Lecture 3: Modeling with differential algebraic equations

Moritz Diehl and Armin Nurkanović

Systems Control and Optimization Laboratory (syscop)

Summer School on Direct Methods for Optimal Control of Nonsmooth Systems
September 11-15, 2023

universität freiburg

Outline of the lecture

Differential algebraic equations

Let:

- $t \in \mathbb{R}$ be the time
- $x(t) \in \mathbb{R}^{n_x}$ the differential states
- $u(t) \in \mathbb{R}^{n_u}$ a given control function
- denote by $\dot{x}(t) = \frac{\mathrm{d}x(t)}{\mathrm{d}t}$

Ordinary differential and differential algebraic equations

Differential algebraic equations

Let:

- $t \in \mathbb{R}$ be the time
- $x(t) \in \mathbb{R}^{n_x}$ the differential states
- $u(t) \in \mathbb{R}^{n_u}$ a given control function
- denote by $\dot{x}(t) = \frac{\mathrm{d}x(t)}{\mathrm{d}t}$

Ordinary differential and differential algebraic equations

- Let $F : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$ be a function such that the **Jacobian $\frac{\partial F}{\partial \dot{x}}(\cdot)$ is invertible**. The system of equations:

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

is called an Ordinary Differential Equation (ODE).

Differential algebraic equations

Let:

- $t \in \mathbb{R}$ be the time
- $x(t) \in \mathbb{R}^{n_x}$ the differential states
- $u(t) \in \mathbb{R}^{n_u}$ a given control function
- denote by $\dot{x}(t) = \frac{\mathrm{d}x(t)}{\mathrm{d}t}$

Ordinary differential and differential algebraic equations

- Let $F : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$ be a function such that the **Jacobian $\frac{\partial F}{\partial \dot{x}}(\cdot)$ is invertible**. The system of equations:

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

  is called an Ordinary Differential Equation (ODE).
- .. if the **Jacobian $\frac{\partial F}{\partial \dot{x}}(\cdot)$is NOT invertible**, then the system of equations:

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

  is called an Differential Algebraic Equation (DAE).

Some historical remarks

DAE theory is much more recent than ODE theory

In the old days pioneered by:

- Euler-Lagrange equations in 1788 :
  J. L. Lagrange, *Mechanique analytique*.
  Libraire chez la Veuve Desaint, Paris

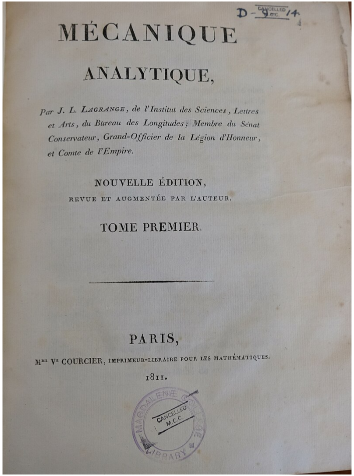


image source: wikipedia

Some historical remarks

DAE theory is much more recent than ODE theory

In the old days pioneered by:

- Euler-Lagrange equations in 1788 :
  J. L. Lagrange, *Mechanique analytique*. Libraire chez la Veuve Desaint, Paris
- Kirchhoff's laws in 1847:
  G. Kirchhoff *Ueber die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Vertheilung galvanischer Ströme geführt wird.* Annalen der Physik 148.12 (1847): 497-508.

1847. ANNALEN №. 12
DER PHYSIK UND CHEMIE.
BAND LXXII.

I. *Ueber die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Vertheilung galvanischer Ströme geführt wird;*
von G. Kirchhoff.

Ist ein System von n Drähten: 1, 2 ... n gegeben, welche auf eine beliebige Weise unter einander verbunden sind, und hat in einem jeden derselben eine beliebige elektromotorische Kraft ihren Sitz, so findet man zur Bestimmung der Intensitäten der Ströme, von welchen die Drähte durchflossen werden, $I_1, I_2 \dots I_n$, die nöthige Anzahl linearer Gleichungen durch Benutzung der beiden folgenden Sätze [1]):

I. Wenn die Drähte $k_1, k_2, \dots$ eine geschlossene Figur bilden, und w_k bezeichnet den Widerstand des Drahtes k, E_k die elektromotorische Kraft, die in demselben ihren Sitz hat, nach derselben Richtung positiv gerechnet als I_k, so ist, falls $I_{k1}, I_{k2}, \dots$ alle nach *einer* Richtung als positiv gerechnet werden:

$$w_{k1} I_{k1} + w_{k2} I_{k2} + \dots = E_{k1} + E_{k2} + \dots$$

II. Wenn die Drähte $\lambda_1, \lambda_2, \dots$ in einem Punkte zusammenstofsen, und $I_{\lambda 1}, I_{\lambda 2}, \dots$ alle nach diesem Punkte zu als positiv gerechnet werden, so ist:

$$I_{\lambda 1} + I_{\lambda 2} + \dots = 0.$$

Ich will jetzt beweisen, dafs die Auflösungen der Gleichungen, welche man durch Anwendung dieser Sätze für $I_1, I_2 \dots I_n$ erhält, vorausgesetzt, dafs das gegebene System von Drähten nicht in mehrere völlig von einander getrennte zerfällt, sich folgendermafsen allgemein angeben lassen:

Es sey m die Anzahl der vorhandenen Kreuzungspunkte, d. h. der Punkte, in denen zwei oder mehrere Drähte zusammenstofsen, und es sey $\mu = n - m + 1$, dann ist

1) Bd. 64, S. 513 dieser Annalen.

Poggendorff's Annal. Bd. LXXII. 32

Some historical remarks[1]

DAE theory is much more recent than ODE theory

In the modern days:

- Charles W. Gear first mathematician of modern time who studied DAEs
- first occurrence of the term "Differential-Algebraic Equation" in the title of Gear's paper" *Simultaneous numerical solution of differential-algebraic equations.* IEEE transactions on circuit theory 18.1 (1971): 89-95.

Simultaneous Numerical Solution of Differential–Algebraic Equations

CHARLES W. GEAR, MEMBER, IEEE

Abstract—A unified method for handling the mixed differential and algebraic equations of the type that commonly occur in the transient analysis of large networks or in continuous system simulation is discussed. The first part of the paper is a brief review of existing techniques of handling initial value problems for stiff ordinary differential equations written in the standard form $y' \; f(y, t)$. In the second part one of these techniques is applied to the problem $F(y, y', t)=0$. This may be either a differential or an algebraic equation as $\partial F/\partial y'$ is nonzero or zero. It will represent a mixed system when vectors F and y represent components of a system. The method lends itself to the use of sparse matrix techniques when the problem is sparse.

I. Introduction

MANY problems in transient network analysis and continuous system simulation lead to systems of ordinary differential equations which require the solution of a simultaneous set of algebraic equations each time that the derivatives are to be evaluated. The textbook form of a system of ordinary differential equations is

$$w' = f(w, t) \tag{1}$$

where w is a vector of dependent variables, f is a vector of functions of w and time t of the same dimension as w, and w' is the time derivative of w. Most methods discussed in the literature required the equations to be expressed in this form. The textbook extension to a simultaneous system of differential and algebraic equations (DAEs) could be

$$\begin{aligned} w' &= f(w, u, t) \\ 0 &= g(w, u, t) \end{aligned} \tag{2}$$

where u is a vector of the same dimension as g (but not necessarily the same as w).

