Lecture 4

Simulation of differential-algebraic equations

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Outline

- *Structural index - introduction and definition*
- *Consistent initial conditions*
- *Pantelides algorithm – initial conditions and structural index*
- *Index reduction with dummy derivatives*
- *Summary*

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Structural index

An important step in the procedure to transfer the model to C code is to perform index reduction (and find consistent initial conditions). Index reduction requires that you know the index of the model. As we know it is a difficult problem in general to determine index; a method based on model structure is typically used.

Structural index can be defined in many ways. One way, for the DAE

$$A\dot{x} + Bx = 0$$

the structural index is the index the DAE has for *almost all* A and B with the same structure.

- direct generalization to non-linear systems
- can be computed with Pantelides algorithm, which will be used also for other purposes

Structural index - introductory example

Let $x = (x_1, x_2) \in \mathbb{R}^2$ and consider the index 1 model

$$\begin{aligned} \dot{x}_1 &= x_1 + x_2 + u \\ 0 &= -2x_1 + x_2 \end{aligned}$$

	$\dot{x}_1$	x_2
e_1	X	X
e_2		X

The highest differentiated variables are $x_{hd} = (\dot{x}_1, x_2)$

DAE has index 1 for almost all coefficients in front of the x variables, only when coefficients in front of $\dot{x}_1$ in e_1 or x_2 in e_2 is 0 we have a problem.

Conclusions: we can from the table on the right determine that this model has (structural-)index 1.

$$F(\dot{x}_1, x_1, x_2) = 0$$

has low index (locally) if

$$\left.\frac{\partial F(\dot{x}_1, x_1, x_2)}{\partial x_{hd}}\right|_{\dot{x}_1 = x_1^{\prime,*}, x_1 = x_1^*, x_2 = x_2^*}$$

has full rank

Structural index - introductory example

Let $x = (x_1, x_2, x_3) \in \mathbb{R}^3$

$$\begin{aligned} \dot{x}_1 &= x_1 + x_2 + x_3 + u \\ 0 &= -2x_1 + x_2 \\ 0 &= x_1 + x_2 + u \end{aligned}$$

	$\dot{x}_1$	x_2	x_3
e_1	X	X	X
e_2		X	
e_3		X	

From the table on the right we see that *regardless* of which coefficient we have for the variables, the DAE has index > 1. The DAE has a unique solution since

$$|\lambda E - A| = \lambda + 3 \neq 0, \quad (x_1, x_2, x_3) = (-\frac{1}{3}u, -\frac{2}{3}u, -\frac{1}{3}\dot{u})$$

Turns out you can determine structural index only by looking at the tables on the right. This is also direct to automatically do for large scale models in general purpose simulation environments.

Structural index vs. the differential index

Let ν and ν_{str} be the index and the structural index respectively for

$$F(t, y', y) = 0$$

Unfortunately, both the situations below are possible

$$\nu < \nu_{str}, \qquad \nu \leq \nu_{str}$$

$$\nu_{str} < \nu, \qquad \nu_{str} \leq \nu$$

What is the consequence of this for a method that relies on a structural algorithm for index reduction?

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Now, what was the problem with initial conditions?

For an initial value problem for an ODE

$$\dot{x} = f(x, t), \quad x(t_0) = x_0$$

there are no limitations (except domain for f) for the initial condition x_0.

For a DAE

$$F(t, y, \dot{y}) = 0$$

it is not sufficient that $\dot{y}(t_0)$ and $y(t_0)$ fulfills

$$F(t_0, y_0, \dot{y}(t_0)) = 0$$

Now, what was the problem with initial conditions?

For example, remember the DAE from the first DAE lecture

$$\begin{aligned} \dot{x}_1 + x_2 + x_3 &= f_1 \\ \dot{x}_2 + x_1 &= f_2 \\ x_2 &= f_3 \end{aligned} \qquad \begin{aligned} x_1(t) &= f_2(t) - \dot{f}_3(t) \\ x_2(t) &= f_3(t) \\ x_3(t) &= f_1(t) - f_3(t) - \dot{f}_2(t) + \ddot{f}_3(t) \end{aligned}$$

Here, no freedom at all and the initial conditions has to satisfy

$$\begin{aligned} x_1(t_0) &= f_2(t_0) - \dot{f}_3(t_0) \\ x_2(t_0) &= f_3(t_0) \\ x_3(t_0) &= f_1(t_0) - f_3(t_0) - \dot{f}_2(t_0) + \ddot{f}_3(t_0) \end{aligned}$$

Problem

We do not want to solve the DAE to find initial conditions!

Pantelides algorithm - consistent initial conditions

Finding a consistent initial condition $(y(t_0), \dot{y}(t_0), t_0)$ for a DAE

$$F(y, \dot{y}, t) = 0$$

with unknown index is a difficult problem in general. By differentiation we can obtain "hidden" conditions on the initial condition.

Pantelides algorithm

Graph theoretical approach to find the conditions that has to be satisfied and solved by a numerical equation solver.

- Good because based on equation structure only, possible to make automatic
- Bad based on equation structure only, does not give analytical results

- Can be used to compute differential index
- Can be used for index reduction. Will come back to this.

