Lecture 2 – Simulation of differential-algebraic equations

Simulation of DAE models and index reduction

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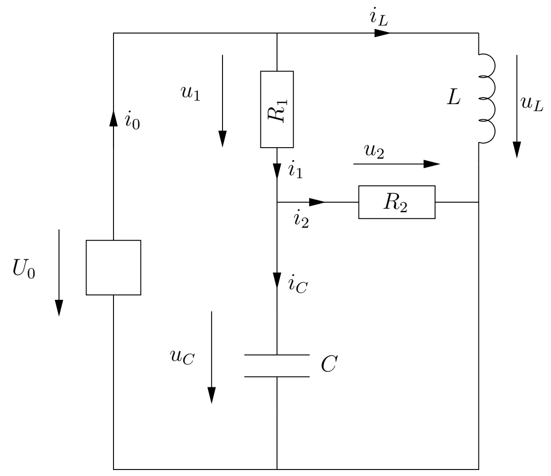
Simple circuit model, index 1



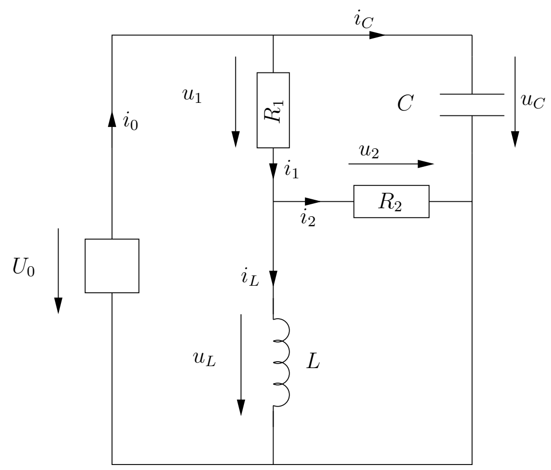
$$
\begin{aligned}
e_1 &: u_0 = f(t)\\
e_2 &: u_1 = R_1 i_1\\
e_3 &: u_2 = R_2 i_2\\
e_4 &: i_C = C\frac{du_c}{dt}\\
e_5 &: u_L = L\frac{di_L}{dt}\\
e_6 &: i_0 = i_1 + i_L\\
e_7 &: i_1 = i_2 + i_C\\
e_8 &: u_0 = u_1 + u_C\\
e_9 &: u_L = u_1 + u_2\\
e_{10} &: u_C = u_2
\end{aligned}
$$

$x_1 = (u_c, i_L)$, $x_2 = (u_2, i_2, u_0, u_1, u_L, i_1, i_C, i_0)$

Computational form of model

$$
\begin{aligned}
e_1 &: u_0 = f(t)\\
e_2 &: u_1 = R_1 i_1\\
e_3 &: u_2 = R_2 i_2\\
e_4 &: i_C = C\frac{du_c}{dt}\\
e_5 &: u_L = L\frac{di_L}{dt}\\
e_6 &: i_0 = i_1 + i_L\\
e_7 &: i_1 = i_2 + i_C\\
e_8 &: u_0 = u_1 + u_C\\
e_9 &: u_L = u_1 + u_2\\
e_{10} &: u_C = u_2
\end{aligned}
\quad\Rightarrow\quad
\begin{aligned}
e_4 &: \frac{du_c}{dt} = \frac{1}{C} i_C\\
e_5 &: \frac{di_L}{dt} = \frac{1}{L} u_L\\
\\
e_{10} &: u_2 := u_C\\
e_3 &: i_2 := \frac{1}{R_2} u_2\\
e_1 &: u_0 := f(t)\\
e_8 &: u_1 := u_0 - u_C\\
e_9 &: u_L := u_1 + u_2\\
e_2 &: i_1 := \frac{1}{R_1} u_1\\
e_7 &: i_C := i_1 - i_2\\
e_6 &: i_0 := i_1 + i_L
\end{aligned}
$$

