for trapezoidal rule, respectively.

- These methods have global convergence order 2 for smooth functions.
- Goal: Modify methods such that they preserve convergence properties even for large number of kinks.
Piecewise Linearization
We propose two methods to approximate locally Lipschitz continuous functions with piecewise affine functions:

(a) Tangent mode linearization

(b) Secant mode linearization
The proposed approximations have the form

\[
F(x) = F(\hat{x} + \Delta x) \approx F(\hat{x}) + \Delta F(\hat{x}; \Delta x)
\]

\[
F(x) = F(\hat{x} + \Delta x) \approx \frac{1}{2} [F(\hat{x}) + F(\hat{x})] + \Delta F(\hat{x}, \hat{x}; \Delta x)
\]

for tangent mode and for secant mode, respectively, where \( \hat{x} = \frac{1}{2}(\hat{x} + \hat{x}) \).

**Definition**

A function is called **composite piecewise smooth**, if it can composed out of some set of smooth elementary functions and the absolute value function, i.e. it can be represented as a **directed, acyclic graph** with nodes \( (v_i)_{i \in I} \), where \( v_{i+1} = \varphi_{i+1}(v_i) \) with \( \varphi_i \in C^{1,1} \) or abs or a binary operation.

\[\Rightarrow\] We can construct approximations with AD-like methods.
Propagation Rules I

We define the following propagation rules to produce the piecewise linearization in tangent mode

\[
\begin{align*}
\Delta v_i &= \Delta v_j \pm \Delta v_k & \text{for } v_i &= v_j \pm v_k \\
\Delta v_i &= \Delta v_j \cdot \dot{v}_k + \dot{v}_j \cdot \Delta v_k & \text{for } v_i &= v_j \cdot v_k \\
\Delta v_i &= (\Delta v_j \cdot \dot{v}_k - \dot{v}_j \cdot \Delta v_k) / \dot{v}_k^2 & \text{for } v_i &= v_j / v_k \\
\Delta v_i &= \hat{c}_{ij} \cdot \Delta v_j & \text{for } v_i &= \varphi_i(v_j)
\end{align*}
\]

where we have \( \hat{c}_{ij} = \varphi'_i(\dot{v}_j) \) for \( \varphi_i \in C^{1,1} \) and

\[
\Delta v_i = \text{abs}(\dot{v}_{i-1} + \Delta v_{i-1}) - \dot{v}_i \quad \text{for } \varphi_i = \text{abs}.
\]
For secant mode the basic propagation rules stay the same, but here

$$\hat{c}_{ij} = \begin{cases} 
\varphi_i'(\hat{v}_j) & \text{if } \hat{x} = \check{x} \\
\hat{v}_i - \check{v}_i & \text{else}
\end{cases}$$

and for $\varphi_i = \text{abs}$ we have that

$$\hat{v}_i = \frac{1}{2}(\bar{v}_i + \check{v}_i) = \frac{1}{2} [\text{abs}(\bar{v}_j) + \text{abs}(\check{v}_j)]$$.

Obviously for $\check{x} = \hat{x}$ both rules coincide.
In a similar way we can propagate a bound on the Lipschitz constant of $F$. 

**Calculation of $\beta_F$**

\[
\begin{align*}
  v &= \varphi(u) \quad \Rightarrow \quad \beta_v = \beta_u |\varphi'(\hat{u})| \\
  v &= \text{abs}(u) \quad \Rightarrow \quad \beta_v = \beta_u \\
  v &= u + w \quad \Rightarrow \quad \beta_v = \beta_u + \beta_w \\
  v &= uw \quad \Rightarrow \quad \beta_v = \beta_u |\hat{w}| + |\hat{u}| \beta_w \\
  v &= \frac{u}{w} \quad \Rightarrow \quad \beta_v = \frac{\beta_u |\hat{w}| + |\hat{u}| \beta_w}{|\hat{w}|^2}
\end{align*}
\]

For this constant it holds:

\[ \| F(x) - F(\tilde{x}) \| \leq \beta_F \| x - \tilde{x} \| \]
We can also propagate a constant $\gamma_F$:

