Chapter 3: Approximation of Differential-Algebraic Equations

Michael Hanke

Mathematical Models, Analysis and Simulation, Part I

The Problem

Consider the differential equation

$$\boxed{A(t,x)x' + g(t,x) = 0}$$

or, more generally, $F(t,x,x') = 0$. Here, all involved functions $x : I \to \mathbb{R}^n$ etc are vector-valued functions!

Applications:

- Electrical circuits
- Constraint mechanical multibody systems
- Discretization of multiphysics systems
- Singular perturbed problems

How can daes reliably be solved?

Are there any differences to explicit odes?

Numerical Approximation

- Consider the dae $F(t,x,x') = 0$.
- Use the θ-method ($0 \le \theta \le 1, h = t_n - t_{n-1}$):

$$x'(t_{n-1} + \theta h) \approx \frac{x(t_n) - x(t_{n-1})}{h},$$
$$x(t_{n-1} + \theta h) \approx (1-\theta)x(t_{n-1}) + \theta x(t_n)$$

  such that

$$F\left(t_{n-1} + \theta h, (1-\theta)x_{n-1} + \theta x_n, \frac{x_n - x_{n-1}}{h}\right) = 0$$

- Some special cases:
  $\theta = 0$ Explicit Euler method.
  $\theta = 1/2$ Midpoint rule.
  $\theta = 1$ Implicit Euler method.

The θ-Method For Linear Daes

Let

$$EAF = \begin{pmatrix} I & 0 \\ 0 & J \end{pmatrix}, \quad EBF = \begin{pmatrix} W & 0 \\ 0 & I \end{pmatrix}$$

be the Kronecker canonical form of (A,B)

Make the transformation

$$\begin{pmatrix} y_n \\ z_n \end{pmatrix} = F^{-1}x_n$$

as before and scale by E:

$$\frac{y_n - y_{n-1}}{h} + (1-\theta)Wy_{n-1} + \theta W y_n = p(t_{n-1} + \theta h),$$
$$J\frac{z_n - z_{n-1}}{h} + (1-\theta)z_{n-1} + \theta z_n = r(t_{n-1} + \theta h).$$

Compare to the continuous problem:

$$y' + Wy = p(t)$$
$$Jz' + z = r(t)$$

- The discretization of the ode (first row) works as expected.
- For $\mu = 0$, the second row is missing.

The Index 1 Case

$$(1-\theta)z_{n-1}+\theta z_n = r(t_{n-1}+\theta h) =: r_n$$

- If $\theta = 0$, z_n cannot be computed. Hence, the method must be implicit!
- If $\theta \neq 0$, the recursion becomes

$$z_n = -\frac{1-\theta}{\theta}z_{n-1} + \frac{1}{\theta}r_n$$

- This recursion is stable if and only if $|1-\theta/(\theta)| < 1$, i.e.

$$1/2 < \theta \leq 1.$$

- For $\theta = 1/2$, the recursion is weakly unstable.
- For $0 < \theta < 1/2$, this recursion is (exponentially) unstable!

Conclusion: The explict Euler is not feasible, the trapezoidal rule becomes unstable. It is the implicit Euler method which can be used!

The Index 2 Case

- Consider the implicit Euler method, only. Computation as above provides

$$z_n = r_n - \frac{1}{h}J(r_n - r_{n-1}).$$

- If there are no errors in the computation of $(1/h)J(r_n - r_{n-1})$, z_n remains bounded.
- Inexact starting values as well as round-off give rise to a *weak instability*, i.e., the errors are amplified by h^{-1}.

Note: For $\mu \geq 3$, the amplification factor becomes $h^{1-\mu}$.

Conclusions

1. Singular systems of index μ are mixed regular differential equations and equations including $\mu - 1$ differentiations.
2. Consistent initial values are *not* easy to compute in practice.
3. Integration methods handle the inherent regular ode as expected.
4. Numerical integration methods must be *implicit*. Moreover, additional conditions must be fulfilled to ensure *stability in the algebraic variables* (or their equivalent).
5. Errors in the starting values are amplified by $h^{1-\mu}$ in the best case, but only the components z_n are effected.
6. Index 0,1,2 daes can be solved numerically. *Not those with $\mu \geq 3$.*

For *general* nonlinear equations, (3), (5) are no longer true. But often, numerial methods work as expected.

Finite Difference Methods for DAEs

- For general DAEs, most often BDF based codes are used. (ex. DASSL)
- Radau-IIA methods have the same stability problems. However, the implementation is tricky. (ex. RADAU5)
- If the system has special structure, use it as much as you can! (ex. Projected RK methods)
- Many implicit methods can be adapted to be used with DAEs. However, their applicability (read: efficiency) is usually restricted to special areas of applications.

The Gear/Hsu/Petzold Example

$$A(t)x'(t) + B(t)x(t) = q(t),$$
$$A = \begin{pmatrix} 0 & 0 \\ 1 & \eta t \end{pmatrix}, B = \begin{pmatrix} 1 & \eta t \\ 0 & 1+\eta t \end{pmatrix}.$$

This is an index-2 system. Apply the implicit Euler method:

$$x_{2,n} = \frac{\eta}{1+\eta} x_{2,n-1} + \frac{1}{1+\eta} q_{2,n} - \frac{1}{1+\eta} \frac{q_{1,n} - q_{1,n-1}}{h}$$

if and only if $1+\eta \neq 0$.