Simple circuit model, index > 1



$$
\begin{aligned}
e_1 &: u_0 = f(t)\\
e_2 &: u_1 = R_1 i_1\\
e_3 &: u_2 = R_2 i_2\\
e_4 &: i_C = C\frac{du_c}{dt}\\
e_5 &: u_L = L\frac{di_L}{dt}\\
e_6 &: i_0 = i_1 + i_C\\
e_7 &: i_1 = i_2 + i_L\\
e_8 &: u_0 = u_1 + u_L\\
e_9 &: u_C = u_1 + u_2\\
e_{10} &: u_L = u_2
\end{aligned}
$$

$x_1 = (u_C, i_L)$, $x_2 = (u_2, i_2, u_0, u_1, u_L, i_1, i_C, i_0)$

Differential index

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

Definition

The minimum number of times the DAE has to be differentiated with respect to t to be able to determine $\dot{y}$ as a function of t och y is called the (differential-) index of the DAE.

- index might be solution dependent, uniform index
- There are several types of index, the above is called differential index.
- Perturbation index
- variants of the above (see paper)

Anyhow: index is a measure how far from an ODE the DAE is.

Outline

- Simulation of high index DAE:s, key problems
- Simulation of index 1 DAE:s
  - State-space method
  - ϵ-embedding
  - BDF
- Index reduction
  - Index reduction by differentiation
  - Drift stabilization

Simulation of DAE with index > 1

$$\begin{aligned} A\dot{y}(t) + By(t) &= g(t), \text{ linear, constant coefficients} \\ A(t)\dot{y}(t) + B(t)y(t) &= g(t), \text{ linear, time-varying coefficients} \\ F(\dot{y}, y, t) &= 0, \text{ general DAE} \end{aligned}$$

- Start with a linear DAE with constant coefficients, this is sufficient to illustrate the main reasons why high index problems are difficult
- Consider the index-3 problem

$$\begin{aligned} x(t) &= g(t) \\ \dot{x} &= y \\ \dot{y} &= z \end{aligned}$$

which has the solution $x(t) = g(t)$, $y(t) = \dot{g}(t)$, and $z(t) = \ddot{g}(t)$.

Backward Euler, fix step length

A backward Euler on the problem gives the equations

$$\begin{aligned} x_n &= g_n \\ y_n &= \frac{x_n - x_{n-1}}{h} \\ z_n &= \frac{y_n - y_{n-1}}{h} \end{aligned}$$

Direct substitutions of x_n and y_n give

$$\begin{aligned} x_n &= g_n \\ y_n &= \frac{g_n - g_{n-1}}{h} = \dot{g}_n + \mathcal{O}(h) \\ z_n &= \frac{g_n - 2g_{n-1} + g_{n-2}}{h^2} = \ddot{g}_n + \mathcal{O}(h) \end{aligned}$$

This looks great!

$$x(t_n) - x_n = 0, \quad y(t_n) - y_n = \mathcal{O}(h), \quad z(t_n) - z_n = \mathcal{O}(h)$$

Fix step length

Theorem

If a k step BDF ($k < 7$) is applied to

$$A\dot{y}(t) + By(t) = g(t)$$

the solution will be $O(h^k)$ after max $(m-1)k+1$ steps.

This would indicate that an algorithm with fixed step length would work fine also for high index.

Unfortunately, this breaks down for variable step length integrators.

Constant DAE, variable step length

Now assume variable step length, i.e., the algorithm becomes

$$x_n = g_n$$
$$y_n = \frac{x_n - x_{n-1}}{h_n}$$
$$z_n = \frac{y_n - y_{n-1}}{h_n}$$

Now, examining the error in z_n we obtain

$$z_n - g_n'' = \cdots = \frac{1}{2}\left(\frac{h_{n-1}}{h_n} - 1\right)\ddot{g}_n + O(h)$$

This means that the error will diverge(!) with decreasing h_n, $O(h_n^{-1})$ (index > 2). The error in y will be $O(1)$ (index 2).

