Applying Taylor on Non-smooth DAEs with Flow Network Structure

Tom Streubel
Overview

• Expanding Piecewise Differentiable Functions with Faà di Bruno and Taylor

• A PD-Taylor Method for Non-smooth DAEs
  – Derivation of the Non-smooth Method (Involving The Collocation Method)
  – Numerical Experiment #1: An Academical Example
  – Recap: Gas Networks, Control Valves and Setpoint Values
  – Numerical Experiment #2: The Control Valve
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kth-order Taylor Polynomial Expansions

**Taylor’s Theorem:** Let $f : \mathbb{R}^n \to \mathbb{R}^k$ be a $k + 1$ times continuously differentiable function and let $\hat{x}, \Delta x \in \mathbb{R}^n$ be a reference point and a linear increment of a polynomial expansion:

$$
\mathcal{T}_f[\hat{x}](\Delta x) = \sum_{|\alpha| \leq k} \frac{\partial^\alpha f(\hat{x})}{\alpha!} \Delta x^\alpha
$$

then the following estimation holds true:

$$
f(\hat{x} + \Delta x) - \mathcal{T}_f[\hat{x}](\Delta x) = O(\|\Delta x\|^{k+1})
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using the following Notion of higher order curvature increments/multivariate-monomial increments:

\[
\Delta^{(j)} f(\hat{x}; \Delta x) \equiv \sum_{|\alpha|=j} \frac{\partial^\alpha f(\hat{x})}{\alpha!} \Delta x^\alpha
\]

we can simplify the notion above into a sum of increments
kth-order Taylor Polynomial Expansions

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\[
\mathcal{T}_f[\hat{x}](\Delta x) = \sum_{|\alpha| \leq k} \frac{\partial^{\alpha} f(\hat{x})}{\alpha!} \Delta x^{\alpha} = f(\hat{x}) + \sum_{j=1}^{k} \Delta^{(j)} f(\hat{x}; \Delta x)
\]

then the following estimation holds true:

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we can simplify the notion above into a sum of increments
A function $f : \mathbb{R}^n \to \mathbb{R}^k$ is said to have an **Abs Normal Form (ANF)** if $0 \leq s \in \mathbb{N}$ and

- there is $G_f \in C^{d,1}(\mathbb{R}^n \times \mathbb{R}^s \to \mathbb{R}^s)$ with $\partial_w G(x, w)$ strictly lower triangular
- there is $F_f \in C^{d,1}(\mathbb{R}^n \times \mathbb{R}^s \to \mathbb{R}^k)$

such that

$$z(x) = G_f(x, |z(x)||)$$
$$f(x) = F_f(x, |z(x)||)$$

(ANF)

apply Taylor polynomial expansion to $F_f$ and $G_f$

$$\mathcal{T}^d_{G_f}[\hat{x}, \hat{w}](x, w) = \sum_{j=0}^d \Delta^{(j)} G_f(\hat{x}, \hat{w}; \Delta x, \Delta w)$$
$$\mathcal{T}^d_{F_f}[\hat{x}, \hat{w}](x, w) = \sum_{j=0}^d \Delta^{(j)} F_f(\hat{x}, \hat{w}; \Delta x, \Delta w)$$
Multivariate Abs Polynomial or Taylor Spline Expansions

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such that

$$z(x) = G_f(x, |z(x)|)$$

and hence

$$x(\tau) = \dot{x} + \tau \Delta x$$

$$[z \circ x](\tau) = G_f(x(\tau), |z(x(\tau))|)$$

$$[f \circ x](\tau) = F_f(x(\tau), |z(x(\tau))|)$$

**parametrized ANF**

apply Taylor polynomial expansion to $F_f$ and $G_f$

$$\mathcal{T}^d_{G_f}[\dot{x}, \dot{w}](x, w) = \sum_{j=0}^{d} \Delta^{(j)} G_f(\dot{x}, \dot{w}; \Delta x, \Delta w)$$

$$\mathcal{T}^d_{F_f}[\dot{x}, \dot{w}](x, w) = \sum_{j=0}^{d} \Delta^{(j)} F_f(\dot{x}, \dot{w}; \Delta x, \Delta w)$$
Multivariate **Abs Polynomial or Taylor Spline Expansions**