This recursion is

- weakly unstable like h^{-1} if $\eta > -1/2$
- weakly unstable like h^{-2} if $\eta = -1/2$
- unstable like $\exp(1/h)$ if $\eta < -1/2$, $\eta \neq -1$

Strange things happen if the nullspace $\ker A(x,t)$ of $A(x,t)$ varies!

Fortunately, very often, this nullspace is constant.

Note: The implicit Euler method is both the simplest BDF method and the simplest Radau IIA method.

Index Reductions

Start with a semiexplicit index-1 system,

$$y' = -B_{11}y - B_{12}z + p,$$
$$0 = -B_{21}y - B_{22}z + r.$$

This dae has index 1 if and only if B_{22} is nonsingular.

Differentiate the constraint in the original dae:

$$0 = -B_{21}y' - B_{22}z' + r'$$

Then, the system reads:

$$\begin{pmatrix} I & 0 \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} y' \\ z' \end{pmatrix} + \begin{pmatrix} B_{11} & B_{12} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} p \\ r' \end{pmatrix}.$$

This is an index-0 dae (an ode)

Index Reductions (cont.)

Conclusion: By differentiation of the algebraic constraint, the index can be reduced by one.

- The index-reduced system is *not* equivalent to the original one!
- The new system has more degrees of freedom (initial values for z).
- How to do that in more implicitely given systems?
- Do there exist better index reduction methods?

Problems With a Structure: Hessenberg Index-2 Systems

$$y' = f(y,z),$$
$$0 = h(y)$$

sucht that $h_y(y) f_z(y,z)$ is nonsingular for all (y,z).

Note that both h_y and f_z are rectangular!

Differentiate as before: $0 = h_y(y)y' = h_y(y) f(y,z)$.

Do it a second time (omitting arguments):

$$0 = h_{yy}(y', f(y,z)) + h_y(f_y y' + f_z z') = h_{yy}(f(y,z), f(y,z)) + h_y f_y f(y,z) + h_y f_z z'.$$

Hessenberg Index-2 systems (cont.)

Hence,

$$z' = (h_y f_z)^{-1} G(y,z).$$

The original system has (differentiation) index 2.

The system

$$y' = f(y,z),$$
$$0 = h_y(y) f(y,z)$$

is a semiexplicit system with index 1. This can be further reduced to become an index-0 system (I.e., an explicit ode).

Hessenberg Systems (cont)

- The index-0 system can be approximated by any numerical method.
- For the index-1 system, an implicit method must be used. It can be much simplified by collocation, $0 = h_y(y_n) f(y_n, z_n)$.

Are the systems equivalent? **No**

Let the initial value $(y(0), z(0))$ for the index-1 system such that $h(y(0)) = 0$.

$$0 = \int_0^t h_y(y(s)) f(y(s), z(s)) ds = h(y(t)) - h(y(0)) = h(y(t))$$

Equivalence, if and only if the initial values are consistent.

This property gets lost during integration. Drift-off

Stabilization of Constraints

The system

$$y' = f(y,z),$$
$$0 = h(y),$$
$$0 = h_y(y) f(y,z)$$

is equivalent to the original one, but overdetermined.

Baumgarte's idea: Choose a parameter $\alpha > 0$ and replace the algebraic constraint by

$$0 = (d/dt)h + \alpha h.$$

The solution becomes $h(y(t)) = h(y(0)) \exp(-\alpha t)$.

Pro: Any drift-off is suppressed.

Contra: The system becomes stiff. How to choose α?

Note: Baumgarte proposed this idea for index-3 CMBS.

Stabilization of Invariants

Assume that we have an ode

$$y' = \hat{f}(y), y(0) = y_0$$

such that the solution fulfills

$$h(y(t)) \equiv 0.$$

Examples:

- Charges in an electrical circuit.
- Mass under chemical reactions.

A common integrator will *not* preserve the invariant

Gear/Gupta/Leimkuhler: Consider the dae

$$y' = \hat{f}(y) - H^T(y) z,$$
$$0 = h(y).$$

Both systems have the same solution y while $z \equiv 0$.

This system has index 2!

A Stiff Pendulum

- Consider a planar spring of length l and mass m with spring constant ε^{-1} $(0 < \varepsilon \ll 1)$ with one end attached to the origin.
- Let $r = \sqrt{p_1^2 + p_2^2}$. Then

$$mp'' = -\varepsilon^{-1}\frac{r-1}{r}p - \begin{pmatrix} 0 \\ g \end{pmatrix}.$$

- Introduce $\lambda = \varepsilon^{-1}(r-1)$. Then,

$$mp'' = -\frac{\lambda}{r}p - \begin{pmatrix} 0 \\ g \end{pmatrix},$$
$$\varepsilon\lambda = r - 1.$$

- For small ε, this system is very hard to solve numerically (extremely stiff).
- For $\varepsilon \to 0$ we obtained the reduced system,

$$mp'' = -\frac{\lambda}{r}p - \begin{pmatrix} 0 \\ g \end{pmatrix},$$
$$0 = r - 1.$$

  This system is no longer stiff! In fact, it is easier to solve than the original one, even if it has index 3!

The Pendulum: Conclusion

- A higher-index dae can often be simpler that, or result as a simplification of, an ode or a lower index dae.
- A dae can in a sense be very close to another dae with a different index.

It is wrong in general to consider a dae as an infinitely stiff ode!!!

Note: The important property of BDF and Radau IIA methods applied to DAEs is stability in the recursions for the algebraic components, not their stiff stability.