Pantelides algorithm

We know that given a DAE

$$F(\dot{y}, y, t) = 0$$

we can differentiate well chosen equation a suitable number of times to obtain a model including all constraints for the initial condition.

$$\begin{aligned} F(\dot{y}, y, t) &= 0 \\ \frac{d}{dt} F(\dot{y}, y, t) &= 0 \\ \frac{d^2}{dt^2} F(\dot{y}, y, t) &= 0 \\ &\vdots \\ \frac{d^j}{dt^j} F(\dot{y}, y, t) &= 0 \end{aligned}$$

Two questions:

- which equations?
- differentiate how many times?

The small example again

$$e_1 : \dot{x}_1 + x_2 + x_3 = f_1$$
$$e_2 : \dot{x}_2 + x_1 = f_2$$
$$e_3 : x_2 = f_3$$

Differentiate e_2 once and e_3 twice and collect the equations. These 6 equations can be solved for the 6 variables $(x_1(0), \dot{x}_1(0), x_2(0), \dot{x}_2(0), \ddot{x}_2(0), x_3(0))$ for a consistent initial condition

$$e_1 : \dot{x}_1 + x_2 + x_3 = f_1$$
$$e_2 : \dot{x}_2 + x_1 = f_2$$
$$\dot{e}_2 : \ddot{x}_2 + \dot{x}_1 = \dot{f}_2$$
$$e_3 : x_2 = f_3$$
$$\dot{e}_3 : \dot{x}_2 = \dot{f}_3$$
$$\ddot{e}_3 : \ddot{x}_2 = \ddot{f}_3$$

The new DAE $(e_1, \dot{e}_2, \ddot{e}_3)$ is index 1 (see next slide) and we had to differentiate e_3 twice. This is no coincidence.

The small example again

$$e_1 : \dot{x}_1 + x_2 + x_3 = f_1$$
$$\dot{e}_2 : \ddot{x}_2 + \dot{x}_1 = \dot{f}_2$$
$$\ddot{e}_3 : \ddot{x}_2 = \ddot{f}_3$$

$$\Rightarrow$$

$$\ddot{e}_3 : \ddot{x}_2 = \ddot{f}_3$$
$$\dot{e}_2 : \dot{x}_1 = \dot{f}_2 - \ddot{f}_3$$
$$e_1 : x_3 = f_1 - \dot{x}_1 + x_2 = f_1 - \dot{f}_2 - \ddot{f}_3 + x_2$$

Initial condition, example

For the model (1-DOF)

$$e_1: \ \dot{x}_1 + \dot{x}_2 = a(t), \quad e_2: \ x_1 + x_2^2 = b(t)$$

we can differentiate equation e_2 to obtain the constraint

$$\dot{e}_2: \ \dot{x}_1 + 2x_2\dot{x}_2 = b'(t)$$

and we are done since $(\dot{x}_1, \dot{x}_2)$ can be solved for in $(e_1, \dot{e}_2)$ (if $1 \neq 2ax_2$).

The initial condition is therefore obtained by solving

$$\begin{aligned}
\dot{x}_1(t_0) + \dot{x}_2(t_0) &= a(t_0) \\
x_1(t_0) + x_2^2(t_0) &= b(t_0) \\
\dot{x}_1(t_0) + 2x_2(t_0)\dot{x}_2(t_0) &= \dot{b}(t_0)
\end{aligned}$$

for $(x_1(t_0), x_2(t_0), \dot{x}_1(t_0), \dot{x}_2(t_0))$. With 4 unknowns and three equations, 1-DOF which we kind of knew.

Initial condition, example, cont.

For the model

$$\dot{x}_1 = x_1 + x_2, \quad 0 = x_1 + 2x_2 + a$$

we can not obtain any new constraints on the initial condition by differentiating the equations.

For every new differentiation, we get a new variable. Differentiation gives

$$\begin{aligned} \ddot{x}_1 &= \dot{x}_1 + \dot{x}_2 \\ 0 &= \dot{x}_1 + 2\dot{x}_2 + \dot{a} \end{aligned}$$

These can *always* be satisfied by choosing a suitable value for $\ddot{x}_1(t_0)$ and $\dot{x}_2(t_0)$.

From this you can conclude that it is sufficient to solve the original equations for $(x_1(t_0), \dot{x}_1(t_0), x_2(t_0))$. (This we already knew since the DAE is index 1)

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New constraints, when?

What does the situation look like when we can, and cannot, obtain new constraints by differentiating? What separates the two examples?

$$
\begin{aligned}
\dot{x}_1 + \dot{x}_2 &= a(t) \\
x_1 + x_2^2 &= b(t)
\end{aligned}
\qquad\qquad
\begin{aligned}
\dot{x}_1 &= x_1 + x_2 \\
0 &= x_1 + 2x_2 + a
\end{aligned}
$$

New constraints exists — No new constraints

- Difference is the index of the DAE:s
- A sufficient condition for a DAE to have at most index 1 is that it is possible to solve for highest differentiated variables.
- For semi-explicit DAE:s it is also a necessary condition

Differentiation a set of equations

Assume a DAE

$$f(x, \dot{x}, y, t) = 0, \quad f : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}^{n+m}$$

The highest differentiated variables are interesting, let $z = (\dot{x}, y)$ be a vector with the highest derivatives

$$f(x, z, t) = 0$$

Find a subset with k equations

$$\bar{f}(\bar{x}, \bar{z}, t) = 0,\ \bar{x} \in \mathbb{R}^q,\ \bar{z} \in \mathbb{R}^l$$

- k - number of equations in $\bar{f}$
- l - number of highest derivatives in $\bar{f}$

Assume a well-formed model, e.g., no dependent set of equations.