- starting from Taylor polynomial expansions

\[
\mathcal{T}_{G_f}^d[\tilde{x}, \tilde{\omega}](x, \omega) = \sum_{j=0}^{d} \Delta^{(j)} G_f(\tilde{x}, \tilde{\omega}; \Delta x, \Delta \omega)
\]

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x(\tau) = \dot{x} + \tau \Delta x
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[z \circ x](\tau) = G_f(x(\tau), |z(x(\tau))|)
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(parametrized ANF)
Multivariate Abs Polynomial or Taylor Spline Expansions

- starting from Taylor polynomial expansions

\[ T^d_{G_f} [\hat{x}, \hat{w}] (x, w) = \sum_{j=0}^{d} \Delta (j) G_f (\hat{x}, \hat{w}; \Delta x, \Delta w) \]
\[ T^d_{F_f} [\hat{x}, \hat{w}] (x, w) = \sum_{j=0}^{d} \Delta (j) F_f (\hat{x}, \hat{w}; \Delta x, \Delta w) \]

- There is a generalized version Faà di Bruno’s formula, with

\[ T^d_{z \circ x} [0] (\tau) = T^d_{G_f} [\hat{x}, z(\hat{x})] \circ \text{Faà} (T^d_x [0], |T^d_{z \circ x} [0]|) (\tau) \]
\[ T^d_{f \circ x} [0] (\tau) = T^d_{F_f} [\hat{x}, z(\hat{x})] \circ \text{Faà} (T^d_x [0], |T^d_{z \circ x} [0]|) (\tau) \]

Abs-Polynomial Form (APF)

\[ x(\tau) = \hat{x} + \tau \Delta x \]
\[ [z \circ x](\tau) = G_f (x(\tau), |z(x(\tau))|) \]
\[ [f \circ x](\tau) = F_f (x(\tau), |z(x(\tau))|) \]
Multivariate Abs Polynomial or Taylor Spline Expansions

- starting from Taylor polynomial expansions

\[ T_{G_f}^d [\hat{x}, \hat{w}] (x, w) = \sum_{j=0}^{d} \Delta^{(j)} G_f (\hat{x}, \hat{w}; \Delta x, \Delta w) \]

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such that

\[ [f \circ x] (\tau) = T_{f \circ x}^d [0] (\tau) + \mathcal{O}(|\tau|^{d+1}) \]

→ effectively a Theorem of Taylor for piecewise differentiable functions
Multivariate **Abs Polynomial** or **Taylor Spline Expansions**

- starting from Taylor polynomial expansions
  \[ T_{G_f}^d[\hat{x}, \hat{w}](x, w) = \sum_{j=0}^{d} \Delta^{(j)}G_f(\hat{x}, \hat{w}; \Delta x, \Delta w) \]
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- There is a generalized version **Faà di Bruno**’s formula, with
  \[ T_{z\circ x}^d[0](\tau) = T_{G_f}^d[\hat{x}, |z(\hat{x})|] \circ \text{Faà}(T_{x}^d[0], |T_{z\circ x}^d[0]|)(\tau) \]
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\[ [f \circ x](\tau) = T_{f\circ x}^d[0](\tau) + \mathcal{O}(|\tau|^{d+1}) \]

→ effectively a **Theorem of Taylor for piecewise differentiable functions**

Can I raise \( d \in \mathbb{N} \)? If \( G_f \) & \( F_f \) are real analytic then
\[ f(x(\tau)) = T_{f\circ x}[0]^\infty(\tau) \]
Multivariate Abs Polynomial or Taylor Spline Expansions