One of the exercises is to show ... in the expression.
Hint: Taylor expansion around $t = t_n$.

Constant DAE, variable step length, cont.

One result for variable step length

Theorem

If a k step BDF ($k < 7$) is applied on

$$A\dot{y}(t) + By(t) = g(t)$$

and the ratio between successive step lengths are bounded, then the solution will be $O(h^q_{max})$ where $q = min(k, k-m+2)$.

- This gives that an index 6 problem could be solved by a 6-step BDF, or?
- Which precondition is here questionable, and why?
- One step backwards Euler with fixed step length is a recommended approach for linear high-index problems with constant coefficients.

Linear, non-constant DAE:s

For a DAE

$$A(t)\dot{y}(t) + B(t)y(t) = g(t)$$

you can define local index at time t and global index via a transformation to a canonical form by $y(t) = H(t)z(t)$ and $G(t)$ to

$$G(t)A(t)(H'(t)z(t) + H(t)\dot{z}(t)) + G(t)B(t)H(t)z(t) = G(t)g(t)$$

such that

$$G(t)A(t)H(t) = \begin{bmatrix} I & 0 \\ 0 & E \end{bmatrix}, G(t)A(t)H'(t) + G(t)B(t)H(t) = \begin{bmatrix} C(t) & 0 \\ 0 & I \end{bmatrix}$$

where E is nilpotent, i.e., the same canonical form as previously shown for linear, constant, DAE:s

$$\dot{z}_1 + C(t)z_1 = G_1(t)g(t)$$
$$E\dot{z}_2 + z_2 = G_2(t)g(t)$$

Linear, non-constant DAE:s, cont.

- If we can transform the DAE, all is well. Then the time variable problem is no more difficult than the time invariant.
- Problem: Finding the transformation matrices is not easy
- What happens if you "go with it" anyway with a fixed step length BDF for a time variable system?

From Gear, Petzold:

> *If the local index is two, we may have a stability problem depending on how fast the matrices change with time. If the local index is larger than 2, we almost always have a stability problem.*

Important to note: Stability problem, not an accuracy problem

What is the origin of the stability problem?

A DAE with local index m can be transformed into

$$(P_nEQ_n)z' + (P_nQ_n)z = P_nq_n$$

where P_n and Q_n are time variable transformation matrices and the constant matrix E is in the form ($m = 3$)

$$E = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad E^m = 0$$

Apply BDF on the DAE

$$(P_nEQ_n)(z_n - z_{n-1}) + h(P_nQ_n)z_n = hP_nq_n$$

which then can be written as

$$(P_nEQ_n + hP_nQ_n)z_n = P_nEQ_nz_{n-1} + hP_nq_n$$

Simplify to

$$(E + hI)Q_nz_n = EQ_nz_{n-1} + hq_n$$

Now, solve for z_n according to

$$z_n = Q_n^{-1}(E + hI)^{-1}EQ_nz_{n-1} + hQ_n^{-1}(E + hI)^{-1}q_n = S_nz_{n-1} + u_n$$

The real solution satisfies

$$z(t_n) = S_nz(t_{n-1}) + u_n - \frac{h^2}{2}S_nz_n''(\xi)$$

With $e_n = z_n - z(t_n)$ we get the recursion

$$e_n = S_ne_{n-1} + \frac{h^2}{2}S_nz_n''(\xi)$$

Now we have a (recursive) expression for the simulation error, time to analyze!