Differentiation a set of equations, cont.

Differentiate the set of equations $\bar{f}$ w.r.t. t

$$\bar{f}_{\bar{x}}\dot{\bar{x}} + \bar{f}_{\bar{z}}\dot{\bar{z}} + \bar{f}_t = 0$$

The number r of "new" highest derivatives $\dot{\bar{z}}$ appearing in the differentiated equation is determined by rank $\bar{f}_{\bar{z}}$.

$$r \leq \min(k, l) = \min(\#\text{eq. in } \bar{f}, \#z \text{ in } \bar{f})$$

- k - number of new equations from differentiation
- r - number of new highest derivatives

The conclusion so far is then:

- we get $k - r$ additional equations/constraints in the existing variables when differentiating $\bar{f}$.
- all subsets of equations where $k > r$ are therefore useful to obtain such "hidden" constraints

Differentiation a set of equations, cont.

Since r (number of new highest derivatives) can not be larger than l (number of highest derivatives in $\bar{f}$), a sufficient condition for $k > r$ is

$$l < k$$

The above property implies that the set of equations $\bar{f}$ contains fewer highest ordered derivatives than equations.

Set of equations is overdetermined with respect to the highest ordered differentiated variables.

New constraints, when? Revisited!

What does the situation look like when we can, and cannot, obtain new constraints by differentiating? What separates the two examples?

$$e_1 : \dot{x}_1 + \dot{x}_2 = a(t)$$
$$e_2 : x_1 + x_2^2 = b(t)$$

New constraints exists, equation e_2 contains none of the highest ordered differentiated variables $\dot{x}_1$ or $\dot{x}_2$.

With $\bar{f}$ equal to e_2 then $k = 1$ and $l = r = 0 \Rightarrow$ $k - r = 1 - 0 = 1$ new constraints.

$$e_1 : \dot{x}_1 = x_1 + x_2$$
$$e_2 : 0 = x_1 + 2x_2 + a$$

No new constraints. Both e_1 and e_2 each contain one of the highest ordered differentiated variables $\dot{x}_1$ and x_2 respectively.

With $\bar{f}$ equal to e_1 or e_2 then $k = 1$ and $l = r = 1 \Rightarrow$ $k - r = 1 - 1 = 0$ new constraints.

Sketch of Pantelides algorithm

Sketch of the basic principles for Pantelides algorithm for a DAE $f(\dot{x}, x, y, t) = 0$.

1. Define $z = (\dot{x}, y)$
2. Find all subsets of equations where $l < k$, i.e., overdetermined w.r.t. the highest ordered derivatives. If none exists, exit.
3. Differentiate these equations and extend the model with the new equations. Go to step 1.

- There are many possible, very many, subsets. This has to be done in a smart way to not run into complexity problems.
- Solvable!

Pantelides algorithm

A graph theoretical algorithm that do the above efficiently for large systems with no symbolic computations.

An implementation of the algorithm, courtesy Mattias Krysander, can be downloaded from the course website, can come in handy when solving some of the exercises.

Matching - a useful graph theoretical concept

$$\begin{aligned} f_1(x_1, x_2, x_3, y) &= 0 \\ f_2(x_1, x_2, y) &= 0 \\ f_3(x_2, x_3, y) &= 0 \end{aligned}$$

	x_1	x_2	x_3
e_1	X	X	X
e_2	X	X	
e_3		X	X

Implicit function theorem gives that there exists a local solution for x in the equation $f(x, y) = c$ at $x = x_0$ if

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_0} = \left.\begin{pmatrix} \star & \star & \star \\ \star & \star & 0 \\ 0 & \star & \star \end{pmatrix}\right|_{x=x_0}$$

has full column rank.

Matching

(here) A pairing of equations with variables

Matching - a useful graph theoretical concept

$$f_1(x_1, x_2, x_3, y) = 0$$
$$f_2(x_1, x_2, y) = 0$$
$$f_3(x_2, x_3, y) = 0$$

	x_1	x_2	x_3
e_1	X	X	X
e_2	X	X	
e_3		X	X

Implicit function theorem gives that there exists a local solution for x in the equation $f(x, y) = c$ at $x = x_0$ if

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_0} = \left.\begin{pmatrix} \star & \star & \star \\ \star & \star & 0 \\ 0 & \star & \star \end{pmatrix}\right|_{x=x_0}$$

has full column rank.

