Symbolic-Numeric Techniques for Improving Structural Analysis of DAEs

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Outline

What are differential-algebraic equations (DAEs)?

- Simple pendulum

$$0 = A = x'' + x\lambda$$
$$0 = B = y'' + y\lambda - G$$
$$0 = C = x^2 + y^2 - L^2 \qquad G\text{: gravity; } L\text{: length}$$

- $A,\ B$: differential equations; C: algebraic
- $x,\ y$: differential variables; λ: algebraic
- Write in an ODE form $Y' = \mathbf{f}(t, Y)$?

E.g.,
$$\begin{aligned} x' &= u \\ y' &= v \\ u' &= -x\lambda \\ v' &= -y\lambda + G \\ \lambda' &= f_5(t, x, y, u, v, \lambda) =? \end{aligned}$$

constraints:

$$C = x^2 + y^2 - L^2 = 0$$
$$C' = 2(xx' + yy') = 0$$

What are DAEs? (cont.)

- Need to differentiate C three times to determine λ'
- Differentiation index ν_d: the minimum number of differentiations required to express $Y' = \mathbf{f}(t, Y)$
- E.g., for pendulum, $\nu_d = 3$

Goal:

- Identify the constraints
- Find consistent initial values to start integrating a DAE initial value problem
- E.g., x, x', y, y' that satisfy

$$C = x^2 + y^2 - L^2 = 0 \qquad \text{(obvious)}$$
$$C' = 2(xx' + yy') = 0 \qquad \text{(hidden)}$$

Structural Analysis (SA) of DAEs

- Preprocessing stage
- Determines
  - structural index: ν_S
  - number of degrees of freedom: DOF
  - variables and derivatives to initialize
  - constraints
- Prescribes a solution scheme

SA methods

- Pantelides's algorithm, Pryce's Σ-method, ...
- Both succeed on many problems of practical interest
- but not all ...

The DAE problem

- General form:

$$F(\, t, \text{ the } x_j \text{ and derivatives of them}\,) = 0$$

  - n sufficiently differentiable functions: $F = (f_1, \ldots, f_n)$
  - n state variables: $x_j(t)$, $j = 1 : n$

- d/dt can appear anywhere in F
- It can be fully implicit

$$\text{E.g.,} \qquad 0 = f_1 = \frac{\big((x_1' \sin t)'\big)^2}{1 + (x_2')^2} + t^2 \cos x_2$$

- No restrictions on order and index of DAE

The Σ-method

- Form the $n \times n$ signature matrix $\Sigma = (\sigma_{ij})$ where

$$\sigma_{ij} = \begin{cases} \text{highest-order derivative of } x_j \text{ in } f_i, \text{ and} \\ -\infty \qquad \text{if } x_j \text{ does not occur in } f_i \end{cases}$$

- Example: pendulum

$$\begin{aligned} 0 &= A = x'' + x\lambda \\ 0 &= B = y'' + y\lambda - G \\ 0 &= C = x^2 + y^2 - L^2 \end{aligned} \qquad \Sigma = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} x & y & \lambda \end{array} \\ \begin{bmatrix} 2 & -\infty & 0 \\ -\infty & 2 & 0 \\ 0 & 0 & -\infty \end{bmatrix} \end{array}$$

- Find a set T of n positions (i, j), one in each row & column, such that $\sum_{(i,j)\in T} \sigma_{ij}$ is maximized
- This sum is $\text{Val}(\Sigma) = 2$
- T is a Highest Value Transversal (HVT) in Σ

- If $\mathrm{Val}(\Sigma)$ is finite, find the smallest nonnegative equation & variable offsets

  $\mathbf{c} = (c_1, \ldots, c_n), \quad \mathbf{d} = (d_1, \ldots, d_n)$:

  $d_j - c_i \geq \sigma_{ij}$ for all i, j, with equality on HVT

- structural index $\nu_S = \max_i c_i + \begin{cases} 1 & \text{if some } d_j = 0 \\ 0 & \text{otherwise} \end{cases}$

  Theorem. $\nu_S \geq \nu_d$ if SA succeeds; often the same

- Degrees of freedom $\mathrm{DOF} = \mathrm{Val}(\Sigma)$

$$\text{E.g.,} \quad \Sigma = \begin{array}{c|ccc|c} & x & y & \lambda & c_i \\ A & 2 & & 0 & 0 \\ B & & 2 & 0 & 0 \\ C & 0 & 0 & & 2 \\ d_j & 2 & 2 & 0 & \end{array}$$

