Newton-like Methods for Solving Piecewise Smooth Systems of Equations - Based on Successive Piecewise Tangent or Secant Linearization

Tom Streubel$^{1,2}$, Andreas Griewank$^3$, Richard Hasenfelder$^2$

1) Zuse Institute Berlin  
2) Humboldt University of Berlin  
3) Yachay Tech
Introduction

**basic idea**

- replace differentiable elementals by their **linear** tangent/secant model
- replace the **piecewise linear** absolute value function by itself

\[ v = \max(u, w) = \frac{(u + w + |u - w|)}{2} \]
\[ f(x) = \sin \left( x + |\exp(x + |3x|)| \right) \]

function expression

assume \( f : \mathbb{R}^n \to \mathbb{R}^m \) to be a chain of \( C^{1,1} \) functions from some Library \( \Phi \) and the absolute value function \( \text{abs}(\cdot) \)

the expression can be recast as single assignment code

\[
\begin{align*}
v_0 &= x \\
z_0 &= 3v_0 \\
v_1 &= |z_0| \\
v_2 &= v_0 + v_1 \\
z_1 &= \exp(v_2) \\
v_3 &= |z_1| \\
v_4 &= v_0 + v_3 \\
v_5 &= \sin(v_4) \\
f(x) &= v_5
\end{align*}
\]

here \( \prec \) is a dependence relation generating a partial order

acyclic directed computational graph
either choose

- one reference point \( \hat{x} \in \text{dom}(F) \) \( \hat{v} = v(\hat{x}) \) (tangent mode)

- two reference points \( \hat{x}, \hat{x} \in \text{dom}(F) \) \( \hat{v} = \frac{1}{2}(v(\hat{x}) + v(\hat{x})) \) (secant mode)

For any single assignment evaluate an increment

\[
\begin{align*}
\Delta v_i &= \alpha \Delta v_j \pm \beta \Delta v_k \quad \text{for } v_i = \alpha v_j \pm \beta v_k \\
\Delta v_i &= \hat{v}_j \cdot \Delta v_k + \hat{v}_k \cdot \Delta v_j \quad \text{for } v_i = v_j \cdot v_k \\
\Delta v_i &= \phi \cdot \Delta v_j \quad \text{for } v_i = \phi(v_j), \text{ where } \phi \neq \text{abs} \\
\Delta v_i &= |\hat{v}_j + \Delta v_j| - \hat{v}_i \quad \text{for } v_i = |v_j| \\
\end{align*}
\]

\[
c\phi = \begin{cases} 
\phi'(\hat{v}_j) & \text{tangent mode or } \hat{v}_j = \hat{v}_i \\
\frac{\phi(\hat{v}_j) - \phi(\hat{v}_j)}{\hat{v}_j - \hat{v}_j} & \text{secant mode and } \hat{v}_j \neq \hat{v}_i 
\end{cases}
\]

These increments depend on reference point(s) and preceding increments. So we write

- \( \Delta v_i(\hat{x}; \Delta x) \equiv \Delta v_i \) (tangent mode)

- \( \Delta v_i(\hat{x}, \hat{x}; \Delta x) \equiv \Delta v_i \) (secant mode)
Algorithmic Piecewise Linearization

$\Delta F(\hat{x}; \cdot)$ is called **tangent** piecewise linear model of $F$ at $\hat{x}$ and satisfies

$$F(x) = F(\hat{x}) + \Delta F(\hat{x}; x - \hat{x}) + \mathcal{O}(\|x - \hat{x}\|^2)$$

Inhomogeneous tangent model  $\dot{\hat{x}} F(x) = F(\hat{x}) + \Delta F(\hat{x}; x - \hat{x})$

$\Delta F(\ddot{x}, \hat{x}; \cdot)$ is called **secant** piecewise linear model of $F$ at $\ddot{x}, \hat{x}$ if

$$F(x) = \hat{F} + \Delta F(\ddot{x}, \hat{x}; x - \hat{x}) + \mathcal{O}(\|x - \ddot{x}\| \cdot \|x - \hat{x}\|)$$

where

$$\hat{F} = \frac{1}{2}[F(\ddot{x}) + F(\hat{x})] \quad \ddot{x} = \frac{1}{2}(\ddot{x} + \hat{x})$$

Inhomogeneous secant model  $\dot{\hat{x}} \dot{F}(x) = \hat{F} + \Delta F(\ddot{x}, \hat{x}; x - \hat{x})$
Approximation properties of PL models

\[ \| \Diamond_{\ddot{x}} F(x) - \Diamond_{\ddot{y}} F(x) \| \leq L \left[ \| \ddot{x} - \ddot{y} \| \max(\| x - \ddot{x} \|, \| x - \ddot{y} \|) \right] \]

For some (algorithmically computable) Lipschitz constant \( L \)

\[ \Diamond_{\ddot{x}} F(x) \equiv F(\ddot{x}) + \Delta F(\ddot{x}; x - \ddot{x}) \]

\[ \uparrow \text{simplifies to, if } \ddot{x} = \hat{x} \]

\[ \| \Diamond_{\ddot{x}} F(x) - \Diamond_{\ddot{y}} F(x) \| \leq L \max \left[ \| \ddot{x} - \ddot{y} \| \max(\| x - \ddot{x} \|, \| x - \ddot{y} \|), \| \ddot{x} - \ddot{y} \| \max(\| x - \hat{x} \|, \| x - \ddot{y} \|) \right] \]

