Notes on Solving Non-Linear Equation Systems in OpenModelica

Status and Plans on Solving Non-Linear Equation Systems

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Motivation

You've never heard of Chaos theory? Non-linear equations? Strange attractors?

Michael Crichton, Jurassic Park

- Current status:
  - Which methods do we use?
  - How are details solved?
- Work in progress

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Outline

Systems of Non-Linear Equations

What are Algebraic Loops?

Transformation steps for simulation

$$\underline{0} = \underline{f}(\underline{x}(t), \underline{\dot{x}}(t), \underline{y}(t), \underline{u}(t), \underline{p}, t)$$

$$\Downarrow$$

$$\underline{0} = \underline{f}(\underline{x}(t), \underline{z}(t), \underline{u}(t), \underline{p}, t), \ \underline{z}(t) = \begin{pmatrix} \underline{\dot{x}}(t) \\ \underline{y}(t) \end{pmatrix}$$

$$\Downarrow$$

$$\underline{z}(t) = \begin{pmatrix} \underline{\dot{x}}(t) \\ \underline{y}(t) \end{pmatrix} = \underline{g}(\underline{x}(t), \underline{u}(t), \underline{p}, t)$$

$$\Downarrow$$

$$\underline{\dot{x}}(t) = \underline{h}(\underline{x}(t), \underline{u}(t), \underline{p}, t)$$
$$\underline{y}(t) = \underline{k}(\underline{x}(t), \underline{u}(t), \underline{p}, t)$$

Transformation example

$$\begin{aligned} f_2(z_2) &= 0 \\ f_4(z_1, z_2) &= 0 \\ f_3(z_2, z_3, z_5) &= 0 \\ f_5(z_1, z_3, z_5) &= 0 \\ f_1(z_3, z_4) &= 0 \end{aligned}$$

Algebraic loop (SCC)

$$\begin{aligned} f_3(z_2, z_3, z_5) &= 0 \\ f_5(z_1, z_3, z_5) &= 0 \end{aligned}$$

General form

$$f_1(x_1, x_2, \ldots x_n) = 0$$
$$f_2(x_1, x_2, \ldots x_n) = 0$$
$$\vdots$$
$$f_m(x_1, x_2, \ldots x_n) = 0$$

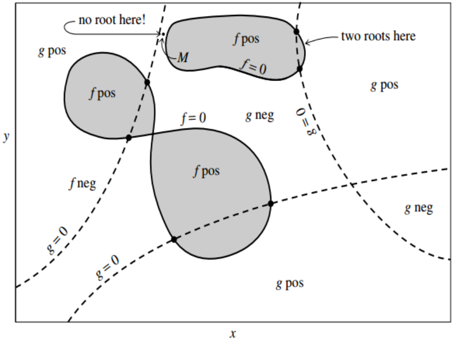
in compact matrix form:

$$\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$$

$$\boldsymbol{f}(\underline{x}) = 0$$

Example

$$f_1(x_1, x_2) = 0$$
$$f_2(x_1, x_2) = 0$$

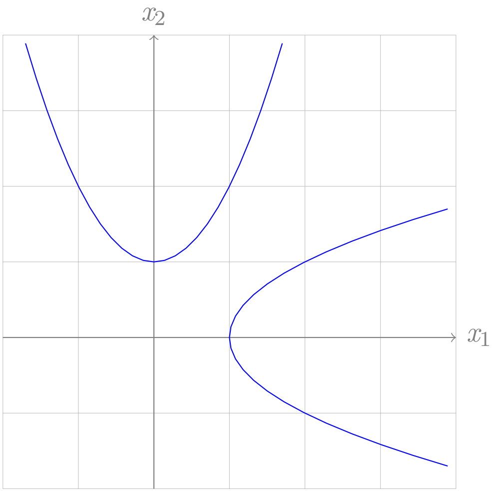


Example

$$x_1{}^2 - x_2 + \alpha = 0$$
$$-x_1 + x_2{}^2 + \alpha = 0$$

Solutions

- $\alpha = 1 \Rightarrow$ no solution.
- $\alpha = \frac{1}{4} \Rightarrow$ one solution $x_1 = x_2 = \frac{1}{2}$.
- $\alpha = 0 \Rightarrow$ two solutions $x_1 = x_2 = 0$ and $x_1 = x_2 = 1$.
- $\alpha = -1 \Rightarrow$ four solutions.