- starting from Taylor polynomial expansions
  \[ T^d_{G_f}[\hat{x}, \hat{w}](x, w) = \sum_{j=0}^{d} \Delta^{(j)} G_f(\hat{x}, \hat{w}; \Delta x, \Delta w) \]
  \[ T^d_{F_f}[\hat{x}, \hat{w}](x, w) = \sum_{j=0}^{d} \Delta^{(j)} F_f(\hat{x}, \hat{w}; \Delta x, \Delta w) \]

- There is a generalized version Faà di Bruno’s formula, with
  \[ T^d_{\Delta \circ x}[0](\tau) = T^d_{G_f}[\hat{x}, |z(\hat{x})|] \circ \text{Faà}(T^d_{x}[0], |T^d_{\Delta \circ x}[0]|)(\tau) \]
  \[ T^d_{f \circ x}[0](\tau) = T^d_{F_f}[\hat{x}, |z(\hat{x})|] \circ \text{Faà}(T^d_{x}[0], |T^d_{\Delta \circ x}[0]|)(\tau) \]

such that

\[ [f \circ x](\tau) = T^d_{f \circ x}[0](\tau) + \mathcal{O}(|\tau|^{d+1}) \]

→ effectively a Theorem of Taylor for piecewise differentiable functions

Can I raise \( d \in \mathbb{N} \)? If \( G_f \) & \( F_f \) are real analytic then

\[ f(x(\tau)) = T^\infty_{f \circ x}[0](\tau) \]

Splines are kept invariant due to the abs polynomial expansion process
Example of Taylor Expansion

\[ F(x, y) = |\exp(x) - |y|| \]

reference point of expansion will be: \((\hat{x}, \hat{y}) = (0, 1)\)
Example of Taylor Expansion

\[ \mathcal{F}(x, y) = |\exp(x) - |y|| \]

expansion of order 1

reference point of expansion is: \((\hat{x}, \hat{y}) = (0, 1)\)
Example of Taylor Expansion

\[ \mathcal{F}(x, y) = |\exp(x) - |y|| \]

Expansion of order 2

Reference point of expansion is: \((\hat{x}, \hat{y}) = (0, 1)\)
Example of Taylor Expansion

$F(x, y) = |\exp(x) - |y||$

Expansion of order 3

Reference point of expansion is: $(\bar{x}, \bar{y}) = (0, 1)$
Example of Taylor Expansion

\[ F(x, y) = |\exp(x) - |y|| \]

expansion of order 4

reference point of expansion is: \((\hat{x}, \hat{y}) = (0, 1)\)
Example of Taylor Expansion

\[ F(x, y) = |\exp(x) - |y|| \]

expansion of order 5

reference point of expansion is: \((\bar{x}, \bar{y}) = (0, 1)\)
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A Smooth Collocation Method

consider a differential-algebraic equation (DAE): $0 = f(\dot{x}(t), x(t), t)$ with $x_0 = x(t_0)$, where $f : \mathcal{D} \subseteq (\mathbb{R}^n \times \mathbb{R}^n \times [t_0, T]) \rightarrow \mathbb{R}^n$ is the system function of the DAE

i. use a polynomial as “Ansatz”-function for the solution:

$$p_x(t) = x_0 + \sum_{j=1}^{m} a_j (t - t_0)^j$$

$$\dot{p}_x(t) = \sum_{j=1}^{m} j \cdot a_j (t - t_0)^{j-1}$$

ii. solve $0 = [f(\dot{p}_x(t_0 + \frac{i}{m} h), p_x(t_0 + \frac{i}{m} h), t_0 + \frac{i}{m} h)]_{i=1}^{m}$ to determine coefficients $a_j$

iii. compute $x_1 = p_x(t_0 + h)$
A Smooth Collocation Method with Taylor

consider a differential-algebraic equation (DAE): \( 0 = f(x(t), x(t), t) \) with \( x_0 = x(t_0) \), where \( f : \mathcal{D} \subseteq (\mathbb{R}^n \times \mathbb{R}^n \times [t_0, T]) \to \mathbb{R}^n \) is the system function of the DAE