A simple method for initial value problems such as Euler's method has the form

$$w_n = w_{n-1} + hf(w_{n-1}, u_{n-1}, t_{n-1}) \tag{3}$$

where $h = t_n - t_{n-1}$ is the time increment. Since only w_{n-1} is known from the previous time step or the initial values, the algebraic equations

$$0 = g(w_{n-1}, u_{n-1}, t_{n-1}) \tag{4}$$

must be solved for u_{n-1} before each time step.

The properties of the DAEs typically encountered are

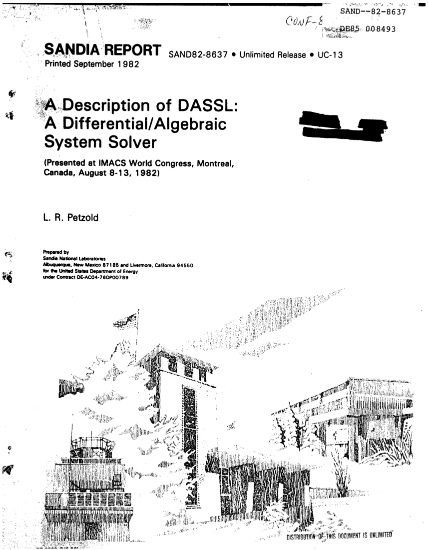
1) differential equations
   large
   sparse
   stiff
2) algebraic equations
   large
   sparse
   mildly nonlinear.

Manuscript received May 19, 1970; revised July 28, 1970. This work was supported in part by the U. S. Atomic Energy Commission.

The author is with the Stanford Linear Accelerator Center, Stanford University, Stanford, Calif. 94305. He is on leave from the University of Illinois, Urbana, Ill.

In the modern days:

- Charles W. Gear first mathematician of modern time who studied DAEs
- first occurrence of the term "Differential-Algebraic Equation" in the title of Gear's paper" *Simultaneous numerical solution of differential-algebraic equations.* IEEE transactions on circuit theory 18.1 (1971): 89-95.
- DASSL code in the 1980s by Linda Petzold - first DAE simulation code



SAND--82-8637
CONF-8
DE85 008493

SANDIA REPORT SAND82-8637 • Unlimited Release • UC-13
Printed September 1982

A Description of DASSL:
A Differential/Algebraic
System Solver

[redacted]

(Presented at IMACS World Congress, Montreal, Canada, August 8-13, 1982)

L. R. Petzold

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789

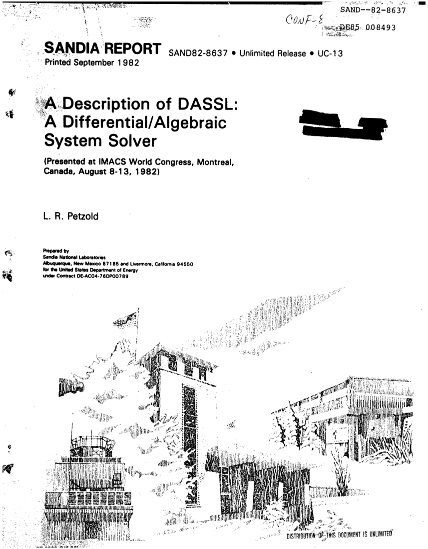
DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Some historical remarks[1]

DAE theory is much more recent than ODE theory

In the modern days:

- Charles W. Gear first mathematician of modern time who studied DAEs
- first occurrence of the term "Differential-Algebraic Equation" in the title of Gear's paper" *Simultaneous numerical solution of differential-algebraic equations.* IEEE transactions on circuit theory 18.1 (1971): 89-95.
- DASSL code in the 1980s by Linda Petzold - first DAE simulation code
- electric circuits and mechanical systems still drive the development of DAEs



SAND--82-8637
CONF-8
DE85 008493

SANDIA REPORT SAND82-8637 • Unlimited Release • UC-13
Printed September 1982

A Description of DASSL: A Differential/Algebraic System Solver

[redacted]

(Presented at IMACS World Congress, Montreal, Canada, August 8-13, 1982)

L. R. Petzold

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

[1] Reference for historical overview: Simeon, Bernd. *On the history of differential-algebraic equations: a retrospective with personal side trips*. Springer International Publishing, 2017.

Consider the system of equations

$$F(x,\dot{x}) = \begin{bmatrix} x_1 - \dot{x}_1 + 1 \\ \dot{x}_1 x_2 + 2 \end{bmatrix} = 0.$$

Consider the system of equations

$$F(x,\dot{x}) = \begin{bmatrix} x_1 - \dot{x}_1 + 1 \\ \dot{x}_1 x_2 + 2 \end{bmatrix} = 0.$$

The Jacobian

$$\frac{\partial F(\dot{x},x)}{\partial \dot{x}} = \begin{bmatrix} -1 & 0 \\ x_2 & 0 \end{bmatrix},$$

is not invertible.

Consider the system of equations

$$F(x, \dot{x}) = \begin{bmatrix} x_1 - \dot{x}_1 + 1 \\ \dot{x}_1 x_2 + 2 \end{bmatrix} = 0.$$

The Jacobian

$$\frac{\partial F(\dot{x}, x)}{\partial \dot{x}} = \begin{bmatrix} -1 & 0 \\ x_2 & 0 \end{bmatrix},$$

is not invertible.

Solve $\dot{x}_1 = x_1 + 1$ and obtain

$$\hat{F}(x, \dot{x}) = \begin{bmatrix} x_1 + 1 - \dot{x}_1 \\ (x_1 + 1)x_2 + 2 \end{bmatrix} = 0.$$

- There is no $\dot{x}_2$ in the equations,
- The variable x_2 is an **algebraic variable**.

Some examples

Example 2 - ODE or DAE?

Consider the system of equations

$$F(x, \dot{x}) = p\dot{x} + x = 0.$$

The Jacobian is

$$\frac{\partial F(\dot{x}, x)}{\partial \dot{x}} = p.$$

- If $p \neq 0$, we have a *pure* ODE: $\dot{x} = -\frac{x}{p}$.
- If $p = 0$, we have an algebraic equation $x = 0$.

Consider the system of equations

$$F(x, \dot{x}) = \begin{bmatrix} \dot{x}_1 + x_1 \\ (x_1 - x_2)\dot{x}_2 + x_1 - x_2 \end{bmatrix} = 0.$$

The Jacobian

$$\frac{\partial F(\dot{x}, x)}{\partial \dot{x}} = \begin{bmatrix} 1 & 0 \\ 0 & x_1 - x_2 \end{bmatrix},$$

is for $x_1 = x_2$ not invertible. Depending on the state we can have a DAE or ODE:

- If $x_1 = x_2$ we have a DAE: $\begin{bmatrix} \dot{x}_1 + x_1 \\ x_1 - x_2 \end{bmatrix} = 0.$
- If $x_1 \neq x_2$ we have an ODE: $\begin{cases} \dot{x}_1 = -x_1 \\ \dot{x}_2 = -1 \end{cases}.$

Differential algebraic equations are usually nicer

- General DAEs include problems may not be mathematically well-defined or very difficult to discretize directly.
- However, in practice DAEs are much nicer:

$$F(t, \dot{x}(t), x(t), z(t), u(t)) = 0, \quad t \in [0, T],$$
$$x(0) = x_0.$$

Clear distinction between:

