Differential Algebraic Equations

Contents:

1. Introduction
2. Differential Algebraic Equations
3. Linear DAE
4. The Notion of Index
5. Numerical Methods
6. Summary

Goal:

- To develop a basic understanding of differential-algebraic equations

Introduction

- Cut a system into subsystems
- Use object orientation to structure the system
- Write mass, momentum and energy balances for each subsystem
- Assemble equations as differential algebraic equations
- Let software (Modelica) handle bookkeeping and transformations
- Build component libraries

Numerics

- Carl Runge, Martin Wilhelm Kutta $\approx$ 1900
- From desk calculators and people to computers and Numerical Mathematics $\approx$ 1900
- Use of computers for modeling and simulation late 1950's
- Besk 1956
- Germund Dahlquist. Stability and Error Bounds in the Numerical Solution of Ordinary Differential Equations 1958 (Fritz Carlsson Lars Hörmander)
- Electric circuits and DAE
- IBM 1960's ASTAP
- Berkeley SPICE1 Nagel Pederson 1973
- Charles William (Bill) Gear Cambridge UK, Urbana Ill, IBM 1960–62
- Linda Petzold DASSL 1982

A Question?

- Why should we know about these things, is it not handled by the software?
- Unfortunately not!
- Numerical linear algebra OK
- ODE good but not perfect
- Kjell Gustafsson: Pitfalls in simulation
- Kjell Gustafsson och Bill Gear

Ordinary Differential Equations

The initial value problem for the differential equation

$$\frac{dx}{dt} = f(x,t), \qquad x(0) = x_0$$

exists and is unique if the function $f(x,t)$ is Lipschitz continuous meaning that

$$|f(x,t) - f(y,t)| \le K|x-y|$$

Picard-Lindelöf or Cauchy-Lipschitz

Lack of Existence and Uniqueness

- Solutions may not exist for all t

$$\frac{dx}{dt} = x^2, \quad x(t) = \frac{1}{1-t}$$

- There may be many solutions,

$$\frac{dx}{dt} = 2\sqrt{x}, \quad x(0) = 0, \quad x(t) = \begin{cases} 0 & \text{if } t \le a \\ (t-a)^2 & \text{if } t > a \end{cases}$$

- Bad modeling?
- Good indicator!
- Numerical solutions require care!

Lecture 2 - Differential Algebraic Equations

1. Introduction
2. **Differential Algebraic Equations**
3. Linear DAE
4. The Notion of Index
5. Numerical Methods
6. Summary

Differential-Algebraic Equations

$$F(\dot z, z, t) = 0$$

A special case (semi-explicit)

$$\frac{dx}{dt} = f(x,y,t)$$
$$0 = g(x,y,t)$$

Singular perturbations

$$\frac{dx}{dt} = f(x,y,t)$$
$$\epsilon\frac{dy}{dt} = g(x,y,t)$$

More complicated than ODE

- Initial values must be consistent with algebraic equation
- Solutions less continuous than inputs
- The notion of index
- Existence and uniqueness
- Differential geometry is the natural tool
- Numerics: DASSL, RADAU

Will return to existence later!

References

W. Gear (1971) Simultaneous numerical solution of differential-algebraic equations. IEEE Trans Circuit Theory CT-18 89-95.
L. Petzold (1982) Differential-Algebraic Equations are not ODE's SIAM J on Scientific and Statistical Computing. 367-384.
E. Griepentrog and R. März (1986) Differential algebraic equations and their numerical solution Teubner.
K. E. Brenan, S. I. Campbell and L. R. Petzold (1986) Numerical Solution of Initial-Value Problems in Differential Algebraic Systems, SIAM classics in Applied Mathematics 1996.
E. Hairer G. Wanner (1991) Solving Ordinary Differential Equations II - Stiff and Differential Algebraic Equations, Springer.
W. C. Rheinboldt (1984) Differential-algebraic systems as differential equations on manifolds. *Math. Comp.*, (1984), 1473-1482
Code: DASSL (Petzold) RADAU (Hairer)

Lecture 2 - Differential Algebraic Equations

Linearization and Linear DAE

$$F(\dot z, z, t) = 0$$

$$E\frac{dz}{dt} = Az + b$$
$$E = \frac{\partial F}{\partial \dot z}, \quad A = -\frac{\partial F}{\partial z} \quad b = -\frac{\partial F}{\partial t}$$

- If E is regular we have an ODE
- The rank of E may change with z

The matrix $\lambda E - A$ is called a matrix pencil. It is singular if $\det(\lambda E - A) = 0$ for all λ and regular otherwise.