For some (algorithmically computable) Lipschitz constant \( L \)

\[ \Diamond_{\ddot{x}} F(x) \equiv \ddot{F} + \Delta F(\ddot{x}, \hat{x}; x - \ddot{x}) \]

Implications:

- \( \ddot{x} = a = \ddot{y} \) \implies \( \Diamond_{\ddot{a}} F(a) = \Diamond_{\ddot{a}} F(a) = F(a) \)

- \( \ddot{x} = a = \hat{x} \) \implies \( \| F(a) - \Diamond_{\ddot{y}} F(a) \| \leq 2L \| a - \ddot{y} \| \| a - \hat{y} \| \)
Newton via successive piecewise linearization I

Tangent mode

Let $x^*$ be a root of a $PC^{1,1}$ algorithm $F$.

If $\Diamond_{x}^{-1} F(0) \cap B_{\rho}(x^*) \neq \emptyset$ for a fixed radius $\rho > 0$ then

$$x_{j+1} \in \arg \min \{ \| x - x_j \| \mid x \in \Diamond_{x_j}^{-1} F(0) \}$$

is called feasible tangent mode iteration.

Furthermore this iteration scheme simplifies to the classic Newton method in the smooth scenario (when no abs operation occurs in the evaluation graph): $x_{j+1} = x_j - J_F^{-1}(x_j) \cdot F(x_j)$

Secant mode

if $\Diamond_{\{\hat{x},\hat{x}\}}^{-1} F(0) \cap B_{\rho}(x^*) \neq \emptyset$ again for a fixed radius then

$$x_{j+1} \in \arg \min \{ \| x - \hat{x}_j \| \mid x \in \Diamond_{\{x_{j-1}, x_j\}}^{-1} F(0) \}$$

is called feasible secant mode iteration, where $\hat{x}_j = \frac{1}{2} (x_j + x_{j-1})$ and $\Diamond^{-1}$ set-valued inverses
Quadratic or golden ratio convergence rate

**Tangent mode**

Assume feasibility of tangent mode iteration as well as

\[ \exists c > 0 \forall x \in B_\rho(x^*) : \|x - x^*\| \leq c \| \nabla x^* F(x) \| \quad \text{(local strong metric regularity)} \]

satisfied, the tangent mode iteration converges quadratically (rate \( p = 2 \)) to \( x^* \)

**Secant mode**

Assume feasibility of secant mode iteration as well as

\[ \exists c > 0 \forall x \in B_\rho(x^*) : \|x - x^*\| \leq c \| \nabla x^* F(x) \| \quad \text{(local strong metric regularity)} \]

satisfied, then the secant mode iteration converges with

Golden ratio rate \( p = \frac{1}{2}(1 + \sqrt{5}) \) to the root \( x^* \)
strong metric regularity in $x^*$ i.e.

$$\exists c > 0 \forall \hat{x} \in B_\rho(x^*) : \|\hat{x} - x^*\| \leq c\|x^* F(\hat{x})\|$$

is implied by openness of the restriction of $\Diamond_{x^*} F(\cdot)$ to $B_\rho(x^*)$

So far we know

feasibility of both iterations

$$x_{j+1} \in \arg\min \{\|x - x_j\| \mid x \in \Diamond_{x_j}^{-1} F(0)\}$$

$$x_{j+1} \in \arg\min \{\|x - \hat{x}_j\| \mid x \in \Diamond_{\{x_{j-1}, x_j\}}^{-1} F(0)\}$$

is implied by injectivity of $\Diamond_{x^*} F(\cdot)$

Open Newton Conjecture:
feasibility is already guaranteed in case of openness of $\Diamond_{x^*} F(\cdot)$
Propagation of Piecewise Linear Operator

\[ f(x) = \sin \left( x + |\exp(x + |3x|)| \right) \]

function expression

assume \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) to be a chain of \( C^{1,1} \) functions from some Library \( \Phi \) and the absolute value function \( \text{abs}(\cdot) \)

the expression can be recast as single assignment code

\[
\begin{align*}
 v_0 &= x \\
 z_0 &= 3v_0 \\
 v_1 &= |z_0| \\
 v_2 &= v_0 + v_1 \\
 z_1 &= \exp(v_2) \\
 v_3 &= |z_1| \\
 v_4 &= v_0 + v_3 \\
 v_5 &= \sin(v_4) \\
 f(x) &= v_5
\end{align*}
\]

single assignment code

acyclic directed computational graph
Unfolded Evaluation Procedures

\[ z_0 = 3x \]
\[ z_1 = \exp(x + w_0) \]
\[ F(x, w_0, w_1) = \sin(x + w_1) \]

\[(UA)\]

\[
\begin{align*}
  v_0 &= x \\
  z_0 &= 3v_0 \\
  v_1 &= w_0 \\
  v_2 &= v_0 + v_1 \\
  z_1 &= \exp(v_2) \\
  v_3 &= w_1 \\
  v_4 &= v_0 + v_3 \\
  v_5 &= \sin(v_4) \\
  F(x, w_0, w_1) &= v_5
\end{align*}
\]

differential single assignment code

acyclic directed computational graph
Unfolded/Original Evaluation Procedures

\( z_0 = 3x \)