**Calculation of $\gamma_F$**

\[
\begin{align*}
\nu &= \varphi(u) \quad \Rightarrow \quad \gamma \nu &= \gamma u |\varphi'(\dot{u})| + \beta_u^2 |\varphi''(\dot{u})| \\
\nu &= \text{abs}(u) \quad \Rightarrow \quad \gamma \nu &= \gamma u \\
\nu &= u + w \quad \Rightarrow \quad \gamma \nu &= \gamma u + \gamma w \\
\nu &= uw \quad \Rightarrow \quad \gamma \nu &= \gamma u |\dot{w}| + 2 \beta_u \beta_w + |\dot{u}| |w| \\
\nu &= \frac{u}{w} \quad \Rightarrow \quad \gamma \nu &= \frac{\gamma u |\dot{w}|^2 + 2 |\dot{w}| \beta_u \beta_w + 2 |\dot{u}| \beta_w^2 + |\dot{u}| |\dot{w}| \gamma w}{|\dot{w}|^3}
\end{align*}
\]

$\gamma_F$ is a bound on the Lipschitz constant of the derivative of $F$ (everywhere it exists).
The Lipschitz constant $\beta_F$ is also a Lipschitz constant for the piecewise linear model:

Lipschitz Continuity

\[
\| \diamondsuit \dot{x} F(x) - \diamondsuit \dot{x} F(\tilde{x}) \| \leq \beta_F \| x - \tilde{x} \| \quad \text{and} \\
\| \diamondsuit \ddot{x} F(x) - \diamondsuit \ddot{x} F(\tilde{x}) \| \leq \beta_F \| x - \tilde{x} \|
\]

where:

\[
\diamondsuit \dot{x} F(x) \equiv F(\dot{x}) + \Delta F(\dot{x}; x - \dot{x}) \quad \text{and} \\
\diamondsuit \ddot{x} F(x) \equiv \frac{1}{2} (F(\ddot{x}) + F(\ddot{x})) + \Delta F(\ddot{x}, \ddot{x}; x - \ddot{x})
\]
We assume that $F$ is composite piecewise Lipschitz continuous differentiable on an open neighbourhood of a closed, convex domain $\mathcal{H} \subset \mathbb{R}^n$. Then:

**Tangent mode approximation**

$$\forall \hat{x}, x \in \mathcal{H} : \| F(x) - F(\hat{x}) - \Delta F(\hat{x}; x - \hat{x}) \| \leq \gamma_F \| x - \hat{x} \|^2.$$ 

**Secant mode approximation**

$$\forall \hat{x}, \hat{\hat{x}}, x \in \mathcal{H} : \| F(x) - \hat{F} - \Delta F(\hat{x}, \hat{\hat{x}}; x - \hat{x}) \| \leq \gamma_F \| x - \hat{x} \| \| x - \hat{\hat{x}} \|.$$ 

$\gamma_F$ can be computed as mentioned before.
Generalized methods
Idea for construction: We integrate the ODE $\dot{x}(t) = F(x(t))$:

$$x(h) - x(0) = \int_{0}^{h} F(x(t))\,dt$$
Generalized methods

Generalized Midpoint Rule

Idea for construction: We integrate the ODE $\dot{x}(t) = F(x(t))$:

$$\hat{x} - \check{x} := x(h) - x(0) = \int_0^h F(x(t)) \, dt = h \int_{-\frac{1}{2}}^{\frac{1}{2}} F\left(x\left(\frac{h}{2} + \tau h\right)\right) \, d\tau$$
Generalized Midpoint Rule

Idea for construction: We integrate the ODE $\dot{x}(t) = F(x(t))$:

$$\hat{x} - \tilde{x} := x(h) - x(0) = \int_0^h F(x(t))dt = h \int_{-\frac{1}{2}}^{\frac{1}{2}} \underbrace{F \left( x \left( \frac{h}{2} + \tau h \right) \right)}_{F(x) \approx F(\dot{x}) + \Delta F(\dot{x}; \Delta x)} \ d\tau$$
Generalized Midpoint Rule

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$$
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$$

and get

$$
\hat{x} - \check{x} = h \int_{-\frac{1}{2}}^{\frac{1}{2}} F(\hat{x}) + \Delta F(\hat{x}; t(\hat{x} - \check{x}))dt \quad \text{with} \quad \hat{x} = \frac{\hat{x} + \check{x}}{2}
$$
Idea for construction: We integrate the ODE $\dot{x}(t) = F(x(t))$:

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$F(x) \approx \hat{F} + \Delta F(\hat{x}, \check{x}; t(\hat{x} - \check{x}))$
Generalized Trapezoidal Rule

Idea for construction: We integrate the ODE \( \dot{x}(t) = F(x(t)) \):

\[
\hat{x} - \check{x} := x(h) - x(0) = \int_0^h F(x(t)) dt = h \int_{-\frac{1}{2}}^{\frac{1}{2}} F \left( x \left( \frac{h}{2} + \tau h \right) \right) d\tau
\]

\( F(x) \approx \hat{F} + \Delta F(\hat{x}, \check{x}; t(\hat{x} - \check{x})) \)

and get

\[
\hat{x} - \check{x} = h \int_{-\frac{1}{2}}^{\frac{1}{2}} \hat{F} + \Delta F(\hat{x}, \check{x}; t(\hat{x} - \check{x})) dt \quad \text{with} \quad \hat{F} = \frac{F(\hat{x}) + F(\check{x})}{2}
\]
Both rules reduce to familiar rules if $F$ is smooth.

For $F$ piecewise linear we get

$$\hat{x} - \check{x} = h \int_{-\frac{1}{2}}^{\frac{1}{2}} F \left( \frac{\hat{x} + \check{x}}{2} + t(\hat{x} - \check{x}) \right) dt$$

In piecewise linear case method is an AVF method.

Trapezoidal rule yields a $C^{1,1}$-interpolant that has correct tangents at $\hat{x}$ and $\check{x}$.

In both cases to find new point we have to solve a nonlinear, nonsmooth equation.

Can be solved with Picard like method for sufficiently small $h$. 
The above nonlinear equations can be written in fixed point form and with $\dot{x} = 0$ we get

$$x = h \left[ F(x/2) + \int_{1/2}^{1} \Delta F(x/2; xt) \, dt \right] =: hG(x)$$

It can be shown that if we bound $h$ suitably, this equation is contractive. Due to Banach we have a fixed point $x_h$ and it can be shown that it holds

$$x_h - x(h) = \mathcal{O}(h^3)$$

where $x(t)$ solves the equation

$$\dot{x}(t) = F(x(t)) \text{ with } x(0) = 0.$$
A first numerical result

![Graph showing error in x against number of timesteps]

- **Impl. Midpoint**
- **Trapezoidal**
- **Generalized**
Theoretical expectations

- Stable second order convergence **without event handling**
  \[ \implies \text{should be as good as or outperform Trapezoidal Rule/Impl. Midpoint} \]
- Should be able to use (local) **Richardson extrapolation** to gain higher orders
- Possible geometric integration properties
Richardson extrapolation

**With** transversality condition = finitely many kinks

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<thead>
<tr>
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<th>on smooth parts</th>
<th>on kinks</th>
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Richardson extrapolation

**Without** transversality condition

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Error Estimator

\[ \| x(h) - x_h \| = \left\| \int_0^h F(x(t)) dt - \int_0^h \overset{\cdot}{F} + \Delta F(\dot{x}, \dot{x}; t(\dot{x} - \ddot{x})) dt \right\| \]

\[ \leq \int_0^h \| F(x(t)) - F((1 - \frac{t}{h})\ddot{x} + \frac{t}{h}\dot{x}) \| dt \]

\[ + \int_0^h \| F((1 - \frac{t}{h})\ddot{x} + \frac{t}{h}\dot{x}) - \overset{\cdot}{F} + \Delta F(\dot{x}, \dot{x}; t(\dot{x} - \ddot{x})) \| dt \]