- $x \in R^{n_x}$ - differential states (need an initial condition)
- $z \in R^{n_z}$ - algebraic states (initial condition implicit)

Differential algebraic equations are usually nicer

- General DAEs include problems may not be mathematically well-defined or very difficult to discretize directly.
- However, in practice DAEs are much nicer:

$$
\begin{aligned}
&F(t, \dot{x}(t), x(t), z(t), u(t)) = 0, \quad t \in [0, T], \\
&x(0) = x_0.
\end{aligned}
$$

  Clear distinction between:
  - $x \in R^{n_x}$ - differential states (need an initial condition)
  - $z \in R^{n_z}$ - algebraic states (initial condition implicit)
- Difference even more obvious in **semi-explicit** form (most common in practice):

$$
\begin{aligned}
\dot{x}(t) &= f(t, x(t), z(t), u(t)) \\
0 &= g(t, x(t), z(t), u(t)).
\end{aligned}
$$

Differential algebraic equations are usually nicer

- General DAEs include problems may not be mathematically well-defined or very difficult to discretize directly.
- However, in practice DAEs are much nicer:

$$
\begin{aligned}
&F(t, \dot{x}(t), x(t), z(t), u(t)) = 0, \quad t \in [0, T], \\
&x(0) = x_0.
\end{aligned}
$$

  Clear distinction between:
  - $x \in R^{n_x}$ - differential states (need an initial condition)
  - $z \in R^{n_z}$ - algebraic states (initial condition implicit)
- Difference even more obvious in **semi-explicit** form (most common in practice):

$$
\begin{aligned}
\dot{x}(t) &= f(t, x(t), z(t), u(t)) \\
0 &= g(t, x(t), z(t), u(t)).
\end{aligned}
$$

- Very common in electric circuits (linear fully implicit), with M not having full rank:

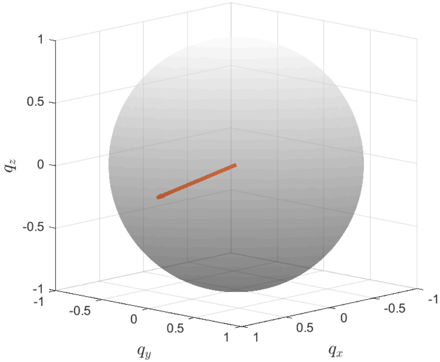
$$
M\dot{x} = Ax + Bu.
$$

A semi-explicit DAE example

Three-dimensional pendulum

$$\begin{aligned} \dot{q} &= v \\ m\dot{v} &= F_{\mathrm{g}} - qz + u \\ 0 &= q^\top q - L^2 \end{aligned}$$

F_{g} - gravitational force



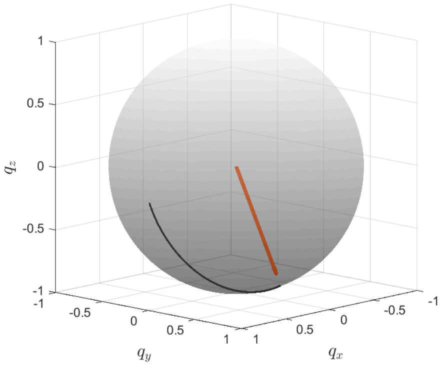
A semi-explicit DAE example

Three-dimensional pendulum

$$
\begin{aligned}
\dot{q} &= v \\
m\dot{v} &= F_{\mathrm{g}} - qz + u \\
0 &= q^\top q - L^2
\end{aligned}
$$

F_{g} - gravitational force

z - is the reaction force along q



A semi-explicit DAE example

Three-dimensional pendulum

$$\dot{q} = v$$
$$m\dot{v} = F_{\mathrm{g}} - qz + u$$
$$0 = q^\top q - L^2$$

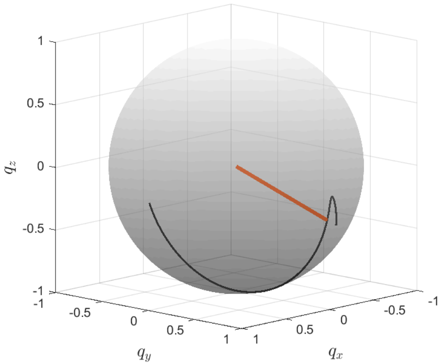
F_{g} - gravitational force

z - is the reaction force along q

The semi-explicit form reads as

$$\dot{x} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m}qz + \frac{u}{m} \end{bmatrix} =: f(x, z, u)$$
$$0 = q^\top q - L^2 =: g(x)$$

with $x = (q, v)$



A semi-explicit DAE example

Three-dimensional pendulum

$$\begin{aligned} \dot{q} &= v \\ m\dot{v} &= F_{\mathrm{g}} - qz + u \\ 0 &= q^\top q - L^2 \end{aligned}$$

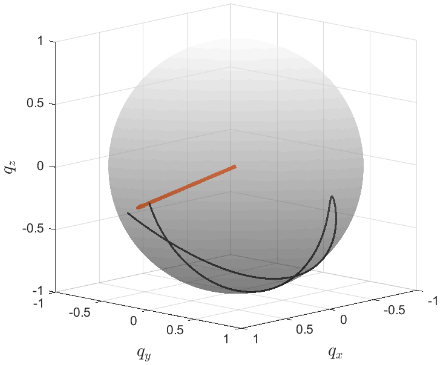
F_{g} - gravitational force

z - is the reaction force along q

The semi-explicit form reads as

$$\begin{aligned} \dot{x} &= \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m}qz + \frac{u}{m} \end{bmatrix} =: f(x, z, u) \\ 0 &= q^\top q - L^2 =: g(x) \end{aligned}$$

with $x = (q, v)$



A semi-explicit DAE example

Three-dimensional pendulum

$$\dot{q} = v$$
$$m\dot{v} = F_{\mathrm{g}} - qz + u$$
$$0 = q^\top q - L^2$$

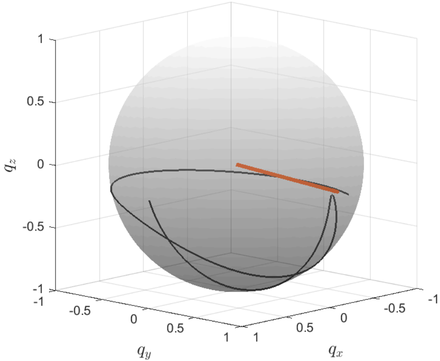
F_{g} - gravitational force

z - is the reaction force along q

The semi-explicit form reads as

$$\dot{x} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} qz + \frac{u}{m} \end{bmatrix} =: f(x, z, u)$$
$$0 = q^\top q - L^2 =: g(x)$$

with $x = (q, v)$



How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

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

How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

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

If for a given (x, u) the matrix $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix}$ is invertible ("index one"),

How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

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

If for a given (x, u) the matrix $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix}$ is invertible ("index one"), then from the implicit function theorem it follows that there exists a function $\psi(x, u)$

$$\begin{bmatrix} \dot{x} \\ z \end{bmatrix} = \psi(x, u) \text{ such that } F(\psi(x, u), x, u) = 0.$$

How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

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

If for a given (x, u) the matrix $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix}$ is invertible ("index one"), then from the implicit function theorem it follows that there exists a function $\psi(x, u)$

$$\begin{bmatrix} \dot{x} \\ z \end{bmatrix} = \psi(x, u) \text{ such that } F(\psi(x, u), x, u) = 0.$$

Semi-explicit DAE

$$F(\dot{x}, z, x, u) = \begin{bmatrix} \dot{x} - f(x, z, u) \\ g(x, z, u) \end{bmatrix} = 0.$$

How to solve DAEs numerically?

