Lecture 19:
Differential Algebraic Equations
Recap

• Differential algebraic equations
  • Semi-explicit
  • Fully implicit
• Simulation via backward difference formulas
Recap

• How suitable are such approaches?

• Consider stirred tank example 1:

\[
\frac{dc_2}{dt} = \frac{Q}{V} (c_1(t) - c_2(t))
\]

\[
c_1(t) = \gamma(t)
\]

Apply backward Euler method:

\[
\left. \frac{dx}{dt} \right|_{t_k} = \frac{x(t_k) - x(t_{k-1})}{t_k - t_{k-1}} + O(t_k - t_{k-1})
\]

\[
c_1(t_k) = \gamma(t_k)
\]

\[
c_2(t_k) = \frac{1}{1 + \frac{Q}{V}(t_k - t_{k-1})} \left( c_2(t_{k-1}) + \frac{Q}{V} (t_k - t_{k-1}) c_1(t_k) \right) + O((t_k - t_{k-1})^2)
\]
Recap

• How suitable are such approaches?

• Consider stirred tank example 2:

\[
\frac{dc_2}{dt} = \frac{Q}{V} (c_1(t) \quad c_2(t))
\]

\[c_2(t) = \gamma(t)\]

Apply backward Euler method:

\[c_2(t_k) = \gamma(t_k)\]

\[c_1(t_k) = c_2(t_k) + \frac{V}{Q} \left( \frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}} \right) + O(t_k - t_{k-1})\]
Recap

- How suitable are such approaches?
- Consider the system of DAEs:

  \[
  \dot{c}_2 = c_1(t) \\
  \dot{c}_3 = c_2(t) \\
  0 = c_3(t) - \gamma(t)
  \]

Apply backward Euler method:

\[
\begin{align*}
  c_3(t_k) &= \gamma(t_k) \\
  c_2(t_k) &= \frac{c_3(t_k) - c_3(t_{k-1})}{t_k - t_{k-1}} + O(t_k - t_{k-1}) \\
  c_1(t_k) &= \frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}} + O(1)
\end{align*}
\]
Recap

- Solution via backward Euler:
  - Stirred-tank example 1:
    - local truncation error: $O(\Delta t^2)$
  - Stirred-tank example 2:
    - local truncation error: $O(\Delta t)$
  - DAE example 3:
    - local truncation error: $O(1)$
Recap

• How suitable are such approaches?

• Consider the system of DAEs:

\[
\begin{aligned}
\dot{c}_1 &= c_1(t) + c_2(t) + c_3(t) \\
\dot{c}_2 &= -c_1(t) - c_2(t) + c_3(t) \\
0 &= c_1(t) + c_2(t)
\end{aligned}
\]

Apply backward Euler method:
# Differential Index

- Consider stirred tank example 1:

\[
\frac{dc_2}{dt} = \frac{Q}{V} (c_1(t) - c_2(t)) \quad (1)
\]

\[
c_1(t) = \gamma(t) \quad (2)
\]

- How many time derivatives are needed to convert to a system of independent ODEs having differentials of all the unknowns?

  derivative of (2)

\[
\frac{dc_1}{dt} = \dot{\gamma}(t) \quad (3)
\]

Called an index-1 DAE.
Differential Index

• Consider stirred tank example 2:

$$\frac{dc_2}{dt} = \frac{Q}{V} (c_1(t) - c_2(t)) \quad (1)$$

$$c_2(t) = \gamma(t) \quad (2)$$

• How many time derivatives are needed to convert to a system of ODEs?

Substitute (1)

$$\frac{dc_2}{V} = \dot{\gamma} \quad \rightarrow \quad c_1(t) = c_2(t) + \frac{V}{Q} \dot{\gamma} \quad (3)$$

Derivative of (2)

$$\frac{dc_1}{dt} - \frac{dc_2}{dt} = \frac{V}{Q} \ddot{\gamma} \quad (4)$$

Called an index-2 DAE.
Differential Index

• Consider DAE example 3:

\[ \dot{c}_2 = c_1(t) \]  (1)

\[ \dot{c}_3 = c_2(t) \]  (2)

\[ 0 = c_3(t) - \gamma(t) \]  (3)

• How many time derivatives are needed to convert to a system of ODEs?

derivative of (3) substitute (2)
\[ \dot{c}_3 = \dot{\gamma} \rightarrow c_2(t) = \dot{\gamma} \]  (4)

↓ substitute (1)

derivative of (4) derivative of (5)
\[ \dot{c}_2 = \ddot{\gamma} \rightarrow c_1(t) = \ddot{\gamma} \]  (5)

\[ \dot{c}_1 = \dddot{\gamma} \]  (6)

Called an index-3 DAE.
The differential index of a semi-explicit DAE system is defined as the minimum number of differentiations required to convert the DAE to a system of independent ODEs.