(blanks in Σ denote $-\infty$)

$\mathrm{Val}(\Sigma) = 2, \ \nu_S = 2 + 1 = 3$

Solution scheme

- Solve DAE by stages, stage number k counts up from $k_d = -\max_j d_j$
- At stage k, solve $f_i^{(c_i+k)} = 0$ for i s.t. $c_i + k \geq 0$
  for unknowns $x_j^{(d_j+k)}$ for j s.t. $d_j + k \geq 0$
- Substitute found values "forward"

E.g., for pendulum, $\mathbf{c} = (0, 0, 2)$, $\mathbf{d} = (2, 2, 0)$, $k_d = -2$

k	solve	for	
-2	$0 = C = x^2 + y^2 - L^2$	x, y	*nonlinear*
-1	$0 = C' = 2(xx' + yy')$	x', y'	*linear*
0	$0 = A = x'' + x\lambda$	x'', y'', λ	*linear*
	$0 = B = y'' + y\lambda - G$		
	$0 = C'' = 2(xx'' + yy'' + x'^2 + y'^2)$		
≥ 1	$0 = (A, B, C'')^{(k)}$	$(x'', y'', \lambda)^{(k)}$	*linear*

Solution scheme (cont.)

Theorem. SA succeeds, locally, if can solve DAE up to stage $k = 0$ and determine $x_j^{(d_j)}$ uniquely

- The $n \times n$ System Jacobian $\mathbf{J} = (\mathbf{J}_{ij})$ where

$$\mathbf{J}_{ij} = \begin{cases} \partial f_i / \partial x_j^{(\sigma_{ij})} & \text{if } d_j - c_i = \sigma_{ij} \\ 0 & \text{otherwise, including } \sigma_{ij} = -\infty \end{cases}$$

- Stage $k = 0$ system (blanks in $\mathbf{J}$ denote 0)

$$\begin{bmatrix} 1 & & x \\ & 1 & y \\ 2x & 2y & \end{bmatrix} \begin{bmatrix} x'' \\ y'' \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ G \\ -2(xx' + yy') \end{bmatrix}$$

Theorem. A local unique solution exists if $\mathbf{J}$ is nonsingular

- For pendulum, $\det(\mathbf{J}) = -2(x^2 + y^2) = -2L^2 \neq 0$, success

Structural Analysis's failure

- Example [Mattsson & Söderlind, 1993]

$$0 = f_1 = x' - ty' + g_1(t), \qquad 0 = f_2 = x - ty + g_2(t)$$

$$\Sigma = \begin{array}{c c} & \begin{array}{cc} x & y \end{array} \quad c_i \\ \begin{array}{c} f_1 \\ f_2 \\ d_j \end{array} & \begin{array}{c} \begin{bmatrix} 1^\bullet & 1 \\ 0 & 0^\bullet \end{bmatrix} \begin{array}{c} 0 \\ 1 \end{array} \\ \begin{array}{cc} 1 & 1 \end{array} \end{array} \end{array} \qquad \mathbf{J} = \begin{array}{c c} & \begin{array}{cc} x & y \end{array} \\ \begin{array}{c} f_1 \\ f_2 \end{array} & \begin{bmatrix} 1 & -t \\ 1 & -t \end{bmatrix} \end{array}$$

- $\mathrm{Val}(\Sigma) = 1$, $\nu_S = 1$, $\det(\mathbf{J}) = 0$; SA fails

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- A simple fix: replace f_1 by $\overline{f}_1 = f_1 - f_2' = y + g_1(t) - g_2'(t)$

$$\overline{\Sigma} = \begin{array}{c c} & \begin{array}{cc} x & y \end{array} \quad c_i \\ \begin{array}{c} \overline{f}_1 \\ f_2 \\ d_j \end{array} & \begin{array}{c} \begin{bmatrix} & 0^\bullet \\ 0^\bullet & 0 \end{bmatrix} \begin{array}{c} 0 \\ 0 \end{array} \\ \begin{array}{cc} 0 & 0 \end{array} \end{array} \end{array} \qquad \overline{\mathbf{J}} = \begin{array}{c c} & \begin{array}{cc} x & y \end{array} \\ \begin{array}{c} \overline{f}_1 \\ f_2 \end{array} & \begin{bmatrix} & 1 \\ 1 & -t \end{bmatrix} \end{array}$$

- $\mathrm{Val}(\overline{\Sigma}) = 0 < 1 = \mathrm{Val}(\Sigma)$, $\det(\overline{\mathbf{J}}) = -1$, SA succeeds

Structural Analysis's failure

- Example [Mattsson & Söderlind, 1993]

$$0 = f_1 = x' - ty' + g_1(t), \qquad 0 = f_2 = x - ty + g_2(t)$$

$$\Sigma = \begin{array}{c} \\ f_1 \\ f_2 \\ d_j \end{array} \begin{array}{c} \begin{array}{cc} x & y \end{array} \\ \begin{bmatrix} 1^\bullet & 1 \\ 0 & 0^\bullet \end{bmatrix} \\ \begin{array}{cc} 1 & 1 \end{array} \end{array} \begin{array}{c} c_i \\ 0 \\ 1 \\ \\ \end{array} \qquad \mathbf{J} = \begin{array}{c} \\ f_1 \\ f_2 \end{array} \begin{array}{c} \begin{array}{cc} x & y \end{array} \\ \begin{bmatrix} 1 & -t \\ 1 & -t \end{bmatrix} \end{array}$$

- $\mathrm{Val}(\Sigma) = 1$, $\nu_S = 1$, $\det(\mathbf{J}) = 0$; SA fails

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- A simple fix: replace f_1 by $\bar{f}_1 = f_1 - f_2' = y + g_1(t) - g_2'(t)$

$$\bar{\Sigma} = \begin{array}{c} \\ \bar{f}_1 \\ f_2 \\ d_j \end{array} \begin{array}{c} \begin{array}{cc} x & y \end{array} \\ \begin{bmatrix} & 0^\bullet \\ 0^\bullet & 0 \end{bmatrix} \\ \begin{array}{cc} 0 & 0 \end{array} \end{array} \begin{array}{c} c_i \\ 0 \\ 0 \\ \\ \end{array} \qquad \bar{\mathbf{J}} = \begin{array}{c} \\ \bar{f}_1 \\ f_2 \end{array} \begin{array}{c} \begin{array}{cc} x & y \end{array} \\ \begin{bmatrix} & 1 \\ 1 & -t \end{bmatrix} \end{array}$$

- $\mathrm{Val}(\bar{\Sigma}) = 0 < 1 = \mathrm{Val}(\Sigma)$, $\det(\bar{\mathbf{J}}) = -1$, SA succeeds

- Another simple fix: change of variables
- Set $z = x - ty$; then $x' - ty' = y + z'$

$$
\begin{aligned}
0 &= f_1 = y + z' + g_1(t) \\
0 &= f_2 = \phantom{y + {}} z \phantom{{}'} + g_2(t)
\end{aligned}
$$

$$
\overline{\Sigma} = \begin{array}{c|cc|c} & y & z & c_i \\ \hline f_1 & 0^\bullet & 1 & 0 \\ f_2 & & 0^\bullet & 1 \\ \hline d_j & 0 & 1 & \end{array}
\qquad
\overline{\mathbf{J}} = \begin{array}{c|cc} & y & z \\ \hline f_1 & 1 & 1 \\ f_2 & & 1 \end{array}
$$

- $\mathrm{Val}(\overline{\Sigma}) = 0 < 1 = \mathrm{Val}(\Sigma)$, $\det(\overline{\mathbf{J}}) = 1$
- SA succeeds; index 2
- Use $x = z + ty$ to recover x

Methods

Problem statement

- **J** is identically singular
- Fix SA's failure in a systematic way

Two conversion methods

- Linear Combination of equations (LC method)
- Expression Substitution (ES method)

Conjecture

- May have a better problem formulation if $\mathrm{Val}(\Sigma)$ is reduced

Example of LC method

$$
\begin{aligned}
0 = f_1 &= -x_1' + x_3 \\
0 = f_2 &= -x_2' + x_4 \\
0 = f_3 &= \quad x_1 x_2 + g_1(t) \\
0 = f_4 &= \quad x_1 x_4 + x_2 x_3 + x_1 + x_2 + g_2(t)
\end{aligned}
$$

$$
\Sigma = \begin{array}{c|cccc|c}
 & x_1 & x_2 & x_3 & x_4 & c_i \\
\hline
f_1 & 1 & & 0^\bullet & & 0 \\
f_2 & & 1^\bullet & & 0 & 0 \\
f_3 & 0^\bullet & 0 & & & 1 \\
f_4 & \boxed{0} & \boxed{0} & 0 & 0^\bullet & 0 \\
\hline
d_j & 1 & 1 & 0 & 0 &
\end{array}
\qquad
\mathbf{J} = \begin{array}{c|cccc|}
 & x_1 & x_2 & x_3 & x_4 \\
\hline
f_1 & -1 & & 1 & \\
f_2 & & -1 & & 1 \\
f_3 & x_2 & x_1 & & \\
f_4 & & & x_2 & x_1
\end{array}
$$