i. use a polynomial as “Ansatz”-function for the solution:
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\begin{align*}
p_x(t) &= x_0 + \sum_{j=1}^{m} a_j (t - t_0)^j \\
p_x(t) &= \sum_{j=1}^{m} j \cdot a_j (t - t_0)^{j-1}
\end{align*}
\]

ii. solve \( 0 = \left[ f(p_x(t_0 + \frac{i}{m}h), p_x(t_0 + \frac{i}{m}h), t_0 + \frac{i}{m}h) \right]_{i=1}^{m} \) to determine coefficients \( a_j \)

iii. compute \( x_1 = p_x(t_0 + h) \)

Alternatively exchange ii. by:

ii.b) solve \( 0 = \left[ \mathcal{T}^d_{f \circ (p_x, p_x, \text{id})} \right]_{i=1}^{m} (t_0 + h)(t_0 + \frac{i}{m}h) \) (Mixed-Colloc-Taylor-Method)
Towards Non-Smoothness

- assume we know certain “events” \( t_\ell \equiv t_0 + \tau_\ell h \) for \( 0 < \tau_1 < \tau_2 < \cdots < \tau_{\mu-1} < 1 \) to “treat”

i. swap our polynomial “Ansatz”-function for an “Ansatz”-spline

\[
s_x(t) = p_x(t) + \sum_{\ell=1}^{\mu-1} \left[ \sum_{j=2}^{m} a_{\ell,j} \max(0, t - t_\ell)^j \right]
\]
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Towards Non-Smoothness

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\]

ii. Solve either:

\[
0 = \begin{bmatrix}
  f(\dot{s}_x(t_0 + \frac{i}{m} \tau_1 h), s_x(t_0 + \frac{i}{m} \tau_1 h), t_0 + \frac{i}{m} \tau_1 h)_{i=1}^{m} \\
  f(\dot{s}_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), s_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), t_{\ell-1} + \frac{i}{m} \tau_\ell h)_{i=2,\ell=2}^{m,\mu}
\end{bmatrix}
\]

ii.b) or: \( 0 = \begin{bmatrix}
  \mathcal{T}^d_{f \circ (s_x, s_x, \text{id})}[t_0 + h](\dot{s}_x(t_0 + \frac{i}{m} \tau_1 h), s_x(t_0 + \frac{i}{m} \tau_1 h), t_0 + \frac{i}{m} \tau_1 h)_{i=1}^{m} \\
  \mathcal{T}^d_{f \circ (s_x, s_x, \text{id})}[t_0 + h](\dot{s}_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), s_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), t_{\ell-1} + \frac{i}{m} \tau_\ell h)_{i=2,\ell=2}^{m,\mu}
\end{bmatrix}
\]

iii. Compute \( x_1 = s_x(t_0 + h) \)
The Full Taylor-Collocation Method

- set $\mu = 1$, $\tau \equiv (\tau_0 = 0 < \tau_\mu = 1)$ and repeat until $\mu$ & $\tau$ settles
  
i. generate “Ansatz”-functions
    
    $$s_x(t) = p_x(t) + \sum_{i=1}^{\mu-1} \left[ \sum_{j=2}^{m} a_{i,j} \max(0, t - \tau_i)^j \right]$$
    $$\dot{s}_x(t) = \dot{p}_x(t) + \sum_{i=1}^{\mu-1} \left[ \sum_{j=2}^{m} j \cdot a_{i,j} \max(0, t - \tau_i)^{j-1} \right]$$
  
  ii. solve:
    
    $$0 = \begin{bmatrix}
    f(\dot{s}_x(t_0 + \frac{i}{m} \tau_1 h), s_x(t_0 + \frac{i}{m} \tau_1 h), t_0 + \frac{i}{m} \tau_1 h)_{i=1}^m, \\
    f(\dot{s}_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), s_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), t_{\ell-1} + \frac{i}{m} \tau_\ell h)_{i=2, \ell=2}^{m,\mu}
    \end{bmatrix}$$
  