\[
\begin{align*}
\frac{dx}{dt} & = f(x, y, t) \\
0 & = g(x, y, t) \\
\frac{dg}{dt} & = g^{(1)}(x, y, \dot{y}, t) \\
\frac{d^2g}{dt^2} & = g^{(2)}(x, y, \dot{y}, t) \\
& \vdots \\
\text{solve for:} \\
\frac{dy}{dt} & = s(x, y, t)
\end{align*}
\]
Consider another example:

\[
\begin{align*}
\dot{c}_1 &= c_1(t) + c_2(t) + c_3(t) \\
\dot{c}_2 &= -c_1(t) - c_2(t) + c_3(t) \\
0 &= c_1(t) + c_2(t)
\end{align*}
\]

How many time derivatives are needed to convert to a system of ODEs?
Differential Index

- The differential index of a semi-explicit DAE system is defined as the minimum number of differentiations required to convert the DAE to a system of ODEs.

- Index-1 example:

\[
\begin{align*}
\frac{dx}{dt} &= f(x, y, t) \quad (1) \\
0 &= g(x, y, t) \quad (2)
\end{align*}
\]

**derivative of (2)**

\[
0 = \frac{dg}{dt} = \frac{\partial g}{\partial x} \frac{dx}{dt} + \frac{\partial g}{\partial y} \frac{dy}{dt} + \frac{\partial g}{\partial t} \rightarrow \frac{\partial g}{\partial y} \frac{dy}{dt} = - \frac{\partial g}{\partial x} f(x, y, t) - \frac{\partial g}{\partial t}
\]

If \( \frac{\partial g}{\partial y} \) is full rank then the DAE is index-1:

\[
\frac{dy}{dt} = - \left( \frac{\partial g}{\partial y} \right)^{-1} \left( \frac{\partial g}{\partial x} f(x, y, t) + \frac{\partial g}{\partial t} \right)
\]
Differential Index

- Example, determine the differential index:

\[ \frac{dc_2}{dt} = \frac{Q_1}{V_1} (c_1(t) - c_2(t)) \]

\[ \frac{dc_4}{dt} = \frac{Q_1}{V_2} c_2(t) + \frac{Q_2}{V_2} c_3(t) - \frac{Q_1 + Q_2}{V_2} c_4(t) \]

\[ c_1(t) = \gamma_1(t) \]

\[ c_3(t) = \gamma_2(t) \]
Differential Index

Example, determine the differential index:

\[ \frac{dc_2}{dt} = \frac{Q_1}{V_1} (c_1(t) - c_2(t)) \]

\[ \frac{dc_4}{dt} = \frac{Q_1}{V_2} c_2(t) + \frac{Q_2}{V_2} c_3(t) - \frac{Q_1 + Q_2}{V_2} c_4(t) \]

\[ c_3(t) = \gamma_1(t) \]

\[ c_4(t) = \gamma_2(t) \]
Example, determine the differential index:

\[ \frac{d c_2}{d t} = \frac{Q_1}{V_1} (c_1(t) - c_2(t)) \]

\[ \frac{d c_4}{d t} = \frac{Q_1}{V_2} c_2(t) + \frac{Q_2}{V_2} c_3(t) - \frac{Q_1 + Q_2}{V_2} c_4(t) \]

\[ c_1(t) = \gamma_1(t) \]

\[ c_2(t) = \gamma_2(t) \]
Dynamics of DAE Systems

- Solution of stirred tank example 1:
  \[ c_2(t) = c_2(0)e^{-(Q/V)t} \]
  \[ c_1(t) = \gamma(t) \]

  \[ + \frac{Q}{V} \int_0^t \gamma(t')e^{-(Q/V)(t-t')} \, dt' \]

index 1

- Solution of stirred tank example 2:
  \[ c_1(t) = \gamma(t) + \frac{V}{Q} \dot{\gamma} \]
  \[ c_2(t) = \gamma(t) \]

index 2

- Solution of DAE example 3:
  \[ c_1(t) = \ddot{\gamma} \]
  \[ c_2(t) = \dot{\gamma} \]
  \[ c_3(t) = \gamma \]

index 3

- Higher index indicates greater sensitivity to changes in forcing function.
Dynamics of DAE Systems

- Physical example: pendulum
  \[
  \dot{x} = v(t) \\
  m\ddot{v} = -k(t)x(t) + mg \\
  \|x(t)\|^2 = L^2
  \]

- position, velocity, stiffness: \(x(t)\) \(v(t)\) \(k(t)\)

- Identify differential and algebraic variables.