$\boxed{}$: $d_j - c_i > \sigma_{ij} \geq 0$

$\det(\mathbf{J}) = 0$

- $\mathrm{Val}(\Sigma) = 1$, $\nu_S = 2$, $\mathbf{J}$ singular; SA fails

LC method: inspiration

$$\mathbf{J} = \frac{\partial(f_1, f_2, f_3', f_4)}{\partial(x_1', x_2', x_3, x_4)} = \begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ d_j \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \end{array} \\ \left[\begin{array}{cccc} -1 & & 1 & \\ & -1 & & 1 \\ x_2 & x_1 & & \\ & & x_2 & x_1 \end{array}\right] \\ \begin{array}{cccc} 1 & 1 & 0 & 0 \end{array} \end{array} \begin{array}{c} c_i \\ 0 \\ 0 \\ 1 \\ 0 \\ \\ \end{array}$$

- Find $u = (x_2, x_1, 1, -1)^T \in \ker(\mathbf{J}^T)$
- u does not depend on x_1', x_2', x_3, x_4—the $x_j^{(d_j)}$'s
- $\bar{f} \leftarrow u^T \cdot (f_1, f_2, f_3', f_4)^T = -x_1 - x_2 + g_1' - g_2$
- $\partial\bar{f}/\partial(x_1', x_2', x_3, x_4) = u^T\mathbf{J} = \mathbf{0}^T$
- Replace an f_i by $\bar{f}$, decrease $\mathrm{Val}(\Sigma)$
- Cannot replace f_3 since f_3' in $\bar{f}$; otherwise f_3 is lost

LC method: inspiration

$$\mathbf{J} = \frac{\partial(f_1, f_2, f_3', f_4)}{\partial(x_1', x_2', x_3, x_4)} = \begin{array}{c|cccc|c} & x_1 & x_2 & x_3 & x_4 & c_i \\ \hline f_1 & -1 & & 1 & & 0 \\ f_2 & & -1 & & 1 & 0 \\ f_3 & x_2 & x_1 & & & 1 \\ f_4 & & & x_2 & x_1 & 0 \\ \hline d_j & 1 & 1 & 0 & 0 & \end{array}$$

- Find $u = (x_2, x_1, 1, -1)^T \in \ker(\mathbf{J}^T)$
- u does not depend on x_1', x_2', x_3, x_4—the $x_j^{(d_j)}$'s
- $\bar{f} \leftarrow u^T \cdot (f_1, f_2, f_3', f_4)^T = -x_1 - x_2 + g_1' - g_2$
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$$\text{Pick} \quad 0 = f_4 = x_1 x_4 + x_2 x_3 + x_1 + x_2 + g_2(t)$$

$$\text{replace it by} \quad 0 = \overline{f} = -x_1 - x_2 + g_1' - g_2$$

$$\overline{\Sigma} = \begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ \overline{f} \\ d_j \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \end{array} \\ \left[\begin{array}{cccc} 1 & & 0^\bullet & \\ & 1 & & 0^\bullet \\ 0 & 0^\bullet & & \\ 0^\bullet & 0 & & \end{array}\right] \\ \begin{array}{cccc} 1 & 1 & 0 & 0 \end{array} \end{array} \begin{array}{c} c_i \\ 0 \\ 0 \\ 1 \\ 1 \\ \\ \end{array} \qquad \overline{\mathbf{J}} = \begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ \overline{f} \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \end{array} \\ \left[\begin{array}{cccc} -1 & & 1 & \\ & -1 & & 1 \\ x_2 & x_1 & & \\ -1 & -1 & & \end{array}\right] \end{array}$$

- $\mathrm{Val}(\overline{\Sigma}) = 0 < 1 = \mathrm{Val}(\Sigma)$, $\det(\overline{\mathbf{J}}) = x_2 - x_1$
- SA succeeds if $x_1 \neq x_2$; index 2
- Since $u_4 = -1 \neq 0$, can always recover