  ii.b) solve:
    
    $$0 = \begin{bmatrix}
    \mathcal{T}^d_{fo(s_x,s_x,id)}[t_0 + h](\dot{s}_x(t_0 + \frac{i}{m} \tau_1 h), s_x(t_0 + \frac{i}{m} \tau_1 h), t_0 + \frac{i}{m} \tau_1 h)_{i=1}^m, \\
    \mathcal{T}^d_{fo(s_x,s_x,id)}[t_0 + h](\dot{s}_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), s_x(t_{\ell-1} + \frac{i}{m} \tau_\ell h), t_{\ell-1} + \frac{i}{m} \tau_\ell h)_{i=2, \ell=2}^{m,\mu}
    \end{bmatrix}$$
  
  iii. determine new events from each component of $\mathcal{T}^d_{fo(s_x,s_x,id)}[t_0 + h]$ and update $\mu$ & $\tau$

- compute $x_1 = s_x(t_0 + h)$ and return
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Numerical Experiment #1: An Academical Example

- consider $f(\dot{x}(t), \dot{y}(t), x(t), y(t), t) = \left[ \frac{2|y(t)|\dot{y}(t) - \dot{x}(t)}{t^3 - t\pi - y(t)} \right]$, $t_0 = -\frac{2h}{\exp(1)}$ for stepsize $h$
- exact solution known $\rightarrow$ compute exact, consistent $x_0, y_0 = x(t_0), y(t_0)$ (initial value)
- first step is forced to cross at $\bar{t} = 0$ where $y(\bar{t}) = y(0) = 0$ and thus $f$ is non-differentiable
Numerical Experiment #1: An Academical Example

- consider \( f(\dot{x}(t), \dot{y}(t), x(t), y(t), t) = \left[ \frac{2|y(t)|\dot{y}(t) - \dot{x}(t)}{t^3 - t\pi - y(t)} \right] \), \( t_0 = -\frac{2h}{\exp(1)} \) for stepsize \( h \)
- exact solution known \( \rightarrow \) compute exact, consistent \( x_0, y_0 = x(t_0), y(t_0) \) (initial value)
- first step is forced to cross at \( \bar{t} = 0 \) where \( y(\bar{t}) = y(0) = 0 \) and thus \( f \) is non-differentiable

![conv plot (order:2)](smooth method)

![conv plot (order:2)](non-smooth method)
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On Real Time Managed Gas-Networks

GasLib-135 network from public data library: gaslib.zib.de
On Real Time Managed Gas-Networks

\[
\begin{align*}
\dot{p}_R &= \kappa \omega \frac{q_R - q_L}{\ell} \\
\dot{q}_L &= -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa \omega}{2D} \frac{q_L |q_L|}{p_L}
\end{align*}
\]
simplified 1D LR-pipe equations

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topological orientation (not necessarily flow direction)

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general flow balance equation

\[ \hat{q}^{(v)} + \sum_{e \rightarrow v} q^{(e)}_R = \sum_{e \leftarrow v} q^{(e)}_L \]

topological orientation

(not necessarily flow direction)
On Real Time Managed Gas-Networks

simplified 1D LR-pipe equations

\[ \dot{p}_R = \kappa \frac{d}{dt} \frac{q_R - q_L}{\ell} \]
\[ \dot{q}_L = -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa}{2D} \frac{d}{dt} \frac{q_L |q_L|}{p_L} \]

general flow balance equation

\[ \hat{q}^{(v)} + \sum_{e \rightarrow v} q_R^{(e)} = \sum_{e \leftarrow v} q_L^{(e)} \]

backward substituted flow balance equation

\[ q_R^{(e_0)} = q_L^{(e_4)} - \hat{q}^{(v)} - \sum_{i=1}^{3} q_R^{(e_i)} \]
On Real Time Managed Gas-Networks