- Identify index of the DAE system.
  \[
  (1) \quad \frac{d}{dt} \|x(t)\|^2 = 2v(t) \cdot x(t) = 0 \\
  (2) \quad \frac{d}{dt} (v(t) \cdot x(t)) = \frac{1}{m} (-k(t)x(t) + mg) \cdot x(t) + \|v(t)\|^2 = 0 \\
  (3) \quad \frac{d}{dt} \left( \frac{1}{m} (-k(t)x(t) + mg) \cdot x(t) + \|v(t)\|^2 \right) \\
  = -\frac{1}{m} \frac{dk}{dt} \|x(t)\|^2 - 2\frac{1}{m} k(t)v(t) \cdot x(t) + g \cdot v + \frac{2}{m} (-k(t)x(t) + mg) \cdot v(t) = 0
  \]
Simulation of DAE Systems

• Consider DAE example 3:

\[
\begin{align*}
\dot{c}_2 &= c_1(t) \\
\dot{c}_3 &= c_2(t) \\
0 &= c_3(t) - \gamma(t)
\end{align*}
\]

\[
\begin{align*}
\dot{c}_1 &= \ddot{\gamma} \\
\dot{c}_2 &= \dot{\gamma} \\
\dot{c}_3 &= \gamma
\end{align*}
\]

• Can’t I just solve the set of ODEs found when determining that the DAE system is index-3?
Simulation of DAE Systems

• In general, index-1 semi-explicit DAEs can be safely handled by certain stiff integrators in MATLAB (ode15s, ode23t)

• For generic DAEs, specific DAE solvers are usually needed (SUNDIALS, DAEPACK)

• Initial conditions for such equations must be prescribed consistently, or numerical errors can occur.

• Consider the pendulum:
  • Can it’s initial position be specified arbitrarily?
  • Can it’s initial velocity be specified arbitrarily?
  • Can the initial stiffness be specified arbitrarily?
Simulation of DAE Systems

- Consistent initialization of initial value problems: \( \{ \dot{x}(0), x(0) \} \)
  - index-0 DAE (ODE-IVP): \( \dot{x} = f(x, t) \)
    1. \( x(0) \rightarrow \dot{x}(0) = f(x(0), 0) \)
    2. \( \dot{x}(0) \) solve \( \dot{x}(0) = f(x(0), 0) \)
    3. \( c(x(0), \dot{x}(0)) = 0 \) solve with \( \dot{x}(0) = f(x(0), 0) \)
  - fully implicit DAE: \( f(x, \dot{x}, t) = 0 \)
    2N unknowns for N equations
    - apparently N degrees of freedom to specify
    - hidden constraints reduce these degrees
  - with differential states \( x \) and algebraic states \( y \),
    \( f(\dot{x}, x, y, t) = 0 \) \( \{ \dot{x}(0), x(0), y(0) \} \)
Simulation of DAE Systems

- Consistent initialization, example stirred tank 1:

\[
\frac{dc_2}{dt} = \frac{Q}{V} \left( c_1(t) \quad c_2(t) \right) \quad (1)
\]

\[
c_1(t) = (t) \quad (2)
\]

Convert to system of ODEs

\[
\frac{dc_1}{dt} = \cdot (t)
\]

\[
\frac{dc_2}{dt} = \frac{Q}{V} \left( c_1(t) \quad c_2(t) \right) \quad (3)
\]

Consistent initial conditions:

- Constrained by algebraic equation (2)
  \[c_1(0) = \gamma(0)\]

- Constrained by differential equation (3)
  \[\dot{c}_2(0) = \frac{Q}{V} (c_1(0) - c_2(0))\]

- Unconstrained
  \[c_2(0) = c_0\]
Simulation of DAE Systems

• Consistent initialization, example stirred tank 2:

\[
\frac{dc_2}{dt} = \frac{Q}{V} (c_1(t) - c_2(t)) \tag{1}
\]

\[
c_2(t) = \gamma(t) \tag{2}
\]

Convert to system of ODEs

\[
\frac{dc_2}{dt} = \dot{\gamma} \tag{3}
\]

\[
\frac{dc_1}{dt} = \frac{V}{Q} \ddot{\gamma} + \frac{Q}{V} (c_1(t) - c_2(t))
\]

Consistent initial conditions:

Constrained by algebraic equation (2)

\[
c_2(0) = \gamma(0)
\]

Constrained by differential equation (1)

\[
c_1(0) = c_2(0) + \frac{V}{Q} \dot{c}_2(0)
\]

Constrained by differential equation (3)

\[
\dot{c}_2(0) = \dot{\gamma}(0)
\]
Simulation of DAE Systems

• Consider another example:

\[
\begin{align*}
\dot{c}_1 &= c_1(t) + c_2(t) + c_3(t) \\
\dot{c}_2 &= -c_1(t) - c_2(t) + c_3(t) \\
0 &= c_1(t) + c_2(t)
\end{align*}
\]

• Derive consistent initial conditions:
Simulation of DAE Systems

- Consider another example:

  \[ \dot{c}_1 = c_1(t) + c_2(t) + c_3(t) \]
  \[ \dot{c}_2 = -c_1(t) - c_2(t) + c_3(t) \]
  \[ 0 = c_1(t) + c_2(t) + 2c_3(t) \]

- Derive consistent initial conditions: