Differential-Algebraic Equations (DAEs) and numerical methods

by Sirui Tan
Definition of DAEs

\[ F(t, y, y') = 0, \]

where \( y: \mathbb{R} \to \mathbb{R}^m \) is the solution, \( F: \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m \) is a given function.

\( \frac{\partial F}{\partial y'} \) nonsingular \( \Rightarrow \) explicit ODE

\[ y' = f(t, y). \]

semi-explicit DAE (or ODE with constraints)

\[ x' = f(t, x, z), \text{(differential equation)} \]
\[ 0 = g(t, x, z). \text{(algebraic equation)} \]
Example 1. simple pendulum

\[
\begin{align*}
\dot{x}_1 &= x_3, \\
\dot{x}_2 &= x_4, \\
\dot{x}_3 &= -z x_1, \\
\dot{x}_4 &= -z x_2 - g,
\end{align*}
\]

\[x_1^2 + x_2^2 = 1.\]

Figure 1. simple pendulum

\(z(t)\) Lagrange multiplier

\[
\begin{align*}
x_1'' &= -z x_1, \\
x_2'' &= -z x_2 - g, \\
x_1^2 + x_2^2 &= 1.
\end{align*}
\]
Index

Minimum number of differentiations of the system which would be required to solve for $y'$ uniquely in terms of $y$ and $t$ (i.e., to obtain an explicit ODE). It measures the distance from a DAE to its related ODE. It reveals the mathematical structure and potential complications in the analysis and the numerical solution of the DAE.

The higher the index of a DAE, the more difficulties for its numerical solution. Example:

- **index-1 DAE**

  \[ y = q(t). \]

  since $y' = q'(t)$ explicit ODE.

- **index-2 DAE**

  \[
  y_1 = q(t), \\
  y_2 = y'_1.
  \]

  since $y_2' = y_1'' = q''(t)$.  


Special DAE forms

• Hessenberg Index-1 system (or semi-explicit index-1 system)

\[ x' = f(t, x, z), \]
\[ 0 = g(t, x, z). \]

Jacobian matrix \( g_z \) nonsingular.

\( x(t) \) differential variables, \( z(t) \) index-1 algebraic variables.

• Hessenberg Index-2 system

\[ x' = f(t, x, z), \]
\[ 0 = g(t, x). \]

\( g_x f_z \) is nonsingular.

\( z(t) \) index-2 variables. Pure index-2 DAE.
Example 2. Navier-Stokes equations

\[
\begin{align*}
    u_t + uu_x + vu_y + p_x - \nu(u_{xx} + u_{yy}) &= 0, \\
    v_t + uv_x + vv_y + p_y - \nu(v_{xx} + v_{yy}) &= 0, \\
    u_x + v_y &= 0.
\end{align*}
\]

after spatial discretization (FD, FV, FE)

\[
M \mathbf{u}' + (K + N(\mathbf{u})) \mathbf{u} + C \mathbf{p} = \mathbf{f},
\]

\[
C^T \mathbf{u} = 0.
\]

\(C^T M^{-1} C\) is a nonsingular matrix with a bounded inverse \(\Rightarrow\) Hessenberg Index-2 system.
Consistent initial values

Index-2 system

\[ x(t) = \sin(t) \]
\[ x'(t) + y(t) = 0. \]

consistent \iff satisfying the algebraic constraint

\[ x(t) = \sin(t) \]

and hidden constraints

\[ y(t) = -x'(t) = -\cos(t). \]

Consistent initial values

\[ x(0) = \sin(0), \]
\[ y(0) = -\cos(0). \]
Applications

- constrained mechanical systems (e.g. simple pendulum, N-S equations)
- electrical circuits
  large but sparse DAE of the form
  \[ M(y) y' + f(y) = q(t). \]
- chemical reaction kinetics
Numerical methods

Semi-explicit index-1 or index-2 DAE

\[ x' = f(t, x, z), \]
\[ 0 = g(t, x, z). \]

limiting case of the singularly perturbed ODE

\[ x' = f(t, x, z), \]
\[ \varepsilon z' = g(t, x, z), \]

where \( 0 \leq \varepsilon \ll 1. \)

Observations: consider methods for stiff ODEs.
Crank-Nicolson method

Explicit ODE

\[ y' = f(t, y). \]

C-N method

\[ \frac{y_n - y_{n-1}}{h} = \frac{1}{2} \left( f(t_n, y_n) + f(t_{n-1}, y_{n-1}) \right). \]

Index-2 DAE

\[ \begin{align*}
  x(t) &= \sin(t) \\
  x'(t) + y(t) &= 0
\end{align*} \]

exact solution

\[ \begin{align*}
  x(t) &= \sin(t), \\
  y(t) &= -\cos(t).
\end{align*} \]

C-N method

\[ \begin{align*}
  \frac{1}{2} (x_n + x_{n-1}) &= \frac{1}{2} \left( \sin(t_n) + \sin(t_{n-1}) \right) \\
  \frac{x_n - x_{n-1}}{h} + \frac{1}{2} (y_n + y_{n-1}) &= 0.
\end{align*} \]
Exact initial values

\[ x_0 = \sin(0), \]
\[ y_0 = -\cos(0). \]