Matching

(here) A pairing of equations with variables

Matching and structural rank

A matrix is said to have full structural rank if all variables can be matched.

	x_1	x_2	x_3
e_1	X	X	X
e_2	X	X	
e_3		X	X

	x_1	x_2	x_3
e_1	X	X	X
e_2		X	
e_3		X	

- If there exists a complete matching with respect to x in the structure for a function $f(x, y)$, the Jacobian $f_x(x, y)$ has full rank for almost all f with the same structure.

Can be computed in Matlab using the `srank` command.

Example: Matching condition for semi-explicit index 1

In a semi-explicit DAE

$$
\begin{aligned}
\dot{x} &= f(x, y) \\
0 &= g(x, y)
\end{aligned}
$$

the highest differentiated variables $z = (\dot{x},\ y)$. DAE has (local) index 0/1 if

$$
\frac{\partial}{\partial z} \begin{pmatrix} f(x, y) \\ g(x, y) \end{pmatrix} \Bigg|_{z=z_0}
$$

has full column rank.

Convince yourselves that the DAE has structural index 0/1 if the structure of the DAE has a complete matching with respect to the variables z.

Pantelides on an index 3 DAE

Step 1

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$e_3 : 0 = h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
e_3			

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE

Step 1

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$e_3 : 0 = h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
e_3			

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE

Step 1

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$e_3 : 0 = h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
e_3			

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Step 2

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$\dot{e}_3 : 0 = \frac{d}{dt}\, h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
$\dot{e}_3$	X		

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE

Step 1

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$e_3 : 0 = h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
e_3			

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Step 2

$$e_1 : \dot{x} = f(x, y)$$
$$e_2 : \dot{y} = g(x, y, z)$$
$$\dot{e}_3 : 0 = \frac{d}{dt}\, h(x)$$

	$\dot{x}$	$\dot{y}$	z
e_1	X		
e_2		X	X
$\dot{e}_3$	X		

Highest differentiated variables: $(\dot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE, cont.

Step 3

$$\dot{e}_1 : \ddot{x} = \frac{d}{dt} f(x, y)$$

$$e_2 : \dot{y} = g(x, y, z)$$

$$\ddot{e}_3 : 0 = \frac{d^2}{dt^2} h(x)$$

	$\ddot{x}$	$\dot{y}$	z
$\dot{e}_1$	X	X	
e_2		X	X
$\ddot{e}_3$	X		

Highest differentiated vars: $(\ddot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE, cont.

Step 3

$$\dot{e}_1 : \ddot{x} = \frac{d}{dt} f(x,y)$$

$$e_2 : \dot{y} = g(x,y,z)$$

$$\ddot{e}_3 : 0 = \frac{d^2}{dt^2} h(x)$$

	$\ddot{x}$	$\dot{y}$	z
$\dot{e}_1$	X	X	
e_2		X	X
$\ddot{e}_3$	X		

Highest differentiated vars: $(\ddot{x}, \dot{y}, z)$

Pantelides on an index 3 DAE, cont.

Step 3

$$\dot{e}_1 : \ddot{x} = \frac{d}{dt}\ f(x,y)$$
$$e_2 : \dot{y} = g(x,y,z)$$
$$\ddot{e}_3 : 0 = \frac{d^2}{dt^2}\ h(x)$$

	$\ddot{x}$	$\dot{y}$	z
$\dot{e}_1$	X	$\boxed{X}$	
e_2		X	$\boxed{X}$
$\ddot{e}_3$	$\boxed{X}$		

Highest differentiated vars: $(\ddot{x}, \dot{y}, z)$

Resulting system of equations (6 equations in 6 unknowns)

$$e_1 : \dot{x} = f(x,y)$$
$$\dot{e}_1 : \ddot{x} = d/dt\ f(x,y)$$
$$e_2 : \dot{y} = g(x,y,z)$$
$$e_3 : 0 = h(x)$$
$$\dot{e}_3 : 0 = d/dt\ h(x)$$
$$\ddot{e}_3 : 0 = d^2/dt^2\ h(x)$$

	x	$\dot{x}$	$\ddot{x}$	y	$\dot{y}$	z
e_1	X	X		$\boxed{X}$		
$\dot{e}_1$	X	X	X	X	$\boxed{X}$	
e_2	X			X	X	$\boxed{X}$
e_3	$\boxed{X}$					
$\dot{e}_3$	X	$\boxed{X}$				
$\ddot{e}_3$	X	X	$\boxed{X}$			

Example: Pendulum equations

$$\begin{aligned} m\,\ddot{x} &= Tx \\ m\,\ddot{y} &= Ty - m\,g \\ 0 &= x^2 + y^2 - L^2 \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{x} &= w \\ \dot{y} &= z \\ m\,\dot{w} &= Tx \\ m\,\dot{z} &= Ty - m\,g \\ 0 &= x^2 + y^2 - L^2 \end{aligned}$$

Highest differentiated variables are $(\dot{x}, \dot{y}, \dot{w}, \dot{z}, T)$

	T	$\dot{x}$	$\dot{w}$	$\dot{y}$	$\dot{z}$
e_1		X			
e_2				X	
e_3	X		X		
e_4	X				X
e_5					