With \( \| x(t) - p(t) \| \in O(h^3) \) we get:

\[ \| x(h) - x_h \| \leq \beta_F \int_0^h \| p(t) - \ddot{x} - \frac{t}{h}(\dot{x} - \ddot{x}) \| dt + \frac{1}{12} \gamma_F \| \dot{x} - \ddot{x} \|^2 h \]

\[ \rightarrow \eta_1 \]

\[ \rightarrow \eta_2 \]
Error Estimator

Local Error and Estimators

- Error
- Trap. Error Est.
- Gen. Error Est.
Experiments
\[
\ddot{x} = -V'(x) \quad \text{with}
\]
\[
V(x) = \begin{cases} 
\frac{1}{2}(1-x)^2 & \text{if } x \geq 1 \\
\frac{1}{2}(1+x)^2 & \text{if } x \leq -1 \\
0 & \text{else}
\end{cases}
\]
\[
-V'(x) = \begin{cases} 
1-x & \text{if } x \geq 1 \\
x-1 & \text{if } x \leq -1 \\
0 & \text{else}
\end{cases}
\]
\[
= \min(\max(-x-1, 0), 1-x)
\]
\[
= -x - \frac{1}{2}|x-1| + \frac{1}{2}|x+1|
\]

Figure: RHS of Rolling Stone
Exact solution

\[ x(0) = 1, \quad \dot{x}(0) = 1 \]

\[ x(t) = \begin{cases} 
1 + \sin(t) & \text{if } t \in [0, \pi) \\
1 - (t - \pi) & \text{if } t \in [\pi, \pi + 2) \\
-2 - \sin(2 - t) & \text{if } t \in [\pi + 2, 2\pi + 2) \\
t - 3 - 2\pi & \text{if } t \in [2\pi + 2, 2\pi + 4) 
\end{cases} \]

The total period is \(2\pi + 4\).

Figure: Exact solution
Convergence

Experiments

Rolling Stone

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Numerical integration via PL models

10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7

10^2 10^3 10^4

Number of timesteps $n$

Error in $x$

Impl. Midpoint
Trapezoidal
Generalized

Number of timesteps $n$
Error in $x$
Impl. Midpoint
Trapezoidal
Generalized
Convergence with Romberg extrapolation

![Graph showing convergence with Romberg extrapolation](image)

- Generalized
- Gen. Romberg
- Trapezoidal
- Impl. Midpoint
- Trap. Romberg

Number of steps: $10^{-12}$ to $10^5$

Error: $10^{-12}$ to $10^0$
Energy of the System

Summed energy loss: $\| V(x) + \frac{1}{2} \dot{x}^2 - \frac{1}{2} \|$
Problem Formulation

\[
\begin{pmatrix}
\dot{x} \\
\dot{y} \\
\dot{z}
\end{pmatrix} = F(x) =
\begin{pmatrix}
1 \\
z \\
-(y - C \sin(\omega x) + g^{-1}(Cz)) \frac{1}{LC}
\end{pmatrix}
\]

with \( g^{-1}(x) = \begin{cases} 
\frac{x}{\alpha} & \text{if } x \geq 0 \\
\frac{x}{\beta} & \text{if } x < 0 
\end{cases} \)

\( L = 10^{-6}, \ C = 10^{-13}, \ \omega = 3 \cdot 10^9, \ \alpha = 2, \ \beta = 0.00001 \)

\( I(t) = z(t) \)
Computed Solution

Figure: Electric Current

Figure: Electric Charge
Convergence

Experiments

Diode-LC-Circuit

Richard Hasenfelder (HU Berlin)  Numerical integration via PL models

Number of timesteps $n$

Error in $x$

Impl. Midpoint
Trapezoidal
Gen. Midpoint
Gen. Trapezoidal
Convergence with Romberg extrapolation

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Convergence of adaptive Solver

![Graph showing convergence of adaptive solvers for Diode-LC-Circuit experiments. The graph plots error against number of steps for different methods: Generalized, Generalized with SSC, Trapezoidal, Trapezoidal with SSC, Gen. Romberg, and Gen. with SSC. The y-axis represents error on a logarithmic scale from $10^{-13}$ to $10^{-7}$, and the x-axis represents number of steps on a logarithmic scale from $10^3$ to $10^6$. The Generalized method shows the best convergence, followed by Generalized with SSC, Trapezoidal with SSC, Gen. Romberg, and Trap. Romberg. Trap. with SSC has the worst convergence.]
Outlook

- Improve efficiency of implementation
- Improve error constant and automatic scaling of error norm
- Regain energy preservation for extrapolation via restoration of time symmetry
- Exact integration of PL systems
- Automatic event handling
- Generalization to discontinuous case
- Application to DAEs
- Application to optimal control problems
- Application to space discretized PDEs
- ODE sensitivity using Clark can be wrong, PL isn’t (cf. K. Khan)