**Figure 2.** C-N method, exact initial values, \( h = 0.04 \).
Perturbed initial values

\[ x_0 = \sin(0) + h^3, \]
\[ y_0 = -\cos(0). \]

**Figure 3.** C-N method, perturbed initial values, \( h = 0.04 \).
Conclusion: A-stability is not enough.

\[ x' = f(t, x, z), \]
\[ \varepsilon z' = g(t, x, z), \]

where \( 0 \leq \varepsilon \ll 1. \)

Set \( \varepsilon = 0 \Rightarrow \) the limit DAE.
Methods with stiff decay

test equation

\[ y' = \lambda (y - g(t)), \]

or

\[ \varepsilon y' = \hat{\lambda} (y - g(t)), \]

where \( \varepsilon = \frac{1}{|\text{Re}(\lambda)|} \), \( \hat{\lambda} = \varepsilon \lambda \). \( |\hat{\lambda}| = 1. \)

Set \( \varepsilon = 0 \Rightarrow y(t) = g(t). \)

The method has stiff decay if \( t_n > 0 \) fixed

\[ y_n \to g(t_n) \text{ as } \varepsilon \to 0^+. \]

C-N method does not have stiff decay.
Backward Euler method

Index-2 DAE

\[
x(t) = \sin(t),
\]
\[
x'(t) + y(t) = 0.
\]

BE method

\[
x_n = \sin(t_n),
\]
\[
\frac{x_n - x_{n-1}}{h} + y_n = 0.
\]
Exact initial values

\[ x_0 = \sin(0), \]
\[ y_0 = -\cos(0). \]

Figure 4. BE method, exact initial values, \( h = 0.04 \).
Perturbed initial values

\[ x_0 = \sin(0) + h, \]
\[ y_0 = -\cos(0). \]

**Figure 5.** BE method, perturbed initial values, \( h = 0.04 \).
**Multistep methods**

The only method with stiff decay is the BDF method.

Semi-explicit index-1 or index-2 DAE

\[
x' = f(t, x, z),
0 = g(t, x, z).
\]

BDF method

\[
\frac{1}{\beta_0 h} \sum_{j=0}^{k} \alpha_j x_{n-j} = f(t_n, x_n, z_n),
0 = g(t_n, x_n, z_n).
\]
Convergence of BDF

**Theorem:** the $k$-step BDF method is convergent of order $p = k$ for $k \leq 6$, i.e.,

$$x_n - x(t_n) = O(h^p), z_n - z(t_n) = O(h^p),$$

whenever the initial values satisfy

- if $k \leq 2$
  $$x_j - x(t_j) = O(h^{p+1}) \text{ for } j = 0, ..., k - 1.$$

- if $k \geq 3$
  $$x_j - x(t_j) = O(h^p) \text{ for } j = 0, ..., k - 1.$$
Multistage methods

If we consider collocation methods, the only method with stiff decay is the Radau method.

Semi-explicit index-1 or index-2 DAE

\[
\begin{align*}
x' &= f(t, x, z), \\
0 &= g(t, x, z).
\end{align*}
\]

Radau method

\[
\begin{align*}
t_i &= t_{n-1} + c_i h, \quad i = 1, \ldots, s, \\
K_i &= f(t_i, X_i, Z_i), \\
X_i &= x_{n-1} + h \sum_{j=1}^{s} a_{ij} K_j, \\
0 &= g(t_i, X_i, Z_i).
\end{align*}
\]

and (since \(a_{sj} = b_j, \quad j = 1, \ldots, s\))

\[
x_n = X_s, \quad z_n = Z_s.
\]
Convergence of the Radau method

**Theorem:** the $s$-stage Radau method is convergent of order $2s - 1$ for $x_n$ and of order $s$ for $z_n$. (No order reduction for $x_n$.)
Practical difficulties

- obtaining a consistent set of initial conditions
  Given $x_0$, solve for $z_0$ from $0 = g(0, x_0, z_0)$. What’s the initial guess?

- ill-conditioning of iteration matrix
  e.g. backward Euler method, iteration matrix

$$
\begin{pmatrix}
  h_n^{-1} I - f_x & -f_z \\
  -g_x & -g_z
\end{pmatrix}
$$

condition number $O(h_n^{-1})$. If $h_n$ small, Newton iteration fails?

- Error estimation for index-2 DAEs
Available codes

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<td>MEBDF</td>
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Table 1. a list of available codes for DAEs
Summary

• DAEs are generalizations of ODEs. The index indicates the distance from its underlying ODE and thus the difficulty. We should be careful when imposing initial conditions.

• Methods with stiff decay perform well for solving DAEs, e.g, BDF method and the Radau collocation method.
References

- Series of lectures on DAEs, URL: http://www.win.tue.nl/casa/meetings/seminar/previous/