Expansion of the recursion gives

$$e_n = S_ne_{n-1} + \frac{h^2}{2}S_nz_n''(\xi)$$

where we have the explicit expression for the fault

$$e_n = \frac{h^2}{2}\sum_{i=1}^{n}\left(\prod_{j=i}^{n}S_j\right)z_i'' + \prod_{j=0}^{n}S_je_0$$

Three problems

- z'' not bounded
- $e_0 \neq 0$
- S_j not bounded

Now we can start answering the questions, why does it work for constant linear DAE:s (no time variable transformations):

$$S_n = S = Q^{-1}(E + hI)^{-1}EQ$$

Then we have that

$$S^k = Q^{-1}((E + hI)^{-1}E)^k Q$$

Some basic algebra gives

$$(E + hI)^{-1}E = \begin{bmatrix} 0 & & & & \\ h^{-1} & & & & \\ -h^{-2} & & & \ddots & \\ h^{-3} & & \ddots & & \\ & \ddots & & & \\ & h^{-3} & h^{-2} & h^{-1} & 0 \end{bmatrix}$$

which gives that $S^m = 0$, i.e., S also is nilpotent of order m, same as E.

Back to the expression

$$e_n = \frac{h^2}{2}\sum_{i=1}^{n}\left(\prod_{j=i}^{n} S_j\right) z_i'' + \prod_{j=0}^{n} S_j e_0$$

Here it is clear that for $n > m$, the second term disappears (that is not influenced by the step length h)

After some thought you can derive the expression

$$e_n = \frac{h^2}{2}\sum_{i=0}^{m-2} S^{i+1} z_{n-i}''$$

Here we see why the limit for one step BDF is at index 1 problems (S factors then contains at most h^{-1})

Then why did it not work for time variable systems?

$$e_n = \frac{h^2}{2}\sum_{i=1}^{n}\left(\prod_{j=i}^{n} S_j\right) z_i'' + \prod_{j=0}^{n} S_j e_0$$

Three problems

- z'' not bounded
- $e_0 \neq 0$
- S_j not bounded

$$S_2 S_1 = Q_2^{-1}(E + hI)^{-1}E \underbrace{Q_2 Q_1^{-1}}_{\neq I}(E + hI)^{-1}EQ_1$$

For time variable/non-linear systems, the matrices are changing all the time and $\prod_{i=1}^{j} S_i \neq 0$ for all j.

Some conclusions

In the general case there is no methods (to my knowledge) for high index problems in the form

$$A(t)\dot{y} + B(t)y = g$$

and even less for

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

Though, sometimes, it might work with a BDF with fixed step length.

- Note that we have a stability issue, not accuracy (although this could also happen, more about that next time)
- Thus, it is not a solution to increase the order of the method or taking shorter steps.
- On the contrary, shorter steps might even make the situation worse
- Classes of DAE:s

Semi-explicit DAE:s and a rule of thumb

If

$$\dot{x} = f(x, y)$$
$$0 = g(x, y)$$

has index ν then

$$\dot{x} = f(x, \dot{u})$$
$$0 = g(x, \dot{u})$$

index $\nu - 1$.

If

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

has index ν then

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

index $\nu + 1$.

Rule of thumb: The semi-explicit case behaves as the general but with a higher index (and vice versa)

Outline

- *Simulation of high index DAE:s, key problems*
- *Simulation of index 1 DAE:s*
  - *State-space method*
  - *ϵ-embedding*
  - *BDF*
- *Index reduction*
  - *Index reduction by differentiation*
  - *Drift stabilization*

Simulation of semi-explicit index 1 DAE:s

- State-space method
- ϵ-embedding
- BDF (DASSL with variants) is a commonly used DAE solver. Can be downloaded online.

  Is described in detail in the nice book "*Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*" by K.E. Brenan, S.L. Campbell and L.R. Petzold. The book is in our library and I have uploaded the chapter on DASSL on the course web page for the interested.

  I will show the basic principles of DASSL at the end of this lecture.
- I can also highly recommend the method descriptions of the SUNDIALs solvers (`https://sundials.readthedocs.io/`).