Weierstrass-Kronecker Normal Form

For a regular matrix pencil $\lambda E - A$ there exist matrices P and Q

$$PEQ = \begin{pmatrix} I & 0 \\ 0 & N \end{pmatrix} \qquad PAQ = \begin{pmatrix} C & 0 \\ 0 & I \end{pmatrix}$$

where $N = \operatorname{diag}(N_1, N_2, ..., N_k)$ is a block diagonal matrix where all elements of N_i are zero except for ones in the super-diagonal, e.g.

$$N_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad N_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

and C is on Jordan form
A regular matrix pencil can be transformed to

$$P(\lambda E - A)Q = \lambda \begin{pmatrix} I & 0 \\ 0 & N \end{pmatrix} + \begin{pmatrix} C & 0 \\ 0 & I \end{pmatrix}$$

Coordinate Changes - Kronecker normal form

$$E\frac{dz}{dt} = Az + b, \qquad z = Q\begin{pmatrix} x \\ y \end{pmatrix}, \qquad Pb = \begin{pmatrix} \mu \\ \nu \end{pmatrix}$$

Then

$$PE\frac{dz}{dt} = PEQ\frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = PAz + Pb = PAQ\begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} \mu \\ \nu \end{pmatrix}$$

Recall

$$PEQ = \begin{pmatrix} I & 0 \\ 0 & N \end{pmatrix} \qquad PAQ = \begin{pmatrix} C & 0 \\ 0 & I \end{pmatrix}$$

and the equations become

$$\frac{dx}{dt} = Cx + \mu$$
$$N\frac{dy}{dt} = y + \nu$$

Example

What is the meaning of

$$N\frac{dy}{dt} = y + \nu$$

We have

$$N\frac{dy}{dt} = y + \nu$$
$$N^2\frac{d^2y}{dt^2} = N\frac{dy}{dt} + N\frac{d\nu}{dt}$$

If $N^2 = 0$

$$0 = y + \mu + N\frac{d\nu}{dt}$$

The output y contains derivatives of the input ν

Lecture 2 - Differential Algebraic Equations

The Differential Index

Transform the linear DAE to Kronecker form

$$\frac{dx}{dt} = Cx + \xi(t)$$
$$N\frac{dy}{dt} = y + \eta(t)$$

The differential index is the smallest integer m such that the matrix N^m is zero.
The DAE has the solution

$$x = e^{Ct}x(0) + \int_0^t e^{A(t-s)}\xi(s)ds$$
$$y = -\eta(t) - N\frac{d\eta(t)}{dt} - \ldots - N^{m-1}\frac{d^{m-1}\eta(t)}{dt^{m-1}}$$

Notice that solution contains $m - 1$ derivatives of the input!

An Intuitive Interpretation

Consider the ODE

$$\frac{dx}{dt} = Ax$$

The poles or the eigenvalues are given by $\det(sI - A)$
For the DAE

$$E\frac{dx}{dt} = Ax$$

the solutions to $\det(sE - A)$ can be interpreted as poles. When E is singular there are "poles" at "infinity" which can be interpreted as differentiators.

Generalization

The differential index m of the DAE

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

is the minimal number of differentiations required to solve for $\dot{z}$

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

Example

$$\begin{aligned} \frac{dx}{dt} &= Cx + \xi(t) \\ N\frac{dy}{dt} &= y + \eta(t) \end{aligned}$$

The solution is

$$\begin{aligned} x &= e^{Ct}x(0) + \int_0^t e^{A(t-s)}\xi(s)ds \\ y &= -\eta(t) - N\frac{d\eta(t)}{dt} - \dots - N^{m-1}\frac{d^{m-1}\eta(t)}{dt^{m-1}} \end{aligned}$$

Differentiating the last equation shows that m differentiations are required to obtain an explicit equation for dy/dt

Perturbation Index

Consider the equation

$$F(\frac{dz}{dt}, z, t) = 0$$

and the perturbed solution

$$F(\frac{d\bar{z}}{dt}, \bar{z}, t) = \delta(t)$$

The equation has perturbation index $p_i = m$ if there is an error estimate of the form

$$|z(t) - \bar{z}(t)| \le C\Big(|z(0) - \bar{z}(0)| + \max|\delta(t)| + \dots + \max\Big|\frac{d^{m-1}\delta(t)}{dt^{m-1}}\Big|\Big)$$

perturbation index $\le 1 +$ *differential index*

Semi-Explicit Forms

- **Index 0:** Solve explicitly for dx/dt ODE!