  $f_4 = (\overline{f} - u_1 f_1 - u_2 f_2 - u_3 f_3')/u_4$

LC method: outline

Compute	Example
symbolic form of $\mathbf{J}$	
$u \in \ker(\mathbf{J}^T)$, $\mathbf{J}^T u = 0$	$u = \left(x_2,\ x_1,\ 1,\ -1\right)^T$
$I = \{\, i :\ u_i \neq 0 \,\}$	$I = \{\, 1, 2, 3, 4 \,\}$
$\theta = \min_{i \in I} c_i$	$\mathbf{c} = (0, 0, 1, 0),\ \ \theta = 0$
$K = \{\, k \in I :\ c_k = \theta \,\}$	$K = \{\, 1, 2, 4 \,\}$
Pick $k \in K$, replace f_k by	$\overline{f} = u_1 f_1 + u_2 f_2 + u_3 f_3' + u_4 f_4$
$\overline{f} = \sum_{i \in I} u_i f_i^{(c_i - \theta)}$	$= -x_1 - x_2 + g_1' - g_2$

LC method: theory

- Replace f_k ($k \in K$) by $\overline{f} = \sum_{i \in I} u_i f_i^{(c_i - \theta)}$
- Theorem. $\mathrm{Val}(\overline{\Sigma}) < \mathrm{Val}(\Sigma)$ if

  $$\text{HOD of } x_j \text{ in } u \; < d_j - \theta \quad \text{for all } j$$

  HOD—highest-order derivatives
- Can proceed iteratively if new **J** still singular
- At most $\mathrm{Val}(\Sigma)$ iterations

Inspiration by LC method

- Combination of rows (equations) in Σ
- What about columns (derivatives)?

LC method: theory

- Replace f_k ($k \in K$) by $\bar{f} = \sum_{i \in I} u_i f_i^{(c_i - \theta)}$
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  HOD—highest-order derivatives
- Can proceed iteratively if new **J** still singular
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Inspiration by LC method

- Combination of rows (equations) in Σ
- What about columns (derivatives)?

ES method

- Linear combination of variables and derivatives
- Common Expression Substitution

Example:

$$0 = f_1 = x_1 + e^{-x_1' - x_2 x_2''} + g_1(t)$$
$$0 = f_2 = x_1 + x_2 x_2' + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1 & 2 & 0 \\ f_2 & 0 & 1 & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c} \\ f_1 \\ f_2 \end{array} \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{bmatrix} -\mu & -\mu x_2 \\ 1 & x_2 \end{bmatrix} \end{array}$$

$$\mu = e^{-x_1' - x_2 x_2''}$$

- $\det(\mathbf{J}) = 0$, SA fails; reports index 1, $\mathrm{Val}(\Sigma) = 2$
- Cannot apply LC since x_1', x_2'' in $u = (1, \mu)^T \in \ker(\mathbf{J}^T)$

$$0 = f_1 = x_1 + e^{-x_1' - x_2 x_2''} + g_1(t)$$
$$0 = f_2 = x_1 + x_2 x_2' + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1^\bullet & 2 & 0 \\ f_2 & 0 & 1^\bullet & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c|cc|} & x_1 & x_2 \\ f_1 & -\mu & -\mu x_2 \\ f_2 & 1 & x_2 \end{array}$$

Step 1: Process SA result

- Find $u \in \ker(\mathbf{J})$ — $u = (x_2, -1)^T$
- $K = \{ j : u_j \neq 0 \}$ — $K = \{1, 2\}$
- $I = \{ i : d_j - c_i = \sigma_{ij}$ for some $j \in K \}$ — $I = \{1, 2\}$
- $C = \max_{i \in I} c_i$ — $C = 1$
- pick $k \in K$ — $k = 2$

$$0 = f_1 = x_1 + e^{-x_1' - x_2 x_2''} + g_1(t)$$
$$0 = f_2 = x_1 + x_2 x_2' + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1^\bullet & 2 & 0 \\ f_2 & 0 & 1^\bullet & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c|cc} & x_1 & x_2 \\ f_1 & -\mu & -\mu x_2 \\ f_2 & 1 & x_2 \end{array}$$

Step 2: Introduce $|K| - 1$ variables

$$y_j = x_j^{(d_j - C)} - \frac{u_j}{u_k} x_k^{(d_k - C)} \qquad \text{for } j \in K \backslash \{ k \}$$