Numerical code

- Matlab have several solvers for DAE (`ode15s`, `ode15i`, `ode23t`)
- Python has good ODE support in SciPy but no DAE solvers, I use the package ODES `https://scikits-odes.readthedocs.io/` which is a wrapper around ...
- SUNDIALS (more on the next slide)
- Julia – probably the environment with the most support for numerical integration (but I think less support for DAE) with the package `DifferentialEquations.jl` (https://github.com/SciML/DifferentialEquations.jl)

SUNDIALS

SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

Software library consisting of 6 different solvers, written in C.
`https://computing.llnl.gov/casc/sundials`

- CVODE(S)
  Solves IVP for ordinary differential equation (ODE) systems. Includes sensitivity analysis capabilities (forward and adjoint).
- IDA(S)
  Solves IVP for differential-algebraic equation (DAE) systems. Includes sensitivity analysis capabilities (forward and adjoint).
- ARKode
  Solves IVP ODE problems with additive Runge-Kutta methods, including support for IMEX methods.
- KINSOL
  solves nonlinear algebraic systems.

Wrappers in Python exists. Specialized Matlab packages utilizes these solvers. Lots of functionality not available in vanilla Matlab/Python.

Simulation software (a slighlty Julia-centric view)

Comparison Of Differential Equation Solver Software

Subject/Item	MATLAB	SciPy	deSolve	DifferentialEquations.jl	Sundials	Hairer	ODEPACK/Netlib /NAG	JitCODE	PyDSTool	FATODE	GSL	BOOST	Mathematica	Maple
Language	MATLAB	Python	R	Julia	C++ and Fortran	Fortran	Fortran	Python	Python	Fortran	C	C++	Mathematica	Maple
Selection of Methods for ODEs	Fair	Poor	Fair	Excellent	Good	Good	Good	Poor	Poor	Good	Poor	Fair	Fair	Fair
Efficiency*	Poor	Poor	Poor	Excellent	Excellent	Good	Good	Good	Good	Good	Fair	Fair	Fair	Good
Tweakability	Fair	Poor	Good	Excellent	Excellent	Good	Good	Fair	Fair	Fair	Fair	Fair	Good	Fair
Event Handling	Good	Good	Fair	Excellent	Good**	None	Good**	None	Fair	None	None	None	Good	Good
Symbolic Calculation of Jacobians and Autodifferentiation	None	None	None	Excellent	None	None	None	None	None	None	None	None	Excellent	Excellent
Complex Numbers	Excellent	Good	Fair	Good	None	None	None	None	None	None	None	Good	Excellent	Excellent
Arbitrary Precision Numbers	None	None	None	Excellent	None	None	None	None	None	None	None	Excellent	Excellent	Excellent
Control Over Linear/Nonlinear Solvers	None	Poor	None	Excellent	Excellent	Good	Depends on the solver	None	None	None	None	None	Fair	None
Built-in Parallelism	None	None	None	Excellent	Excellent	None	None	None	None	None	None	Fair	None	None
Differential-Algebraic Equation (DAE) Solvers	Good	None	Good	Excellent	Good	Excellent	Good	None	Fair	Good	None	None	Good	Good
Implicitly-Defined DAE Solvers	Good	None	Excellent	Fair	Excellent	None	Excellent	None	None	None	None	None	Good	None
Constant-Lag Delay Differential Equation (DDE) Solvers	Fair	None	Poor	Excellent	None	Good	Fair (via DDVERK)	Fair	None	None	None	None	Good	Excellent
State-Dependent DDE Solvers	Poor	None	Poor	Excellent	None	Excellent	Good	None	None	None	None	None	None	Excellent
Stochastic Differential Equation (SDE) Solvers	Poor	None	None	Excellent	None	None	None	Good	None	None	None	None	Fair	Poor
Specialized Methods for 2nd Order ODEs and Hamiltonians (and Symplectic Integrators)	None	None	None	Excellent	None	Good	None	None	None	None	None	Fair	Good	None
Boundary Value Problem (BVP) Solvers	Good	Fair	None	Good	None	None	Good	None	None	None	None	None	Good	Fair
GPU Compatibility	None	None	None	Excellent	Good	None	None	None	None	None	None	Good	None	None
Analysis Addons (Sensitivity Analysis, Parameter Estimation, etc.)	None	None	None	Excellent	Excellent	None	Good (for some methods like DASPK)	None	Poor	Good	None	None	Excellent	None