Example: Pendulum equations

$$
\begin{aligned}
m\,\ddot{x} &= Tx \\
m\,\ddot{y} &= Ty - m\,g \\
0 &= x^2 + y^2 - L^2
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\dot{x} &= w \\
\dot{y} &= z \\
m\,\dot{w} &= Tx \\
m\,\dot{z} &= Ty - m\,g \\
0 &= x^2 + y^2 - L^2
\end{aligned}
$$

Highest differentiated variables are $(\dot{x}, \dot{y}, \dot{w}, \dot{z}, T)$

	T	$\dot{x}$	$\dot{w}$	$\dot{y}$	$\dot{z}$
e_1		X			
e_2				X	
e_3	X		X		
e_4	X				X
e_5					

Differentiate e_5 and extend the model

$$
\begin{aligned}
e_1 &: & \dot{x} &= w \\
e_2 &: & \dot{y} &= z \\
e_3 &: & m\,\dot{w} &= Tx \\
e_4 &: & m\,\dot{z} &= Ty - m\,g \\
e_5 &: & 0 &= x^2 + y^2 - L^2
\end{aligned}
\qquad
e_5' : \quad 0 = 2x\dot{x} + 2y\dot{y}
$$

Highest differentiated variables are $(\dot{x}, \dot{y}, \dot{w}, \dot{z}, T)$

	T	$\dot{x}$	$\dot{w}$	$\dot{y}$	$\dot{z}$
e_1		X			
e_2				X	
e_3	X		X		
e_4	X				X
$\dot{e}_5$		X		X	

Differentiate e_5 and extend the model

$$e_1: \quad \dot{x} = w$$

$$e_2: \quad \dot{y} = z$$

$$e_3: \quad m\,\dot{w} = Tx$$

$$e_4: \quad m\,\dot{z} = Ty - m\,g$$

$$e_5: \quad 0 = x^2 + y^2 - L^2$$

$$e_5': \quad 0 = 2x\dot{x} + 2y\dot{y}$$

Highest differentiated variables are $(\dot{x}, \dot{y}, \dot{w}, \dot{z}, T)$

	T	$\dot{x}$	$\dot{w}$	$\dot{y}$	$\dot{z}$
e_1		X			
e_2				X	
e_3	X		X		
e_4	X				X
$\dot{e}_5$		X		X	

Differentiate e_1, e_2, *and* $\dot{e}_5$

$$
\begin{aligned}
e_1 &: & \dot{x} &= w & e_4 &: & m\,\dot{z} &= Ty - m\,g \\
\dot{e}_1 &: & \ddot{x} &= \dot{w} & e_5 &: & 0 &= x^2 + y^2 - L^2 \\
e_2 &: & \dot{y} &= z & \dot{e}_5 &: & 0 &= 2x\dot{x} + 2y\dot{y} \\
\dot{e}_2 &: & \ddot{y} &= \dot{z} & \ddot{e}_5 &: & 0 &= 2\dot{x}^2 + 2x\ddot{x} + 2\dot{y}^2 + 2y\ddot{y} \\
e_3 &: & m\,\dot{w} &= Tx
\end{aligned}
$$

	T	$\dot{w}$	$\dot{z}$	$\ddot{x}$	$\ddot{y}$
$\dot{e}_1$		X		X	
$\dot{e}_2$			X		X
e_3	X	X			
e_4	X		X		
$\ddot{e}_5$				X	X

$$\nu = (1, 1, 0, 0, 2)$$

Differentiate e_1, e_2, and $\dot{e}_5$

$$
\begin{aligned}
e_1 &: & \dot{x} &= w & e_4 &: & m\,\dot{z} &= Ty - m\,g \\
\dot{e}_1 &: & \ddot{x} &= \dot{w} & e_5 &: & 0 &= x^2 + y^2 - L^2 \\
e_2 &: & \dot{y} &= z & \dot{e}_5 &: & 0 &= 2x\dot{x} + 2y\dot{y} \\
\dot{e}_2 &: & \ddot{y} &= \dot{z} & \ddot{e}_5 &: & 0 &= 2\dot{x}^2 + 2x\ddot{x} + 2\dot{y}^2 + 2y\ddot{y} \\
e_3 &: & m\,\dot{w} &= Tx
\end{aligned}
$$

	T	$\dot{w}$	$\dot{z}$	$\ddot{x}$	$\ddot{y}$
$\dot{e}_1$		X		X	
$\dot{e}_2$			X		X
e_3	X	X			
e_4	X		X		
$\ddot{e}_5$				X	X

$$\nu = (1, 1, 0, 0, 2)$$

Differentiate e_1, e_2, and $\dot{e}_5$

$$
\begin{aligned}
e_1 &: & \dot{x} &= w & e_4 &: & m\,\dot{z} &= Ty - m\,g \\
\dot{e}_1 &: & \ddot{x} &= \dot{w} & e_5 &: & 0 &= x^2 + y^2 - L^2 \\
e_2 &: & \dot{y} &= z & \dot{e}_5 &: & 0 &= 2x\dot{x} + 2y\dot{y} \\
\dot{e}_2 &: & \ddot{y} &= \dot{z} & \ddot{e}_5 &: & 0 &= 2\dot{x}^2 + 2x\ddot{x} + 2\dot{y}^2 + 2y\ddot{y} \\
e_3 &: & m\,\dot{w} &= Tx
\end{aligned}
$$