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Example

$$
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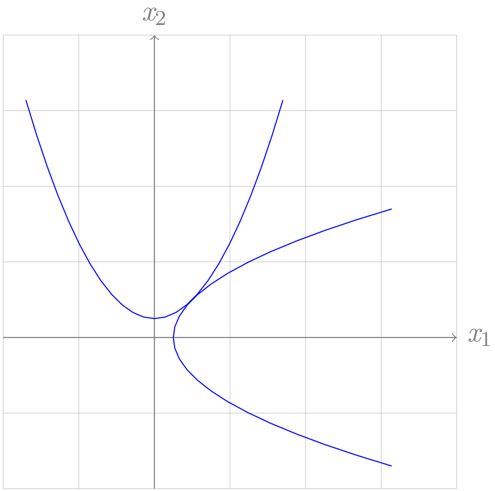

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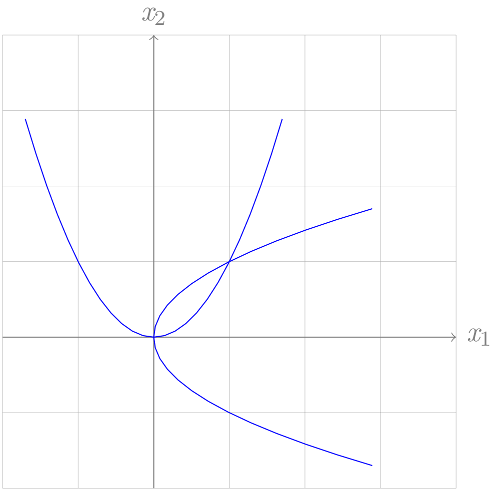

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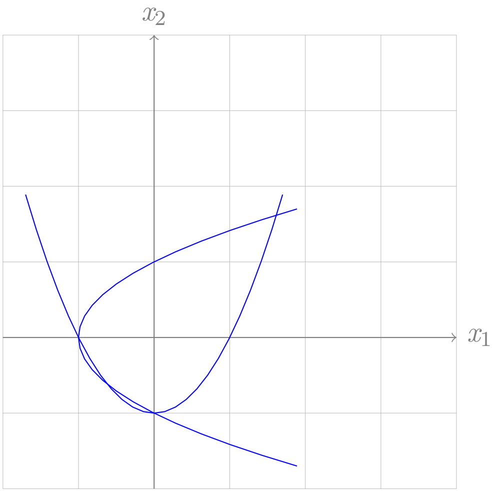
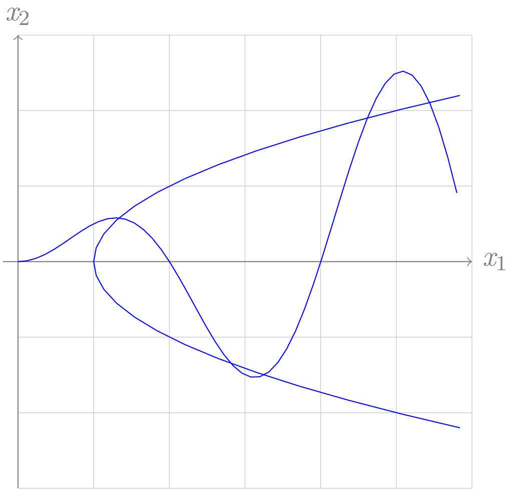


Example

$$\frac{1}{2}x_1 sin(\frac{1}{2}\pi x_1) - x_2 = 0$$
$$-x_1 + {x_2}^2 + 1 = 0$$

solution

- Countable infinite many solutions.



What are the crucial points?

Common things

General form

$$\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$$

$$\boldsymbol{f}(\underline{x}) = 0$$

Iteration instruction:

$$\underline{x}_{i+1} = \Phi(\underline{x}_i)$$

Initial Values: $\underline{x}_0 \in \mathbb{R}^n$

Crucial points

- Good initial values
- Quite accurate derivatives
- Fast linear solver

General problems

- Round-off effects and cancellation
- Modelica asserts

What are the crucial points?

Initial Values

Model with an algebraic loop

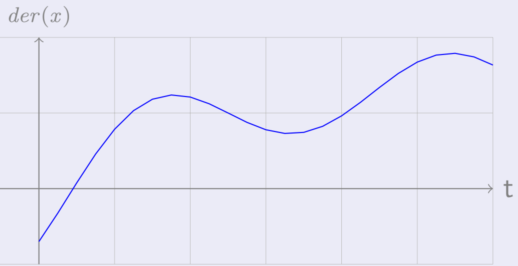
$$f_1(y_1, y_2) = 0$$
$$f_2(y_1, y_2) = 0$$

within

$$\dot{\underline{x}}(t) = functionODE(\underline{x}(t), \underline{u}(t), \underline{y}(t), \underline{p}, t)$$

.

Trajectory



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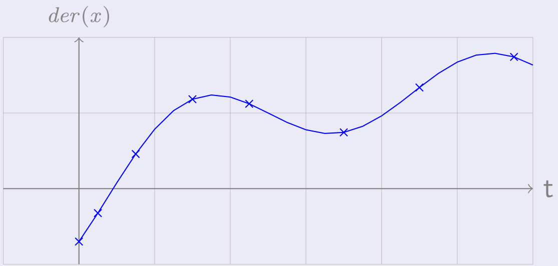
Integrator steps



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Extrapolation

$$y(t_*) = y_{k-1} + \frac{t_* - t_{k-1}}{t_k - t_{k-1}}(y_k - y_{k-1})$$

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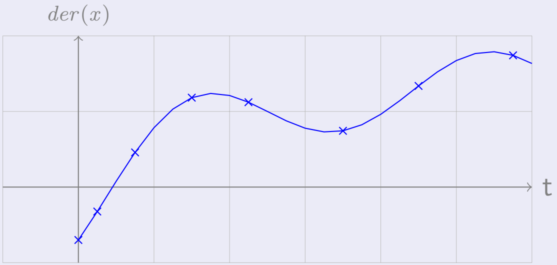

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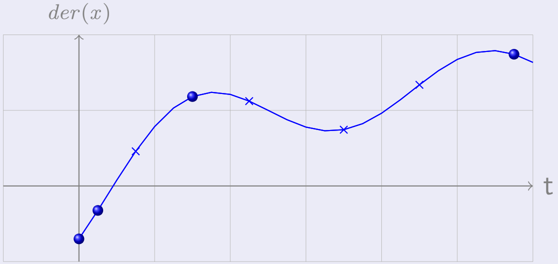
Jacobian evaluations



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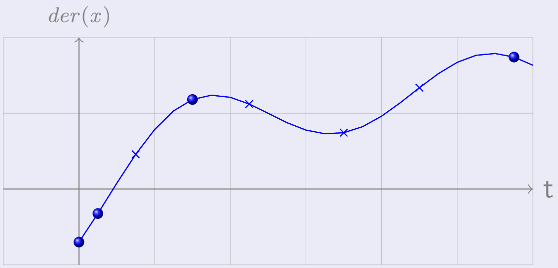

Solution

Every non-linear loop uses now lists for **context dependent extrapolation.**

$$\dot{f}(x) = \frac{(f(x+\delta) - f(x))}{\delta}$$

Drawback

Even if δ is selected optimal:

$$|\frac{\partial f(x)}{\partial x} - \frac{(f(x+\delta_{opt}) - f(x))}{\delta_{opt}}| \approx \sqrt{\epsilon_{RND}}$$

Some significant digits get lost by truncation.

What are the crucial points?

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Approach

Tried to sort such sums by nominal values, if states and derivatives are involved.
+heats=derCalls

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Trying of sorting terms of a sum by leading sign and adding them seperatly and peform the subtraction only once at the end.

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$\Rightarrow$ Use of symbolic jacobians.

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Approach

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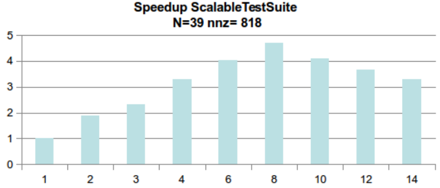
$\Rightarrow$ Use of symbolic jacobians with parallelization `-jacPar=N`



Damped Newton algorithm

- Damping strategy based on expected function decrease and validity of iteration step

Newton iteration step:

$$\begin{aligned} J_{\underline{F}}\left(\underline{x}^{(k)}\right) \cdot \underline{s}^{(k)} &= -\underline{F}\left(\underline{x}^{(k)}\right) \\ \underline{x}^{(k+1)} &= \underline{x}^{(k)} + \tau^{(k)} \underline{s}^{(k)} \end{aligned}$$

Damping parameter:

$$\tau^{(k)} \in [0, 1].$$

MinPack: HYBRID method

- Based on Powell's method, which is based on conjugate direction method.
- Through an Newton corrector step is has the same the convergence rate as it.
- Robostness through QR-Solver.
- $11.5 O(n^2)$

Possible homotopy functions

- Fixpoint-Homotopy:

$$\underline{H}(\underline{x},\lambda) = \lambda \underline{F}(\underline{x}) + (1-\lambda)(\underline{x}-\underline{x}_0) = \underline{0}$$

- Newton-Homotopy:

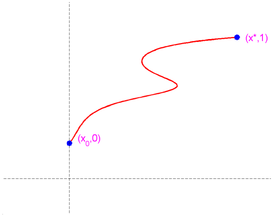
$$\underline{H}(\underline{x},\lambda) = \underline{F}(\underline{x}) - (1-\lambda)\underline{F}(\underline{x}_0) = \underline{0}$$

Simple example

$$f(x) = 2x - 4 + sin(2\pi x),$$

$$x_0 = 0.5, \quad x^* = 2.$$

Homotopy Path (Fixpoint)



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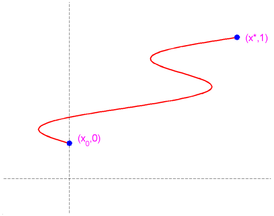
Homotopy Path (Newton)



Newton

- `homotopy`
  - Current default.
  - Total pivot as linear solver
  - Combined damping strategy with Modelica Asserts
- `kinsol`
  - Not in our hand.
  - KLU as linear solver
  - Currently no combination with the homotopy solver.
- `newton`
  - Current testing ground.
  - Lapack as linear solver
  - Currently no combination with the homotopy solver.

Hybrid

- Former default solver.
- Linpack as linear solver
- Developed initial value selection.
- Currently no combination with the homotopy solver.

Outlook

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- Finalize the equality of arms and compare!
- Includes same handling of initial values and homotopy combination.
- Compare own newton vs. kinsol with same linear solver.

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