$$\frac{dx}{dt} = f(x, y)$$

- **Index 1:** g_y regular (cf singular perturbations)

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

Differentiate algebraic equation and solve for dy/dt

$$\begin{aligned} 0 &= g_x\frac{dx}{dt} + g_y\frac{dy}{dt} = g_x f + g_y\frac{dy}{dt} = g_x f + g_y f \\ \frac{dy}{dt} &= -g_y^{-1}g_x f \end{aligned}$$

Semi-Explicit Forms

- **Index 2:** $g_y = 0$ and $g_{xy}f + g_x f_y$ regular

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

Differentiate algebraic equation twice

$$\begin{aligned} 0 &= g_x\frac{dx}{dt} + g_y\frac{dy}{dt} = g_x f \\ 0 &= \Big(g_{xx}f + g_x f_x\Big)\frac{dx}{dt} + \Big(g_{xy}f + g_x f_y\Big)\frac{dy}{dt} \end{aligned}$$

Solve for dy/dt

$$\frac{dy}{dt} = -(g_{xy}f + g_x f_y)^{-1}\Big(g_{xx}f + g_x f_x\Big)f$$

Initial Conditions

Differentiated equations

$$\begin{aligned} \frac{dx}{dt} &= f(x, y) \\ 0 &= g(x, y) \\ 0 &= g_x(x)f(x, y) \\ 0 &= \Big(g_{xx}(x)f(x, y) + g_x(x)f_x(x, y)\Big)f(x, y) + g_x(x)f_y(x, y)\frac{dy}{dt} \end{aligned}$$

Initial conditions must satisfy

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

Finding proper initial conditions is an essential task

Lecture 2 - Differential Algebraic Equations

Numerical Solvers

ODEs

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

Provide a routine for $f(t, x)$.

Runge Kutta methods

Multi-step methods

DAEs

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

Provide a routine for $F(t, x, \dot{x})$.

DASSL – multi-step method

RADAU5 – implicit Runge-Kutta

ODE Methods

Example

$$\frac{dx}{dt} = -\lambda x$$

Forward difference approx

$$\frac{x_{n+1} - x_n}{h} = -\lambda x_n$$

Hence

$$x_{n+1} = (1 - \lambda h)x_n$$

Stable if $\lambda h < 1$ Explicit equations.

Backward difference approx

$$\frac{x_n - x_{n-1}}{h} = -\lambda x_n$$

Hence

$$x_{n+1} = \frac{1}{1 + \lambda h} x_n$$

Stable for all λh, implicit equations.

Implicit methods

Differential equation

$$\frac{dx}{dt} = f(x, t)$$

Approximate derivative by backward difference

$$\frac{dx}{dt} \approx \frac{x_n - x_{n-1}}{h}$$

This gives

$$\frac{dx}{dt} \approx \frac{x_n - x_{n-1}}{h} = f(x_n, t_n)$$

At each step solve for x_n by Gauss-Seidel or Newtons method

DASSL

Consider the DAE

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

A backward difference approximation of $\dot{x}$ gives an algebraic equation to update the equation. Backward Euler gives

$$\dot{x}_n \approx \frac{x_n - x_{n-1}}{h}$$

$$F(t_n, x_n, \frac{x_n - x_{n-1}}{h}) = 0$$

Solve this equation by Newtons method. Analytical Jacobians improves the iterations.

What Happens with the Unusual Part?

Example

$$N\frac{dy}{dt} = y + \eta(t)$$

Example

$$\frac{dy_2}{dt} = y_1 + \eta_1(t)$$
$$0 = y_2 + \eta_2(t)$$

Hence

$$y_1(t_n) = \frac{y_2(t_n) - y_2(t_{n-1})}{h} - \eta_1(t_n)$$
$$y_2(t_n) = -\eta_2(t_n)$$

High Index

- Causes difficulties because of the differentiation
- Index reduction

Index Reduction

$$E\frac{dz}{dt} = Az + b(t)$$

1. Find non-singular matrices P and Q such that

$$PEQ = \begin{pmatrix} E_{11} \\ 0 \end{pmatrix}$$

   with E_{11} of full rank
2. Substitute $y = Qz$, multiply with P from the left

$$\begin{pmatrix} E_{11} \\ 0 \end{pmatrix} \dot{z} = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} z + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

3. Differentiate $A_{21}z + b_2$ to give

---

2. Substitute $y = Qz$, multiply with P from the left

$$\begin{pmatrix} E_{11} \\ 0 \end{pmatrix} \dot{z} = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} z + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

3. Differentiate $A_{21}z + b_2$ to give

$$\begin{pmatrix} E_{11} \\ A_{21} \end{pmatrix} \dot{z} = \begin{pmatrix} A_{11} \\ 0 \end{pmatrix} z + \begin{pmatrix} b_1 \\ -\dot{b}_2 \end{pmatrix}$$

4. Continue until a regular E matrix is obtained

- The equation obtained is an ODE.
- The number of iterations is equal to the differential index.
- The solution may drift away from the algebraic constraint.