	T	$\dot{w}$	$\dot{z}$	$\ddot{x}$	$\ddot{y}$
e_3	$\boxed{X}$	X			
$\dot{e}_1$		$\boxed{X}$		X	
e_4	X		$\boxed{X}$		
$\ddot{e}_5$				$\boxed{X}$	X
$\dot{e}_2$			X		$\boxed{X}$

$$\nu = (1, 1, 0, 0, 2)$$

11 variables and 9 equations, i.e., 2 degrees of freedom. Makes sense ($\approx$ position and velocity)

Structural index

Can be computed by Pantelides algorithm. Determine how in exercise 2.13. (an error in the book by P. Fritzon so you will have to solve it by yourselves)

Remember the non-trivial relationship between index ν and structural index ν_{str}.

$$\nu = \nu_{str}, \quad \nu < \nu_{str}, \quad \nu > \nu_{str}$$

All is possible!

Outline

- Structural index - introduction and definition
- Consistent initial conditions
- Pantelides algorithm – initial conditions and structural index
- Index reduction with dummy derivatives
- Summary

Index reduction

- Differentiate to the underlying ODE is often a not satisfactory solution
- due to that the underlying ODE has a larger solution set
- requires stabilization/projection techniques to avoid violating algebraic constraints
- Objective is then to do index reduction while keeping solution set
- To save all differentiated equations, and not only the underlying ODE, is one such way. The result is a overdetermined index-1 DAE. Consistency etc. is typically violated at discretization, projection etc. is needed.
- Dummy derivatives is a method that solves such problems.

Small example that shows the principle

Index-1 system

$$e_1: \ \dot{x}_1 + \dot{x}_2 = a(t)$$
$$e_2: \ x_1 + x_2^2 = b(t)$$

Differentiate e_2 once gives the *overdetermined* system of equations

$$\begin{aligned} e_1 &: \dot{x}_1 + \dot{x}_2 = a(t) \\ e_2 &: x_1 + x_2^2 = b(t) \\ \dot{e}_2 &: \dot{x}_1 + 2\,x_2\,\dot{x}_2 = \dot{b}(t) \end{aligned}$$

Replace $\dot{x}_1$ for a *new algebraic* variable x_1'

$$e_1 : x_1' + \dot{x}_2 = a(t)$$

$$e_2 : x_1 + x_2^2 = b(t)$$

$$\dot{e}_2 : x_1' + 2\,x_2\,\dot{x}_2 = \dot{b}(t)$$

and solve for (x_1, x_1', x_2). Can be proven to have the *same* solution set as the original equations.

Small example that shows the principle

Index-1 system

$$\begin{aligned} e_1 &: \ \dot{x}_1 + \dot{x}_2 = a(t) \\ e_2 &: \ x_1 + x_2^2 = b(t) \end{aligned}$$

Differentiate e_2 once gives the *overdetermined* system of equations

$$\begin{aligned} e_1 &: \dot{x}_1 + \dot{x}_2 = a(t) \\ e_2 &: x_1 + x_2^2 = b(t) \\ \dot{e}_2 &: \dot{x}_1 + 2\,x_2\,\dot{x}_2 = \dot{b}(t) \end{aligned}$$

Replace $\dot{x}_1$ for a *new algebraic* variable x_1'

$$\begin{aligned} e_1 &: x_1' + \dot{x}_2 = a(t) \\ e_2 &: x_1 + x_2^2 = b(t) \\ \dot{e}_2 &: x_1' + 2\,x_2\,\dot{x}_2 = \dot{b}(t) \end{aligned} \qquad \Rightarrow \qquad \begin{aligned} x_1 &= b(t) - x_2^2 \\ \dot{x}_2 &= \frac{\dot{b}(t) - a(t)}{2x_2 - 1} \end{aligned}$$

and solve for (x_1, x_1', x_2). Can be proven to have the *same* solution set as the original equations.

Index reduction with dummy derivatives, principle

$$F(\dot{x}, x, t) = 0$$
$$\vdots$$
$$\frac{d^j}{dt^j} F(\dot{x}, x, t) = 0$$

If only j is large enough (index) the equations are an index-1 DAE with the exact same solution set as the original DAE. Problem: system is (violently) overdetermined.

Principle for index reduction

1. Let Pantelides algorithm determine the number of times to differentiate
2. Differentiate equations according to Pantelides, collect all equations
3. Simplified: For each differentiated equation, introduce an algebraic variable such that the system becomes exactly determined
4. Result: exactly determined index 1 DAE with the same solution set as the original DAE

Example - a DAE with index 3

$$
\begin{aligned}
(a):&\quad \dot{x} = y && x(t) = f(t)\\
(b):&\quad \dot{y} = z && y(t) = \dot{f}(t)\\
(c):&\quad x = f(t) && z(t) = \ddot{f}(t)
\end{aligned}
$$

Pantelides states that we should differentiate (c) twice and (a) once. Collecting the equations

$$
\begin{aligned}
(c):&\quad x = f(t)\\
(\dot{c}):&\quad \dot{x} = \dot{f}(t)\\
(\ddot{c}):&\quad \ddot{x} = \ddot{f}(t)\\
(a):&\quad \dot{x} = y\\
(\dot{a}):&\quad \ddot{x} = \dot{y}\\
(b):&\quad \dot{y} = z
\end{aligned}
$$

Example, cont.