simplified 1D LR-pipe equations

\[ \dot{p}_R = \kappa \dot{z} \frac{q_R - q_L}{\ell} \]
\[ \dot{q}_L = -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa \dot{z} q_L |q_L|}{p_L} \]

general flow balance equation

\[ \hat{q}^{(v)} + \sum_{e \rightarrow v} q_R^{(e)} = \sum_{e \leftarrow v} q_L^{(e)} \]

backward substituted flow balance equation

\[ q_R^{(e_0)} = q_L^{(e_4)} - \hat{q}^{(v)} - \sum_{i=1}^{3} q_R^{(e_i)} \]

control valve

\[ q_L = q_R = q_{\text{set}} \]
On Real Time Managed Gas-Networks

\[ \dot{p}_R = \kappa \frac{\dot{q}_R - q_L}{\ell} \]
\[ \dot{q}_L = -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa \lambda}{2D} \frac{q_L |q_L|}{p_L} \]

simplified 1D LR-pipe equations

\[ \hat{q}_v + \sum_{e \to v} q_{R(e)}^{(e)} = \sum_{e \leftarrow v} q_{L(e)}^{(e)} \]

general flow balance equation

\[ q_{R(e_0)}^{(e_0)} = q_{L(e_4)}^{(e_4)} - \hat{q}_v - \sum_{i=1}^{3} q_{R(e_i)}^{(e_i)} \]

backward substituted flow balance equation

\[ 0 = \max(-1, \min(1, \max(-q, \min(p_L - p_L, \min(p_R, p_L) - p_R, \max(q_{\text{set}} - q, p_L - \bar{p}_L, \bar{p}_R - p_R)))))) - \dot{q} \]
On Real Time Managed Gas-Networks

simplified 1D LR-pipe equations

\[ \dot{p}_R = \kappa \dot{z} \frac{q_R - q_L}{\ell} \]

\[ \dot{q}_L = -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa \dot{z}}{2D} \frac{q_L |q_L|}{p_L} \]

control valve

\[ q_L = q_R = q_{\text{set}} \]

Numerical Ex. #2

backward substituted flow balance equation

\[ q_R^{(e_0)} = q_L^{(e_4)} - \hat{q}(v) - \sum_{i=1}^{3} q_R^{(e_i)} \]

0 = max(−1, min(1, max(−q, min(p_L − p_L, min(p_R, p_L) − p_R, max(q_{\text{set}} − q, p_L − p_L, p_R − p_R)))))) − \dot{q}
On Real Time Managed Gas-Networks

\[ \dot{p}_R = \kappa \dot{q}_L \frac{q_R - q_L}{\ell} \]
\[ \dot{q}_L = -A \cdot \frac{p_R - p_L}{\ell} - \frac{\lambda \kappa}{2D} \frac{q_L |q_L|}{p_L} \]

simplified 1D LR-pipe equations

general flow balance equation

\[ \dot{q}(v) + \sum_{e \rightarrow v} q_R^{(e)} = \sum_{e \leftarrow v} q_L^{(e)} \]

backwards substituted flow balance equation

\[ q_R^{(e_0)} = q_L^{(e_4)} - \dot{q}(v) - \sum_{i=1}^{3} q_R^{(e_i)} \]

control valve

\( q_L = q_R = q_{\text{set}} \)

\[ 0 = \max(-1, \min(1, \max(-q, \min(p_L - \bar{p}_L, \min(\bar{p}_R, p_L) - p_R, \max(q_{\text{set}} - q, p_L - \bar{p}_L, \bar{p}_R - p_R)))))) - \dot{q} \]

Numerical Ex. #2

Total: ~137 abs values
Numerical Experiment #2: The Control Valve

the scenario …

- top plot are flows
- bottom plot are pressures
- Dashed lines are set point values to control behavior of control valve
Numerical Experiment #2: The Control Valve
Numerical Experiment #2: The Control Valve
Numerical Experiment #2: The Control Valve
Thank you for your attention.