\( z_1 = \exp(x + w_0) \)

\( F(x, w_0, w_1) = \sin(x + w_1) \)

unfolded algorithm

\( z_0 = 3x \)

\( z_1 = \exp(x + |z_0|) \)

\( f(x) \equiv F(x, |z_0|, |z_1|) = \sin(x + |z_1|) \)

nonlinear abs-normal form

\[
\begin{align*}
v_0 &= x \\
z_0 &= 3v_0 \\
v_1 &= w_0 \\
v_2 &= v_0 + v_1 \\
z_1 &= \exp(v_2) \\
v_3 &= w_1 \\
v_4 &= v_0 + v_3 \\
v_5 &= \sin(v_4) \\
F(x, w_0, w_1) &= v_5
\end{align*}
\]

single assignment code

acyclic directed computational graph
Unfolded/Original Evaluation Procedures

\[ \mathcal{F} : \mathbb{R}^n \to \mathbb{R}^m \]  

\[ z = G(x, w) \]  
\[ y = F(x, w) \]  

\[ z = G(x, |z|) \]  
\[ \mathcal{F}(x) = F(x, |z|) \]  

(CPS) \hspace{1cm} \text{piecewise differentiable}

(UA) \hspace{1cm} \text{smooth mapping}

(OA) \hspace{1cm} \text{nonlinear abs-normal form}
Unfolded/Original Evaluation Procedures

\[ z = G(x, w) \]  
\[ y = F(x, w) \]  
\[ z = G(x, |z|) \]  
\[ \mathcal{F}(x) = F(x, |z|) \]

\[ \begin{bmatrix} \Delta z \\ \Delta y \end{bmatrix} = \begin{bmatrix} Z & L \\ J & Y \end{bmatrix} \cdot \begin{bmatrix} \Delta x \\ \Delta w \end{bmatrix} \]

\[ Z = \frac{\partial}{\partial x} G, \quad L = \frac{\partial}{\partial w} G, \quad J = \frac{\partial}{\partial x} F, \quad J = \frac{\partial}{\partial w} F \]
Unfolded/Original Evaluation Procedures

\[ z = G(x, w) \]
\[ y = F(x, w) \quad (UA) \quad \text{smooth mapping} \]

\[ z = G(x, |z|) \]
\[ F(x) = F(x, |z|) \quad (OA) \quad \text{nonlinear abs-normal form} \]

\[
\begin{bmatrix}
\Delta z \\
\Delta F
\end{bmatrix}
= 
\begin{bmatrix}
Z & L \\
J & Y
\end{bmatrix}
\cdot
\begin{bmatrix}
\Delta x \\
|\dot{z} - \Delta z| - |\dot{z}|
\end{bmatrix} 
\quad (ANF)
\]

\[
Z = \frac{\partial}{\partial x} G, \quad L = \frac{\partial}{\partial w} G, \quad J = \frac{\partial}{\partial x} F, \quad J = \frac{\partial}{\partial w} F
\]
Intrinsic parameters are:

- pressures
- (blood volume)
- flow
systemic atrium (left upper chamber):

\[ 0 = IO_{sa} (p_{sa} - p_{sv} - R_{sa} q_{sa} - L_{sa} \dot{q}_{sa}), \]
\[ - (1 - IO_{sa}) q_{sa}, \]
\[ \dot{v}_{sa} = q_{pv1} - q_{sa}, \]
\[ p_{sa} = E_{sa}(v_{sa} - V_{sa}), \quad \text{where} \]
\[ IO_{sa} = c_{sa} \cdot \min(1, \max(0, p_{sa} - p_{sv})) \]
Cardio-Vascular Sys.

Remark: takes up to 3 Newton-like steps per time integration step independently from events caused by closing hearth flaps → *less overhead*
Numerics – Simulated Wiggers Diagram

State of the flap valve

Aortic pressure

Atrial pressure

Ventricular pressure

Ventricular volume

Numerics – Simulated Wiggers Diagram

State of the flap valve

Aortic pressure

Atrial pressure

Ventricular pressure

Ventricular volume
Numerics – Evaluation Points during Transition

- Aortic pressure
- Atrial pressure
- Ventricular pressure
- Ventricular volume
- State of the flap valve

**Graph:**

- $IO_{ss}$ vs. $t$
- $Vo$ vs. $t$
Numerics – Events

- Aortic pressure
- Atrial pressure
- Ventricular pressure
- Ventricular volume
- State of the flap valve
Numerics – Sparsity Structure of ANF

![Graph showing the relationship between state of flap valve, aortic pressure, atrial pressure, and ventricular pressure and volume.](image-url)

- **State of the flap valve**
- **Aortic pressure**
- **Atrial pressure**
- **Ventricular pressure**
- **Ventricular volume**
References


Thank you