The differentiated model is overdetermined (3 unknowns, 6 equations). Introduce an algebraic variable for each differentiated equation

$$x' = \dot{x},\ x'' = \ddot{x},\ y' = \dot{y}$$

Important!! Variables x', x'', y' is here algebraic variables.

$$\begin{aligned}
(c): &\quad & x &= f(t) \\
(\dot{c}): &\quad & x' &= \dot{f}(t) \\
(\ddot{c}): &\quad & x'' &= \ddot{f}(t) \\
(a): &\quad & x' &= y \\
(\dot{a}): &\quad & x'' &= y' \\
(b): &\quad & y' &= z
\end{aligned}$$

Exactly determined, index 1 DAE (6 unknowns, 6 equations)

Somewhat extreme example where the system turns into a purely algebraic system of equations, but it illustrates a simple case.

Principle for index reduction

1. Let Pantelides algorithm determine the number of times to differentiate
2. Differentiate equations according to Pantelides, collect all equations
3. Simplified: For each differentiated equation, introduce an algebraic variable such that the system becomes exactly determined
4. Result: exactly determined index 1 DAE with the same solution set as the original DAE

Step 3 need to be clarified.

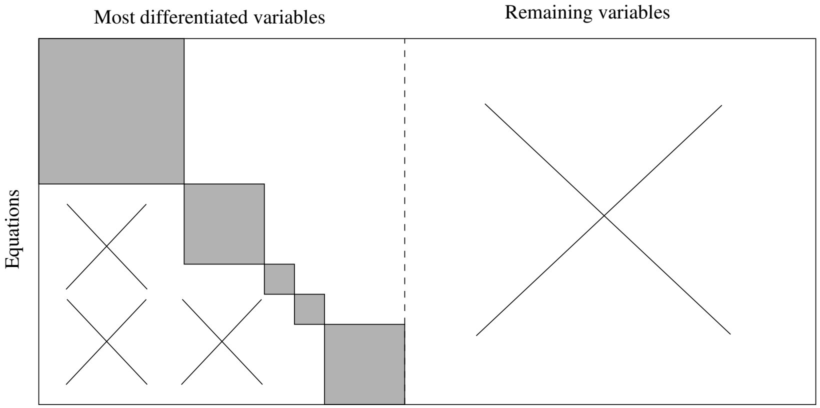
Structure of the differentiated system

Simple if

- Pantelides algorithm only differentiates 1 time and only one new variable is introduced
- How should the situation where equations are differentiated more than once and multiple new variables are introduced simultaneously?

Structure of the differentiated system

take the differentiated system, by permutations of equations and variables you can always get a Block Lower Triangle (BLT) form w.r.t. the most differentiated variables



Consider one block at a time.

Example - a system of index 2

$$
\begin{aligned}
(a):&\quad x_1 + x_2 + u_1 = 0\\
(b):&\quad x_1 + x_2 + x_3 + u_2 = 0\\
(c):&\quad x_1 + \dot{x}_3 + x_4 + u_3 = 0\\
(d):&\quad 2\ddot{x}_1 + \ddot{x}_2 + \ddot{x}_3 + \dot{x}_4 + u_4 = 0
\end{aligned}
$$

Pantelides gives $\nu = (2, 2, 1, 0)$ and the differentiated system $\mathcal{G}x = 0$ is:

$$
\begin{aligned}
(\ddot{a}):&\quad \ddot{x}_1 + \ddot{x}_2 + \ddot{u}_1 = 0\\
(\ddot{b}):&\quad \ddot{x}_1 + \ddot{x}_2 + \ddot{x}_3 + \ddot{u}_2 = 0\\
(\dot{c}):&\quad \dot{x}_1 + \ddot{x}_3 + \dot{x}_4 + \dot{u}_3 = 0\\
(d):&\quad 2\ddot{x}_1 + \ddot{x}_2 + \ddot{x}_3 + \dot{x}_4 + u_4 = 0
\end{aligned}
$$

We have introduced 2+2+1=5 equations, i.e., we need to introduce 5 dummy variables. Which ones? Not as easy as in the first example where there was a one-to-one relation between differentiated equation and new variable. Candidates are $(\dot{x}_1, \ddot{x}_1, \dot{x}_2, \ddot{x}_2, \dot{x}_3, \ddot{x}_3, \dot{x}_4)$, which 5 to choose?

Example - a system of index 2, cont.

The differentiated system $\mathcal{G}x = 0$ is not of the type with one-to-one relation between differentiated equation and variable.