Index Reduction

To avoid that the numerical solution drifts off the algebraic constraints, one may try to obtain a low-index formulation with a solution set identical to the original problem.

Projection methods

1. Retain all original equations and their derivatives.
2. The result is an overdetermined consistent index-1 DAE.
3. Consistency is generally lost when the system is discretized.
4. Use projection techniques (least squares)

Dummy derivatives

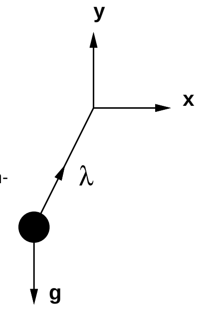
Example — The Pendulum

Unit mass, unit length pendulum

$$\ddot{x} = -\lambda x$$
$$\ddot{y} = -\lambda y - g$$
$$0 = x^2 + y^2 - 1$$

Index 3 problem. Differentiate length constraint twice:

$$0 = x\dot{x} + y\dot{y}$$
$$0 = x\ddot{x} + \dot{x}^2 + y\ddot{y} + \dot{y}^2$$



Example — The Pendulum

$$\ddot{x} = -\lambda x$$
$$\ddot{y} = -\lambda y - g$$
$$0 = x^2 + y^2 - 1$$

More equations are needed to obtain $\dot{x}$, $\dot{y}$, $\ddot{x}$ and $\ddot{y}$. Adding the derivatives we get

$$\ddot{x} = -\lambda x$$
$$\ddot{y} = -\lambda y - g$$
$$0 = x\dot{x} + y\dot{y}$$
$$0 = x\ddot{x} + \dot{x}^2 + y\ddot{y} + \dot{y}^2$$

Notice that these equations do not guarantee that

$$0 = x^2 + y^2 - 1$$

Example — The Pendulum

Use the overdetermined system

$$\ddot{x} = -\lambda x$$
$$\ddot{y} = -\lambda y - g$$
$$0 = x^2 + y^2 - 1$$
$$0 = x\dot{x} + y\dot{y}$$
$$0 = x\ddot{x} + \dot{x}^2 + y\ddot{y} + \dot{y}^2$$

Dummy Derivatives

We need not eliminate $\ddot{y}$ and $\dot{y}$ explicitly:

$$\ddot{x} = -\lambda x$$
$$w = -\lambda y - g$$
$$0 = x^2 + y^2 - 1$$
$$0 = x\dot{x} + yv$$
$$0 = x\ddot{x} + \dot{x}^2 + yw + v^2$$

Add differentiated equations and replace $\ddot{y}$ by w and $\dot{y}$ by v.

- Gives an equivalent index 1 problem.
- Variables w and v are called dummy derivatives.
- The fact that $w \equiv \ddot{y}$ and $v \equiv \dot{y}$ is not explicit in the transformed problem.

Dummy Derivatives Summary

A method for solving high index DAEs:

- Works for a large class of interesting problems.
- Implementable.
- Negligible overhead for explicit or index 1 problems.
- The numerical results for the dummy derivative index 1 model of the pendulum are comparable to the state space model.
  - Use automatic differentiation.
  - Dynamic pivoting

Special Integration Algorithms

In many problems there are physical quantities that are invariants.
There are special algorithem e.g. Symplectic integrators that preserve quantities such as energy or momnetum.
Commonly used for mechanical systems. Hamiltonian systems for space flight.
The general idea is to do discrete approximation that have proper physical interpretations and thus conserve the right quantities.

Lecture 2 - Differential Algebraic Equations

1. Introduction
2. Differential Algebraic Equations
3. Linear DAE
4. The Notion of Index
5. Numerical Methods
6. **Summary**

Summary

- Differential algebraic equations natural for modeling
- DAEs are different from ODEs
- DAEs are not yet mature
- Index and differentiations
- Numerics needed and partially available
- Development inspired by circuit simulation Bill Gear!