Idea: Transform the DAE into an equivalent ODE and use your favorite method.

Fully implicit DAE

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

If for a given (x, u) the matrix $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix}$ is invertible ("index one"), then from the implicit function theorem it follows that there exists a function $\psi(x, u)$

$$\begin{bmatrix} \dot{x} \\ z \end{bmatrix} = \psi(x, u) \text{ such that } F(\psi(x, u), x, u) = 0.$$

Semi-explicit DAE

$$F(\dot{x}, z, x, u) = \begin{bmatrix} \dot{x} - f(x, z, u) \\ g(x, z, u) \end{bmatrix} = 0.$$

Matrix $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} I & \frac{\partial F}{\partial z} \\ 0 & \frac{\partial g}{\partial z} \end{bmatrix}$ invertible if $\frac{\partial g}{\partial z}$ invertible ("semi-explicit DAE of index one").

Example - easy DAE

Consider the DAE

$$F(\dot{x}, x, z) = \begin{bmatrix} x - \dot{x} + 1 \\ \dot{x}z + 2 \end{bmatrix}$$

Example - easy DAE

Consider the DAE

$$F(\dot{x}, x, z) = \begin{bmatrix} x - \dot{x} + 1 \\ \dot{x}z + 2 \end{bmatrix}$$

The matrix

$$\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ z & \dot{x} \end{bmatrix}$$

is invertible for $\dot{x} \neq 0$

Example - easy DAE

Consider the DAE

$$F(\dot{x}, x, z) = \begin{bmatrix} x - \dot{x} + 1 \\ \dot{x}z + 2 \end{bmatrix}$$

The matrix

$$\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ z & \dot{x} \end{bmatrix}$$

is invertible for $\dot{x} \neq 0$

... and we solve the DAE as:

$$\dot{x} = x + 1$$
$$z = -\frac{2}{\dot{x}} = -\frac{2}{x+1}$$

Example - 3D pendulum

The pendulum dynamics

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$
$$0 = q^\top q - L^2$$

Example - 3D pendulum

The pendulum dynamics

$$\begin{aligned}\dot{x} &= \begin{bmatrix}\dot{q}\\ \dot{v}\end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m}qz + \frac{u}{m}\end{bmatrix}\\ 0 &= q^\top q - L^2\end{aligned}$$

In implicit form:

$$F(\dot{x}, z, x, u) = \begin{bmatrix}\dot{x} - f(x,z,u)\\ g(x,z,u)\end{bmatrix} = \begin{bmatrix}\dot{q} - v\\ \dot{v} - (\frac{F_{\mathrm{g}}}{m} - \frac{1}{m}qz + \frac{u}{m})\\ q^\top q - L^2\end{bmatrix} = 0$$

Example - 3D pendulum

The pendulum dynamics

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$
$$0 = q^\top q - L^2$$

In implicit form:

$$F(\dot{x}, z, x, u) = \begin{bmatrix} \dot{x} - f(x, z, u) \\ g(x, z, u) \end{bmatrix} = \begin{bmatrix} \dot{q} - v \\ \dot{v} - (\frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m}) \\ q^\top q - L^2 \end{bmatrix} = 0$$

The matrix

$$\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & \frac{q}{m} \\ 0 & 0 & 0 \end{bmatrix} \text{ is not invertible!}$$

Example - 3D pendulum

The pendulum dynamics

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$
$$0 = q^\top q - L^2$$

In implicit form:

$$F(\dot{x}, z, x, u) = \begin{bmatrix} \dot{x} - f(x, z, u) \\ g(x, z, u) \end{bmatrix} = \begin{bmatrix} \dot{q} - v \\ \dot{v} - (\frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m}) \\ q^\top q - L^2 \end{bmatrix} = 0$$

The matrix

$$\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & \frac{q}{m} \\ 0 & 0 & 0 \end{bmatrix}$$ is not invertible!

How do we deal with such DAEs?

Outline of this lecture

The DAE differential index

Definition (Differential index of fully implicit DAEs)

The DAE differential index is the minimum integer k such that the k-th total time derivative

$$\frac{\mathrm{d}^k}{\mathrm{d}t^k} F(\dot{x}, x, z, u) = 0$$

is a pure ordinary differential equation (in states $x, \dot{x}, \ldots, x^{(k)}$ and $z, \dot{z}, \ldots, z^{(k-1)}$).

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\dot{x}, x, z, u) = \frac{\partial F}{\partial \dot{x}} \ddot{x} + \frac{\partial F}{\partial x} \dot{x} + \frac{\partial F}{\partial z} \dot{z} + \frac{\partial F}{\partial u} \dot{u} = 0$$

The DAE differential index

Definition (Differential index of fully implicit DAEs)

The DAE differential index is the minimum integer k such that the k-th total time derivative

$$\frac{\mathrm{d}^k}{\mathrm{d}t^k} F(\dot{x}, x, z, u) = 0$$

is a pure ordinary differential equation (in states $x, \dot{x}, \ldots, x^{(k)}$ and $z, \dot{z}, \ldots, z^{(k-1)}$).

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\dot{x}, x, z, u) = \frac{\partial F}{\partial \dot{x}} \ddot{x} + \frac{\partial F}{\partial x} \dot{x} + \frac{\partial F}{\partial z} \dot{z} + \frac{\partial F}{\partial u} \dot{u} = 0$$

If $\begin{bmatrix} \frac{\partial F}{\partial \dot{x}} & \frac{\partial F}{\partial z} \end{bmatrix}$ is invertible, then we can define the explicit ODE in states (x, v, z) with $v := \dot{x}$

The DAE differential index

Definition (Differential index of fully implicit DAEs)

The DAE differential index is the minimum integer k such that the k-th total time derivative

$$\frac{\mathrm{d}^k}{\mathrm{d}t^k} F(\dot{x}, x, z, u) = 0$$

is a pure ordinary differential equation (in states $x, \dot{x}, \ldots, x^{(k)}$ and $z, \dot{z}, \ldots, z^{(k-1)}$).

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\dot{x}, x, z, u) = \frac{\partial F}{\partial \dot{x}} \ddot{x} + \frac{\partial F}{\partial x} \dot{x} + \frac{\partial F}{\partial z} \dot{z} + \frac{\partial F}{\partial u} \dot{u} = 0$$

If $\left[\frac{\partial F}{\partial \dot{x}} \quad \frac{\partial F}{\partial z}\right]$ is invertible, then we can define the explicit ODE in states (x, v, z) with $v := \dot{x}$

$$\begin{aligned} \dot{x} &= v \\ \begin{bmatrix} \dot{v} \\ \dot{z} \end{bmatrix} &= -\left[\frac{\partial F}{\partial \dot{x}} \quad \frac{\partial F}{\partial z}\right]^{-1} \left(\frac{\partial F}{\partial x} v + \frac{\partial F}{\partial u} \dot{u}\right) \end{aligned}$$

The DAE differential index - semi-explicit DAEs

Definition (Differential index of semi-explicit DAEs)

The DAE differential index is the minimum integer k such that the

$$\begin{aligned} \dot{x} &= f(x,z,u) \\ 0 &= \frac{\mathrm{d}^k}{\mathrm{d}t^k} g(x,z,u) \end{aligned}$$

is a pure ordinary differential equation.

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} g(x,z,u) = \frac{\partial g}{\partial x} f(x,z,u) + \frac{\partial g}{\partial z}\dot{z} + \frac{\partial g}{\partial u}\dot{u} = 0$$

The DAE differential index - semi-explicit DAEs

Definition (Differential index of semi-explicit DAEs)

The DAE differential index is the minimum integer k such that the

$$\dot{x} = f(x, z, u)$$
$$0 = \frac{\mathrm{d}^k}{\mathrm{d}t^k} g(x, z, u)$$

is a pure ordinary differential equation.

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} g(x, z, u) = \frac{\partial g}{\partial x} f(x, z, u) + \frac{\partial g}{\partial z} \dot{z} + \frac{\partial g}{\partial u} \dot{u} = 0$$

If $\frac{\partial g}{\partial z}$ is invertible, then we can define the explicit ODE (with $v := \dot{x}$)

The DAE differential index - semi-explicit DAEs

Definition (Differential index of semi-explicit DAEs)

The DAE differential index is the minimum integer k such that the

$$\begin{aligned}\dot{x} &= f(x,z,u)\\ 0 &= \frac{\mathrm{d}^k}{\mathrm{d}t^k} g(x,z,u)\end{aligned}$$

is a pure ordinary differential equation.

An index 1 DAE (the "easy" DAEs)

$$\frac{\mathrm{d}}{\mathrm{d}t} g(x,z,u) = \frac{\partial g}{\partial x} f(x,z,u) + \frac{\partial g}{\partial z}\dot{z} + \frac{\partial g}{\partial u}\dot{u} = 0$$

If $\frac{\partial g}{\partial z}$ is invertible, then we can define the explicit ODE (with $v := \dot{x}$)

$$\begin{aligned}\dot{x} &= f(x,z,u)\\ \dot{z} &= -\frac{\partial g}{\partial z}^{-1}\left(\frac{\partial g}{\partial x} f(x,z,u) + \frac{\partial g}{\partial u}\dot{u}\right)\end{aligned}$$

The differential index - examples

Regard the DAE

$$
\begin{aligned}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= z \\
0 &= \frac{1}{2}(x_1^2 + x_2^2 - 2z)
\end{aligned}
$$

The differential index - examples

Regard the DAE

$$\begin{aligned}\dot{x}_1 &= x_2\\ \dot{x}_2 &= z\\ 0 &= \frac{1}{2}(x_1^2 + x_2^2 - 2z)\end{aligned}$$

Differentiate $g(x, z)$ w.r.t. t:

$$\begin{aligned}0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x, z) &= x_1\dot{x}_1 + x_2\dot{x}_2 - \dot{z}\\ 0 &= x_1x_2 + x_2z - \dot{z}\end{aligned}$$

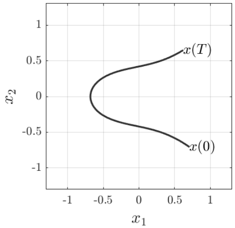
The differential index - examples

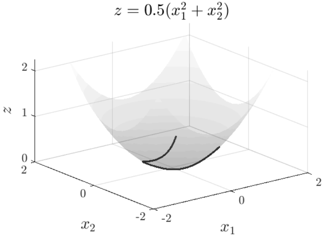
Regard the DAE

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = z$$
$$0 = \frac{1}{2}(x_1^2 + x_2^2 - 2z)$$

Differentiate $g(x,z)$ w.r.t. t:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x,z) = x_1\dot{x}_1 + x_2\dot{x}_2 - \dot{z}$$
$$0 = x_1 x_2 + x_2 z - \dot{z}$$





The DAE is of **index 1**

The differential index - examples

Regard the DAE

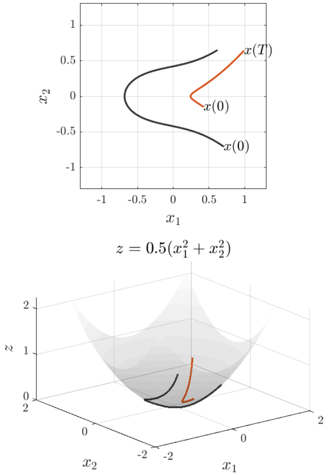
$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= z \\ 0 &= \frac{1}{2}(x_1^2 + x_2^2 - 2z) \end{aligned}$$

Differentiate $g(x,z)$ w.r.t. t:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x,z) = x_1 \dot{x}_1 + x_2 \dot{x}_2 - \dot{z}$$

$$0 = x_1 x_2 + x_2 z - \dot{z}$$

The DAE is of **index 1**



$x(0)$ can take any value

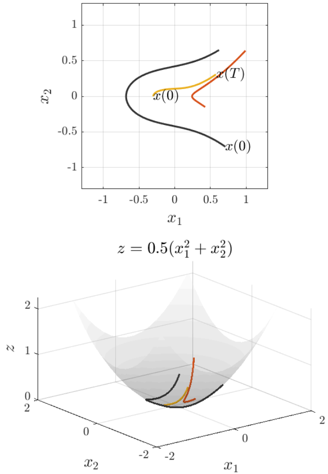
Regard the DAE

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = z$$
$$0 = \frac{1}{2}(x_1^2 + x_2^2 - 2z)$$

Differentiate $g(x,z)$ w.r.t. t:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x,z) = x_1\dot{x}_1 + x_2\dot{x}_2 - \dot{z}$$
$$0 = x_1 x_2 + x_2 z - \dot{z}$$

The DAE is of **index 1**



$x(0)$ can take any value

The differential index - examples

Regard the DAE

$$
\begin{aligned}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= z \\
0 &= \frac{1}{2}(x_1^2 + x_2^2 - 1)
\end{aligned}
$$

The differential index - examples

Regard the DAE

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= z \\ 0 &= \frac{1}{2}(x_1^2 + x_2^2 - 1) \end{aligned}$$

Differentiate $g(x, z)$ w.r.t. t:

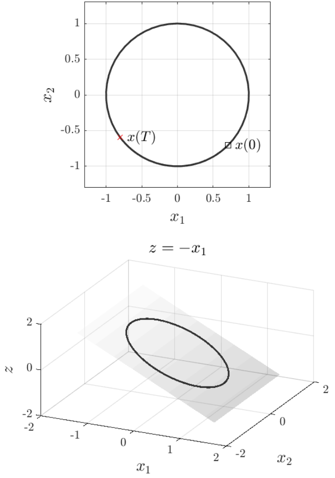
$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x, z) &= x_1 \dot{x}_1 + x_2 \dot{x}_2 \\ 0 &= x_1 x_2 + x_2 z \end{aligned}$$

Regard the DAE

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = z$$
$$0 = \frac{1}{2}(x_1^2 + x_2^2 - 1)$$

Differentiate $g(x,z)$ w.r.t. t:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x,z) = x_1\dot{x}_1 + x_2\dot{x}_2$$
$$0 = x_1 x_2 + x_2 z$$
$$0 = \frac{\mathrm{d}^2}{\mathrm{d}t^2} g(x,z) = \dot{x}_1 x_2 + x_1\dot{x}_2 + \dot{x}_2 z + x_2\dot{z}$$
$$0 = x_2^2 + x_1 z + z^2 + x_2\dot{z}$$



$x(0)$ must satisfy $g(x) = 0$

The differential index - examples

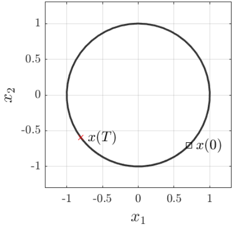
Regard the DAE

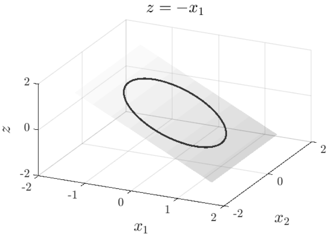
$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = z$$
$$0 = \frac{1}{2}(x_1^2 + x_2^2 - 1)$$

Differentiate $g(x,z)$ w.r.t. t:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} g(x,z) = x_1\dot{x}_1 + x_2\dot{x}_2$$
$$0 = x_1 x_2 + x_2 z$$
$$0 = \frac{\mathrm{d}^2}{\mathrm{d}t^2} g(x,z) = \dot{x}_1 x_2 + x_1\dot{x}_2 + \dot{x}_2 z + x_2\dot{z}$$
$$0 = x_2^2 + x_1 z + z^2 + x_2\dot{z}$$

The DAE is of **index 2**





$x(0)$ must satisfy $g(x) = 0$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \quad (1a)$$

$$0 = q^\top q - L^2 \quad (1b)$$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_g}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

Third differentiation would yield $\dot{z}$ - **index 3 DAE.**

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

Third differentiation would yield $\dot{z}$ - **index 3 DAE.**

- Combining (1) and (2) we have an "easy" **index 1 DAE**, compactly written as

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

Third differentiation would yield $\dot{z}$ - **index 3 DAE.**

Note: we could also analytically obtain z:

$$0 = q^\top \left(\frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \right) + v^\top v$$

$$z = \frac{1}{q^\top q} \left(q^\top F_{\mathrm{g}} + q^\top u + m v^\top v \right)$$

- Combining (1) and (2) we have an "easy" **index 1 DAE**, compactly written as

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

Third differentiation would yield $\dot{z}$ - **index 3 DAE.**

Note: we could also analytically obtain z:

$$0 = q^\top \left(\frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \right) + v^\top v$$

$$z = \frac{1}{q^\top q} \left(q^\top F_\mathrm{g} + q^\top u + m v^\top v \right)$$

- Combining (1) and (2) we have an "easy" **index 1 DAE**, compactly written as

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Lagrange mechanics models are typically index 3 DAEs

The differential index of the 3D pendulum

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix} \tag{1a}$$

$$0 = q^\top q - L^2 \tag{1b}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \quad \text{(first differentiation)}$$

$$\frac{\mathrm{d}^2 g(x)}{\mathrm{d}t^2} = q^\top \dot{v} + v^\top v = 0 \quad \text{(second differentiation)} \tag{2}$$

Third differentiation would yield $\dot{z}$ - **index 3 DAE.**

Note: we could also analytically obtain z:

$$0 = q^\top \left(\frac{F_\mathrm{g}}{m} - \frac{1}{m} q z + \frac{u}{m} \right) + v^\top v$$

$$z = \frac{1}{q^\top q} \left(q^\top F_\mathrm{g} + q^\top u + m v^\top v \right)$$

- Combining (1) and (2) we have an “easy“ **index 1 DAE**, compactly written as

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Lagrange mechanics models are typically index 3 DAEs
- In practice, they are often treated with standard methods after an **index reduction** to a DAE of index 1

Outline of this lecture

Index reduction

In theory, we can always transform a higher index into a lower index DAE. Questions:

1. When can we and when should we do this?
2. Can anything go wrong? (Yes, a lot.)

Index reduction

In theory, we can always transform a higher index into a lower index DAE. Questions:

1. When can we and when should we do this?
2. Can anything go wrong? (Yes, a lot.)

Pros of index reduction

- ✓ obtain ODE or DAE index 1 - use standard methods
- ✓ no new integration code needed
- ✓ rely on nice theory for ODEs and “easy“ DAEs
- ✓ theory of higher index DAEs less mature
- ✓ not always clear how to simulate higher index DAEs
- ✓ no order reduction (treated later)

Index reduction

In theory, we can always transform a higher index into a lower index DAE. Questions:

1. When can we and when should we do this?
2. Can anything go wrong? (Yes, a lot.)

Pros of index reduction

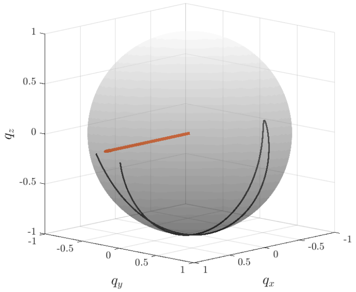
- ✓ obtain ODE or DAE index 1 - use standard methods
- ✓ no new integration code needed
- ✓ rely on nice theory for ODEs and “easy“ DAEs
- ✓ theory of higher index DAEs less mature
- ✓ not always clear how to simulate higher index DAEs
- ✓ no order reduction (treated later)

Cons of index reduction

- ✗ index reduction may be very difficult to perform
- ✗ not all variables have physical interpretation
- ✗ cannot easily exploit structure in specific solver
- ✗ initialization of index reduced DAE difficult (treated next)
- ✗ numerical drift in index reduced DAE (treated next)

Index 3

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$
$$0 = q^\top q - L^2$$



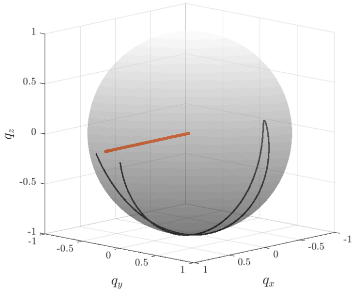
Issues with index reduction - consistent initialization

When are index reduced models equivalent?

Index 3

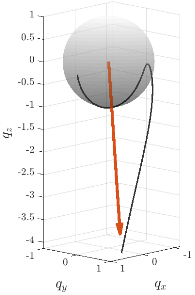
$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$

$$0 = q^\top q - L^2$$



Index 1

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

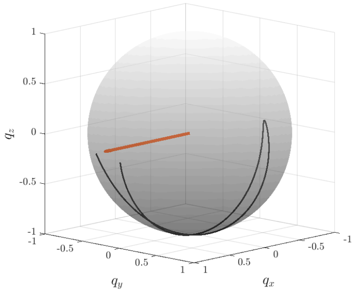


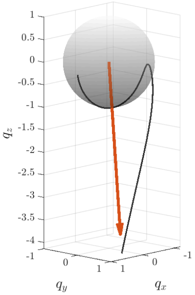
Index 3

$$\dot{x} = \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \frac{F_{\mathrm{g}}}{m} - \frac{1}{m} q z + \frac{u}{m} \end{bmatrix}$$
$$0 = q^\top q - L^2$$

Index 1

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$





What went wrong?

Issues with index reduction - consistent initialization

Index 1 - only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

Issues with index reduction - consistent initialization

Index 1 - only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- We must also regard the constraints

$$g(x) = q^\top q - L^2 = 0 \tag{3a}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \tag{3b}$$

Issues with index reduction - consistent initialization

Index 1 - only imposes $\ddot{g}(x) = 0$

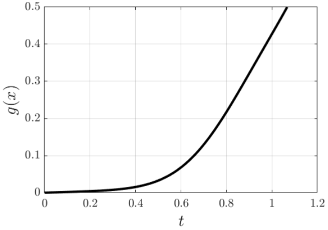
$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

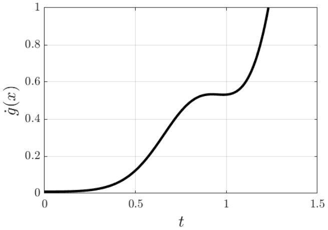
- We must also regard the constraints

$$g(x) = q^\top q - L^2 = 0 \qquad \text{(3a)}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \qquad \text{(3b)}$$

- If initial conditions violate (3) - wrong solution





Issues with index reduction - consistent initialization

Index 1 - only imposes $\ddot{g}(x) = 0$

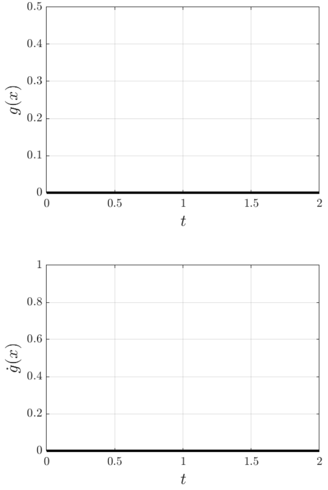
$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- We must also regard the constraints

$$g(x) = q^\top q - L^2 = 0 \qquad \text{(3a)}$$

$$\frac{\mathrm{d}g(x)}{\mathrm{d}t} = q^\top \dot{q} = q^\top v = 0 \qquad \text{(3b)}$$

- If initial conditions violate (3) - wrong solution
- Index reduced DAE must satisfy **consistency conditions** (3) at $t = 0$



Issues with index reduction - constraint drift

Index 1 - only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

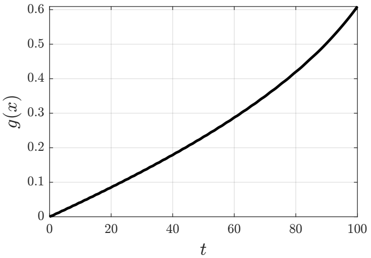
- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$

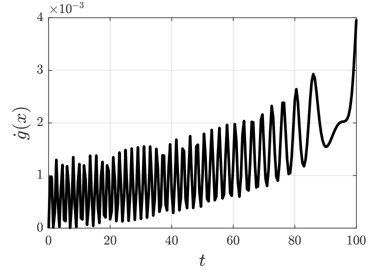
Issues with index reduction - constraint drift

Index 1 - only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$
- Integration errors might still accumulate over time



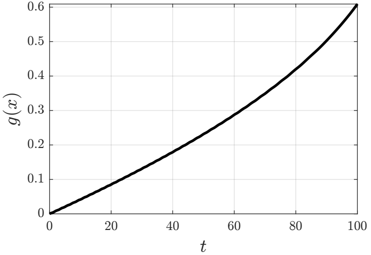


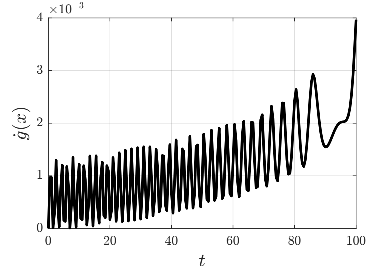
Issues with index reduction - constraint drift

Index 1 - only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$
- Integration errors might still accumulate over time
- **Constraint drift** is a consequence of index reduction



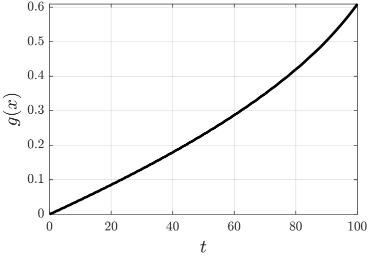


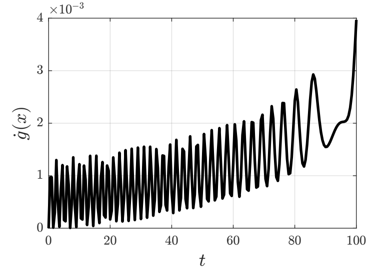
Baumgarte stabilization of the constraint drift for index 3 DAE

After reduction from Index 3 to 1, the resulting DAE only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_{\mathrm{g}} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$





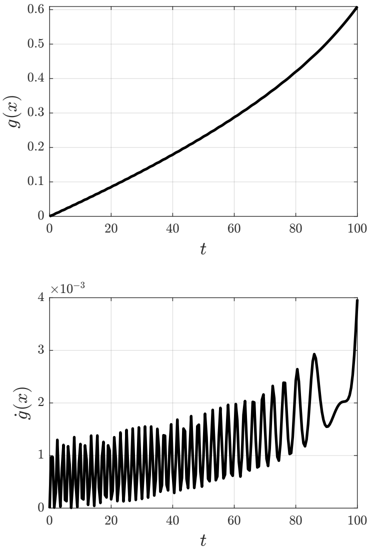
Baumgarte stabilization of the constraint drift for index 3 DAE

After reduction from Index 3 to 1, the resulting DAE only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$
- In index 1 DAE, instead of $\ddot{g}(x) = 0$, impose:

$$\ddot{g}(x) + \kappa_1 \dot{g}(x) + \kappa_0 g(x) = 0$$



Baumgarte stabilization of the constraint drift for index 3 DAE

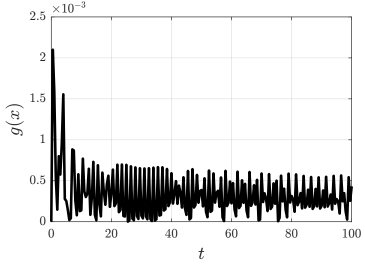
After reduction from Index 3 to 1, the resulting DAE only imposes $\ddot{g}(x) = 0$

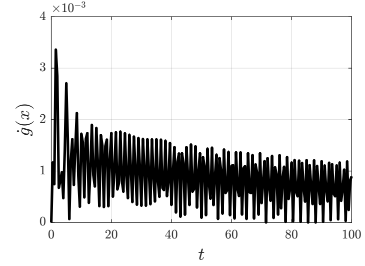
$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$
- In index 1 DAE, instead of $\ddot{g}(x) = 0$, impose:

$$\ddot{g}(x) + \kappa_1 \dot{g}(x) + \kappa_0 g(x) = 0$$

- Pick κ_0 and κ_1 to have stable dynamics (might be tricky)





Baumgarte stabilization of the constraint drift for index 3 DAE

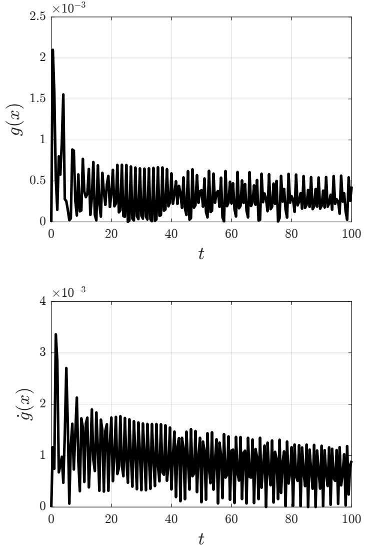
After reduction from Index 3 to 1, the resulting DAE only imposes $\ddot{g}(x) = 0$

$$\begin{bmatrix} m \cdot I & q \\ q^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ z \end{bmatrix} = \begin{bmatrix} F_\mathrm{g} + u \\ -v^\top v \end{bmatrix}$$