*Efficiency takes into account not only the efficiency of the implementation, but the features of the implemented methods (advanced timestepping controls, existence of methods which are known to be more efficient, Jacobian handling)

**Event handling needs to be implemented yourself using basic rootfinding functionality

For more detailed explainations and comparisons, see the following blog post:
http://www.stochasticlifestyle.com/a-comparison-between-differential-equation-solver-suites-in-matlab-r-julia-python-c-and-fortran

Scale	None	Poor	Fair	Good	Excellent
Explanation	Functionality does not exist	Functionality exists, but is feature-incomplete	The basic features exist	The basic features exist and some extra tweakability exists. May include extra methods for efficiency.	Has all of the basic features and more. Extra features for flexibility and efficiency.

from `https://github.com/SciML/DifferentialEquations.jl`

State-space method

$$
\begin{aligned}
y' &= f(y,z) \\
0 &= g(y,z), \quad g_z \text{ invertible}
\end{aligned}
$$

Implicit function theorem then gives that there exists (locally) a function $G(y)$ such that

$$z = G(y)$$

Substitution into the first equations gives the ODE

$$y' = f(y, G(y))$$

which can be solved using your method of choice, no new theory. You can even use an explicit solver if you like.

Lose the structure of the problem which might lead to unnecessary numerical difficulties.

Outline

ϵ-embedding

Write down, for example, a Runge-Kutta for the ODE

$$y' = f(y,z), \quad \epsilon z' = g(y,z), \quad g_z \text{ invertible}$$

You then get

$$\begin{aligned}(Y_{ni} - y_n)_{i=1,\dots s} &= hA(f(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ \epsilon(Z_{ni} - z_n)_{i=1,\dots s} &= hA(g(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ y_{n+1} &= y_n + hb^T(f(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ \epsilon z_{n+1} &= \epsilon z_n + hb^T(g(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\end{aligned}$$

Assume an implicit method which gives that the A matrix is invertible

$$h(g(Y_{nj}, Z_{nj}))_{j=1,\dots,s} = \epsilon A^{-1}(Z_{ni} - z_n)_{i=1,\dots s}$$

ϵ-embedding, cont'.

Now, let $\epsilon \to 0$ and RK becomes

$$\begin{aligned}(Y_{ni} - y_n)_{i=1,\dots s} &= hA(f(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ 0 &= g(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ y_{n+1} &= y_n + hb^T(f(Y_{nj}, Z_{nj}))_{j=1,\dots,s}\\ 0 &= g(y_{n+1}, z_{n+1})\end{aligned}$$

- for a stiffly accurate solver it holds that $z_{n+1} = Z_{ns}$ and the last rewrite is not necessary.
- The solution is identical to the state-space method.
- Methods pretty similar but has some pros and cons respectively
- State-space form does not require an implicit solver
- ϵ-embedding technique possible to generalize to systems not in semi-explicit form (see Hairer-Wanner)

$$My' = f(t,y)$$

Order of solver: RK for semi-explicit index 1

- If the method is stiffly accurate, the solution is equivalent to $y' = f(y, G(y))$ and a p order method gives

  $$y_n - y(t_n) = \mathcal{O}(h^p), z_n - z(t_n) = \mathcal{O}(h^p)$$

  under a Lipschitz assumption on G.
- If the solver is not stiffly accurate, you may lose order on the z-component.
- really the same phenomenon, *order reduction*, as for stiff ODE:s
- Example on page 269 in Ascher-Petzold.

Order reduction

- Stiffly accurate is sufficient for semi-explicit index 1
- Does not apply for higher index
- Stiff decay DIRK (Diagonally Implicit Runge Kutta) methods gets serious order reduction for semi-explicit DAE:s of index 2

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  - Index reduction by differentiation
  - Drift stabilization

BDF

A s step BDF can be directly applied to the general problem

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

without modification with respect to the ODE case.