The highest differentiated variables are $(\ddot{x}_1, \ddot{x}_2, \ddot{x}_3, \dot{x}_4)$ and $\mathcal{G}$ consists of a block g_1, w.r.t. the highest differentiated variables z_1

$$\frac{\partial g_1}{\partial z_1} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 2 & 1 & 1 & 1 \end{pmatrix}$$

In these, the three first equations are differentiated; get that part

$$H_1 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

Choice of variables should be such that index ≤ 1 is retained, i.e., all highest differentiated variables should still be matched. We must choose variables such that the corresponding sub-matrix of H_1 has full rank.

Example - a system of index 2, cont.

We can choose $(\ddot{x}_1, \ddot{x}_3, \dot{x}_4)$ or $(\ddot{x}_2, \ddot{x}_3, \dot{x}_4)$. Choose

$$\hat{z}^{[1]} = (\ddot{x}_1, \ddot{x}_3, \dot{x}_4)$$

these variables will be introduced as dummy variables in the final DAE. We are not done since we yet only have define 3 dummy variables, we must have 5.

Now look at the differentiated equations, with one less differentiation (these also are part of the system)

$$\begin{aligned}
(\dot{a}) : \quad & \dot{x}_1 + \dot{x}_2 + \dot{u}_1 = 0 \\
(\dot{b}) : \quad & \dot{x}_1 + \dot{x}_2 + \dot{x}_3 + \dot{u}_2 = 0 \\
(c) : \quad & x_1 + \dot{x}_3 + x_4 + u_3 = 0
\end{aligned}$$

Candidates for new dummy variables are $(\dot{x}_1, \dot{x}_3, x_4)$. Analyze this sub-model in the same way as before.

Example - a system of index 2, cont.

Extract the differentiated equations

$$(\dot{a}): \quad \dot{x}_1 + \dot{x}_2 + \dot{u}_1 = 0$$

$$(\dot{b}): \quad \dot{x}_1 + \dot{x}_2 + \dot{x}_3 + \dot{u}_2 = 0$$

Highest derivatives are $z_1 = (\dot{x}_1, \dot{x}_3, x_4)$. Differentiate w.r.t. z_1 to obtain

$$H_1^{[2]} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

and here we must choose

$$\hat{z}_1^{[2]} = (\dot{x}_1, \dot{x}_3)$$

as dummy variables and then we have selected our 5 and are done!

Example - a system of index 2, cont.

The final index 1 DAE is then

$$
\begin{aligned}
(a):&\quad x_1 + x_2 + u_1 = 0\\
(\dot{a}):&\quad x_1' + \dot{x}_2 + \dot{u}_1 = 0\\
(\ddot{a}):&\quad x_1'' + \ddot{x}_2 + \ddot{u}_1 = 0\\
(b):&\quad x_1 + x_2 + x_3 + u_2 = 0\\
(\dot{b}):&\quad x_1' + \dot{x}_2 + x_3' + \dot{u}_2 = 0\\
(\ddot{b}):&\quad x_1'' + \ddot{x}_2 + x_3'' + \ddot{u}_2 = 0\\
(c):&\quad x_1 + x_3' + x_4 + u_3 = 0\\
(\dot{c}):&\quad x_1' + x_3'' + x_4' + \dot{u}_3 = 0\\
(d):&\quad 2x_1'' + \ddot{x}_2 + x_3'' + x_4' + u_4 = 0
\end{aligned}
$$

which has the same solution set as the original index 2 DAE.

The 9 unknown variables are$(x_1, x_1', x_1'', x_2, x_3, x_3', x_3'', x_4, x_4')$ out of which all are algebraic except x_2 which appears differentiated of order 2.

Example - a system of index 2, cont.

It is possible to get a simpler solution. Pantelides differentiated for an ODE, it is really sufficient to differentiate until an index 1 DAE.

Rather straightforward changes to the basic principle gives the somewhat simpler system

$$
\begin{aligned}
(a): &\quad x_1 + x_2 + u_1 = 0 \\
(\dot{a}): &\quad x_1' + \dot{x}_2 + \dot{u}_1 = 0 \\
(b): &\quad x_1 + x_2 + x_3 + u_2 = 0 \\
(\dot{b}): &\quad x_1' + \dot{x}_2 + x_3' + \dot{u}_2 = 0 \\
(c): &\quad x_1 + x_3' + x_4 + u_3 = 0 \\
(d): &\quad 2\dot{x}_1' + \ddot{x}_2 + \dot{x}_3' + \dot{x}_4 + u_4 = 0
\end{aligned}
$$

Dummy derivatives summary

- Pantelides algorithm plus a procedure to introduce algebraic variables gives a low-index system with the same solution set as the original DAE
- Is all index related issues thereby solved?
- Pros/cons
- Structural and analytical steps

Outline

- *Structural index - introduction and definition*
- *Consistent initial conditions*
- *Pantelides algorithm – initial conditions and structural index*
- *Index reduction with dummy derivatives*
- *Summary*

Summary

- Three problems have been discussed:
  - consistent initial conditions
  - determining index
  - index reduction
- Pantelides algorithm: a graph theoretical algorithm to find the system of equations to solve for consistent initial conditions given a DAE of arbitrary index
- Pantelides algorithm is a cornerstone for solving all three problems
- Well suited for implementation in a general purpose DAE simulator
- Structural results, not analytical!

Lecture 4

Simulation of differential-algebraic equations

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