Example: $j = 1,\ k = 2,\ C = 1$

$$y_1 = x_1^{(1-1)} - \frac{x_2}{-1} x_2^{(2-1)} = x_1 + x_2 x_2'$$

Identify common expressions

$$0 = f_1 = x_1 + e^{-x_1' - x_2 x_2''} + g_1(t)$$
$$0 = f_2 = x_1 + x_2 x_2' + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1^\bullet & 2 & 0 \\ f_2 & 0 & 1^\bullet & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c|cc|} & x_1 & x_2 \\ f_1 & -\mu & -\mu x_2 \\ f_2 & 1 & x_2 \end{array}$$

Step 3: Replace each $x_j^{(d_j - c_i)}$ by $\left(y_j + \frac{u_j}{u_k} x_k^{(d_k - C)}\right)^{(C - c_i)}$

Example:

replace	by	in
$x_1' = x_1^{(d_1 - c_1)}$	$(y_1 - x_2 x_2')^{(C-c_1)} = y_1' - x_2 x_2'' - x_2'^2$	f_1
$x_1 = x_1^{(d_1 - c_2)}$	$(y_1 - x_2 x_2')^{(C-c_2)} = y_1 - x_2 x_2'$	f_2

Perform expression substitutions

$$0 = \bar{f}_1 = x_1 + e^{-(y_1' - \cancel{x_2 x_2''} - x_2'^2) - \cancel{x_2 x_2''}} + g_1(t)$$
$$0 = \bar{f}_2 = y_1 - \cancel{x_2 x_2'} + \cancel{x_2 x_2'} + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1^\bullet & 2 & 0 \\ f_2 & 0 & 1^\bullet & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c|cc} & x_1 & x_2 \\ f_1 & -\mu & -\mu x_2 \\ f_2 & 1 & x_2 \end{array}$$

Step 3: Replace each $x_j^{(d_j - c_i)}$ by $\left(y_j + \frac{u_j}{u_k} x_k^{(d_k - C)}\right)^{(C - c_i)}$

Example:	replace	by	in
	$x_1' = x_1^{(d_1 - c_1)}$	$(y_1 - x_2 x_2')^{(C - c_1)} = y_1' - x_2 x_2'' - x_2'^2$	f_1
	$x_1 = x_1^{(d_1 - c_2)}$	$(y_1 - x_2 x_2')^{(C - c_2)} = y_1 - x_2 x_2'$	f_2

Perform expression substitutions

$$0 = \bar{f}_1 = x_1 + e^{-y_1' + x_2'^2} + g_1(t)$$
$$0 = \bar{f}_2 = y_1 + x_1^2 + g_2(t),$$

$$\Sigma = \begin{array}{c|cc|c} & x_1 & x_2 & c_i \\ f_1 & 1^\bullet & 2 & 0 \\ f_2 & 0 & 1^\bullet & 1 \\ d_j & 1 & 2 & \end{array} \qquad \mathbf{J} = \begin{array}{c|cc} & x_1 & x_2 \\ f_1 & -\mu & -\mu x_2 \\ f_2 & 1 & x_2 \end{array}$$

Step 4: Simplify each equation

Example:	replace	by	in
	$x_1' = x_1^{(d_1-c_1)}$	$(y_1 - x_2 x_2')^{(C-c_1)} = y_1' - x_2 x_2'' - x_2'^2$	f_1
	$x_1 = x_1^{(d_1-c_2)}$	$(y_1 - x_2 x_2')^{(C-c_2)} = y_1 - x_2 x_2'$	f_2

Perform expression substitutions

$$0 = \bar{f}_1 = x_1 + e^{-y_1' + x_2'^2} + g_1(t)$$
$$0 = \bar{f}_2 = y_1 + x_2^2 + g_2(t)$$
$$0 = g_1 = -y_1 + x_1 + x_2 x_2'$$

$$\overline{\Sigma} = \begin{array}{c|ccc|c} & x_1 & x_2 & y_1 & c_i \\ \bar{f}_1 & 0 & 1 & 1^\bullet & 0 \\ \bar{f}_2 & & 0^\bullet & 0 & 1 \\ g_1 & 0^\bullet & 1 & \boxed{0} & 0 \\ d_j & 0 & 1 & 1 & \end{array} \qquad \overline{\mathbf{J}} = \begin{array}{c|ccc|} & x_1 & x_2 & y_1 \\ \bar{f}_1 & 1 & 2\alpha x_2' & -\alpha \\ \bar{f}_2 & & 2x_2 & 1 \\ g_1 & 1 & x_2 & \end{array}$$

$$\alpha = e^{-y_1' + x_2'^2}$$

Step 5: Append $|K| - 1$ equations

$$0 = g_j = -y_j + x_j^{(d_j - C)} - \frac{u_j}{u_k} x_k^{(d_k - C)} \qquad \text{for } j \in K \backslash \{ k \}$$