- Popular method. "*BDF is so beautiful that it is hard to imagine something else could be better*", Petzold, 1988.
- IDAS/DASSL(DDASRT/DASPK/DASKR), ...
- Last time I checked OpenModelica used ddasrt (Dubbel precision, dassl with root solver), a predecessor to DASKR

DASSL

- DASSL (and successors) is perhaps the most used DAE solver
- Designed to solve DAE:s with index 0 and 1 in the general form

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

- BDF of order 1 to 5. No order reduction
- Variable step length by an extension of fix step length BDF
- Will spend time on lecture to describe the basics

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Index reduction

There are many methods to reduce index.

- Index reduction through differentiation
- Change of variables; think pendulum in polar coordinates. But which coordinate change? Differential-geometry.
- The basic state-space form from control theory

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

- dummy-derivatives, will come back to this next time where automatic methods suitable for large scale models (Modelica) is discussed.
- ...

Index reduction by differentiation

Solving high index problems is difficult. For a DAE with index k

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

we can derive an ODE by differentiating the equations k times

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

This DAE has exactly the same solution set as the original DAE. One major problem: it is overdetermined!

Find the underlying ODE and simulate that one?

Index reduction by differentiation

Consider the index 1 DAE

$$\begin{aligned}\dot{x}_1 &= f(x_1, x_2)\\ 0 &= g(x_1, x_2), \quad g_{x_2}(x_1, x_2) \text{ invertible}\end{aligned}$$

It is direct to differentiate the second equation and derive the ODE

$$\begin{aligned}\dot{x}_1 &= f(x_1, x_2)\\ \dot{x}_2 &= -g_{x_2}(x_1, x_2)^{-1} g_{x_1}(x_1, x_2) f(x_1, x_2)\end{aligned}$$

What will happen with the solution?

Index reduction through differentiation

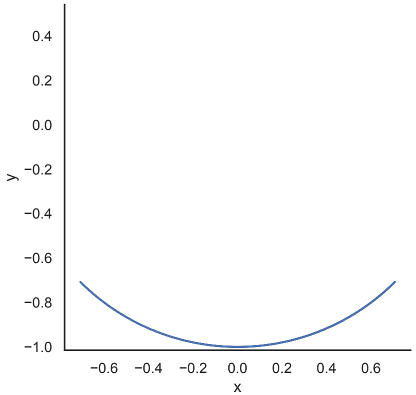
We have done this before, an index 3 example is

$$\begin{aligned}&e_1 : \dot{x} = w, && e_3 : \dot{y} = z, && e_5 : 0 = x^2 + y^2 - l^2\\ &e_2 : m\dot{w} = -x\lambda, && e_4 : m\dot{z} = -y\lambda - mg\end{aligned}$$

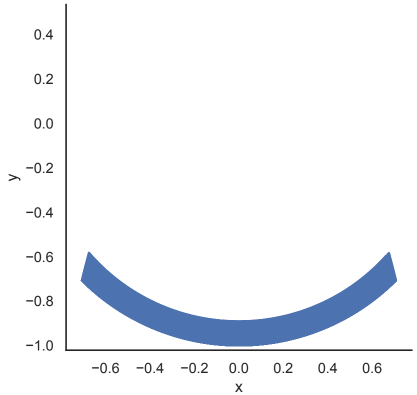
Differentiate the algebraic equation 2 times and we have an index 1 DAE.

- Solution sets to the two
- Initial conditions a difficult problem
- Underlying ODE (UODE) and the original DAE
- Invariants, which are maintained?
- Requires projections or other more or less advanced techniques to fulfill the original algebraic constraints.