These g_j prescribe the substitutions

$$0 = \overline{f}_1 = x_1 + e^{-y_1' + x_2'^2} + g_1(t)$$

$$0 = \overline{f}_2 = y_1 + x_2^2 + g_2(t)$$

$$0 = g_1 = -y_1 + x_1 + x_2 x_2'$$

$$\overline{\Sigma} = \begin{array}{c|ccc|c} & x_1 & x_2 & y_1 & c_i \\ \hline \overline{f}_1 & 0 & 1 & 1^\bullet & 0 \\ \overline{f}_2 & & 0^\bullet & 0 & 1 \\ g_1 & 0^\bullet & 1 & \boxed{0} & 0 \\ \hline d_j & 0 & 1 & 1 & \end{array} \qquad \overline{\mathbf{J}} = \begin{array}{c|ccc} & x_1 & x_2 & y_1 \\ \hline \overline{f}_1 & 1 & 2\alpha x_2' & -\alpha \\ \overline{f}_2 & & 2x_2 & 1 \\ g_1 & 1 & x_2 & \end{array}$$

$$\alpha = e^{-y_1' + x_2'^2}$$

SA result:

- $\mathrm{Val}(\overline{\Sigma}) = 1 < 2 = \mathrm{Val}(\Sigma)$
- SA succeeds if $\det(\overline{\mathbf{J}}) = (2\alpha - 1)x_2 + 2\alpha x_2' \neq 0$
- Index 2

ES method: Outline

- Find $u \in \ker(\mathbf{J})$
- Use u and SA result to find common expressions
- Introduce new variables and substitute them for these expressions in f_i
- Simplify f_i to obtain new $\overline{f}_i$
- Append equations g that prescribe the substitutions
- Theorem. $\text{Val}(\overline{\Sigma}) < \text{Val}(\Sigma)$ if

$$\text{HOD of } x_j \text{ in } u \leq \begin{cases} d_j - C - 1 & \text{if } j \in K \\ d_j - C & \text{otherwise} \end{cases}$$

$$d_j - C \geq 0 \qquad \text{for all } j \in K$$

Progress

- Arbitrarily construct DAEs on which SA fails
- Use LC or ES method to fix them systematically
- Practical problems

Problem	Reference	Method	Result
Robot arm	Campbell et al. (1995)	ES[1], LC	correct index
Transistor amplifier	Mazzia et al. (2003)	LC[2]	correct index
Ring modulator	Mazzia et al. (2003)	LC[2]	correct index
Coupled DAE[3]	Scholz et al. (2013)	LC	correct index
Reissig's DAE	Reissig et al. (1999)	LC	correct index

[1] Done by Pryce (1998)
[2] Done by Nedialkov & Pryce
[3] 4×4 linear constant coefficient DAE

Conclusion

- Identify SA's failure: identically singular **J**
- Remedies: symbolic-numeric conversion methods
  - LC method: Linear Combination of equations
  - ES method: Common Expression Substitutions

  Goal: reduce Val(Σ)
- MATLAB package DAE Structural Analyzer
  `www.cas.mcmaster.ca/~nedialk/daesa`
- Combine DAESA with MATLAB's symbolic toolbox
- A prototype implementation of LC and ES methods

References

- G. Tan, N. Nedialkov, and J. Pryce. *Symbolic-numeric methods for improving structural analysis of DAEs.* arXiv:1505.03445 [cs.SC]. PDF
- *DAESA — a Matlab Tool for Structural Analysis of DAEs: Theory & Algorithm.* To appear in ACM TOMS.
- N. Nedialkov and J. Pryce. Solving Differential-Algebraic Equations by Taylor Series (I), (II), (III)
- J. Pryce. *A simple structural analysis method for DAEs*. BIT, 41(2):364–394, 2001.
- ———. *Solving high-index DAEs by Taylor Series. Numerical Algorithms*. 19:195–211, 1998.