Drift in pendulum



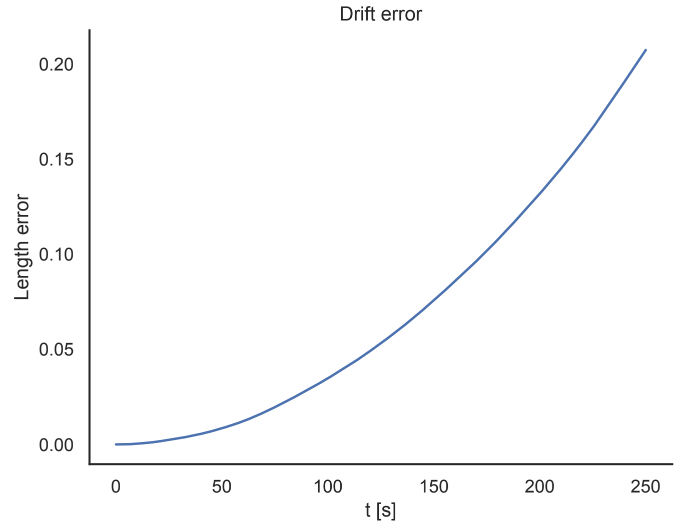
2.5 sec.



250 sec.

Drift in pendulum

- Drift in the pendulum example



Drift

Theorem

If we apply a method of order p we will (in the example from the last slide)

$$\|x^2 + y^2 - 1\| \leq h^p(At_n + Bt_n^2)$$

What can you do about this drift?

- Baumgarte stabilization
- Projection based methods
- Use another index reduction technique

Baumgarte stabilization

The first (1976) method to stabilize drift. The principle is simple, instead of using the second derivative of the algebraic constraint

$$\ddot{g} = 0$$

in the solver you use

$$\ddot{g} + \alpha\dot{g} + \beta g = 0$$

where α and β are chosen such that the zeros of the polynomial

$$s^2 + \alpha s + \beta$$

lies in the left half plane.
Simple to generalize. Kan be tricky to choose parameters α and β with respect to stiffness and other numerical properties.

Baumgarte, example

Consider an index 2 DAE with corresponding differentiated index 1 DAE

$$\begin{aligned} e_1 &: \dot{x} = f(x,y) \qquad & e_1 &: \dot{x} = f(x,y) \\ e_2 &: 0 = g(x) \qquad & \dot{e}_2 &: 0 = \dot{g}(x) = g'(x)f(x,y) \end{aligned}$$

Simulating $\{e_1, \dot{e}_2\}$ will have problems ensuring $g(x) = 0$. Instead, simulate the index 1 DAE

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

and then then

$$g + \alpha g' = 0 \quad \Rightarrow \quad g \sim e^{-\alpha t}$$

Thus, the constant $\alpha > 0$ stabilizes g.

Stabilization through projection

Show the basic principle on a semi-explicit DAE with index 2. Not easy to generalize for higher index, see Hairer-Wanner for further discussions.

$$\begin{aligned} e_1 &: y' = f(y,z) \\ e_2 &: 0 = g(y) \end{aligned}$$

Differentiate once

$$0 = g_y(y)f(y,z)$$

By solving an index 1 DAE (e_1, e_2') we will not necessarily fulfill $g(y_n) = 0$ at each step, even if we start in a consistent starting point.

Stabilization through projection, cont.

Principle

1. Start in a point y_{n-1}, z_{n-1}.
2. Take a step to $\tilde{y}_n, \tilde{z}_n$ with any method.
3. Project! One projection that has been suggested is defined by

$$\min_{y_n} \|\tilde{y}_n - y_n\|, \quad g(y_n) = 0$$

This is a non-linear optimization's problem with constraints.

There are many other ways to project to the surface$\mathcal{M}$.

ODE:s with invariants

$$y' = f(y), \quad \varphi(y) = 0$$

- Invariants from conservation laws, index reduction
- Difference compared to DAE, over determined
- $\varphi(y) = 0$ is called a first integral if $\varphi(y)f(y) \equiv 0$ in the neighborhood of the solution.
- Linear first integrals is fulfilled for most methods of integration
- Quadratic first integrals is fulfilled by, e.g., symplectic Runge-Kutta
- More complex invariants are normally not fulfilled.

Lecture 2 – Simulation of differential-algebraic equations

Simulation of DAE models and index reduction

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