- Suppose that the index reduced DAE satisfies **consistency conditions** (3) at $t = 0$
- In index 1 DAE, instead of $\ddot{g}(x) = 0$, impose:

$$\ddot{g}(x) + \kappa_1 \dot{g}(x) + \kappa_0 g(x) = 0$$

- Pick κ_0 and κ_1 to have stable dynamics (might be tricky)
- Stabilize the constraint drift



Summary on differential index

- Notion of differential index helps to classify DAEs, to determine difficulty, and to pick right method and software
- Two major difficulties in solving DAE:
  1. index reduction
  2. consistent initialization

Summary on differential index

- Notion of differential index helps to classify DAEs, to determine difficulty, and to pick right method and software
- Two major difficulties in solving DAE:
  1. index reduction
  2. consistent initialization
- Higher index DAEs have hidden constraints: Index $k \implies k-1$ hidden constraints
- Constraint drift is consequence of differentiation, might need Baumgarte's stabilization

Summary on differential index

- Notion of differential index helps to classify DAEs, to determine difficulty, and to pick right method and software
- Two major difficulties in solving DAE:
  1. index reduction
  2. consistent initialization
- Higher index DAEs have hidden constraints: Index $k \implies k-1$ hidden constraints
- Constraint drift is consequence of differentiation, might need Baumgarte's stabilization
- The index is a local quantity, might depend on initial state - less common in practical smooth problems
- Nonsmooth ODEs are locally DAEs of different index - very common
- Keeping the index in mind, the integration method has to be chosen carefully (both for smooth and nonsmooth systems)

Introduction to Runge-Kutta methods for DAEs

Two ways to numerically solve DAEs:

1. Direct discretization of the DAE
2. Reformulation (index reduction) and discretization

Some remarks

Introduction to Runge-Kutta methods for DAEs

Two ways to numerically solve DAEs:

1. Direct discretization of the DAE
2. Reformulation (index reduction) and discretization

Some remarks

- direct discretization is desirable since the index reduction might be costly and require expert knowledge
- ... in principle only feasible for index 1 and 2, and for index 3 with some care

Introduction to Runge-Kutta methods for DAEs

Two ways to numerically solve DAEs:

1. Direct discretization of the DAE
2. Reformulation (index reduction) and discretization

Some remarks

- direct discretization is desirable since the index reduction might be costly and require expert knowledge
- ... in principle only feasible for index 1 and 2, and for index 3 with some care
- RK methods in direct discretization: simply impose the algebraic equations at the stage points
- $x(t)$ found through integration, and may be smoother than $z(t)$ - influences accuracy

DAEs in Hessenberg form

DAE of index 1

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

with $\frac{\partial g}{\partial z}$ nonsingular for all t

DAE of index 2

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

with $\frac{\partial g}{\partial x}\frac{\partial f}{\partial z}$ nonsingular for all t

DAE of index 3

$$\dot{x}(t) = f_x(t, x(t), y(t))$$
$$\dot{y}(t) = f_y(t, x(t), y(t), z(t), u(t))$$
$$0 = g(t, x(t), u(t))$$

with $\frac{\partial g}{\partial x}\frac{\partial f_x}{\partial y}\frac{\partial f_y}{\partial z}$ nonsingular for all t

- RK methods most often stated for DAEs in a canonical form
- Often we can get an idea of the differential index by looking at the arguments of $g(\cdot)$

Runge-Kutta methods for index 1 DAEs

Definition (RK method for index 1 DAEs)

Consider an IVP with DAE of index 1 in Hessenberg form. Let n_s be the number of stages. Given the matrix $A \in \mathbb{R}^{n_\mathrm{s} \times n_\mathrm{s}}$ with the entries $a_{i,j}$ for $i, j = 1, \ldots, n_\mathrm{s}$, and the vectors $b, c \in \mathbb{R}^{n_\mathrm{s}}$. Let $t_{n,i} = t_n + c_i h$.

$$
\begin{aligned}
k_{n,i} &= f(t_{n,i}, x_n + h \sum_{j=1}^{n_\mathrm{s}} a_{i,j} k_{n,j}, z_{n,i}, u_n), && i = 1, \ldots, n_\mathrm{s} \\
0 &= g(t_{n,i}, x_n + h \sum_{j=1}^{n_\mathrm{s}} a_{i,j} k_{n,j}, z_{n,i}, u_n), && i = 1, \ldots, n_\mathrm{s} \\
x_{n+1} &= x_n + h \sum_{i=1}^{n_\mathrm{s}} b_i k_{n,i}, \\
0 &= g(t_{n+1}, x_{n+1}, z_{n+1}, u_n).
\end{aligned}
$$

is called a n_s-stage Runge-Kutta (RK) method for DAEs of index 1. Here $z_{n,i},\ i = 1, \ldots, n_\mathrm{s}$ are the stage values for the algebraic variables and z_{n+1} is the approximation of $z(t_{n+1})$.

Runge-Kutta methods for index 2 DAEs

Definition (RK method for index 2 DAEs)

Consider an IVP with DAE of index 2 in Hessenberg form. It is assumed that the initial values x_n and z_n are consistent:

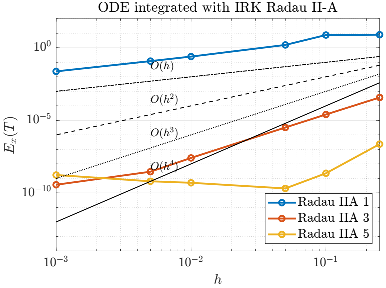
$$g(t_n, x_n, u_n) = 0, \; \frac{\partial}{\partial x} g(t_n, x_n, u_n)^\top f(t_n, x_n, z_n, u_n) = 0.$$

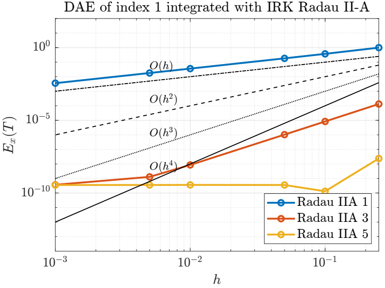
Let n_s be the number of stages. Given the matrix $A \in \mathbb{R}^{n_\mathrm{s} \times n_\mathrm{s}}$ with the entries $a_{i,j}$ for $i, j = 1, \ldots, n_\mathrm{s}$, and the vectors $b, c \in \mathbb{R}^{n_\mathrm{s}}$, a n_s-stage Runge-Kutta (RK) method for DAEs of index 2 is defined by the system of equations:

$$\begin{aligned}
k_{n,i} &= f(t_{n,i}, x_n + h \sum_{j=1}^{n_\mathrm{s}} a_{i,j} k_{n,j}, z_{n,i}, u_n), && i = 1, \ldots, n_\mathrm{s} \\
0 &= g(t_{n,i}, x_n + h \sum_{j=1}^{n_\mathrm{s}} a_{i,j} k_{n,j}, u_n), && i = 1, \ldots, n_\mathrm{s} \\
x_{n+1} &= x_n + h \sum_{i=1}^{n_\mathrm{s}} b_i k_{n,i}
\end{aligned}$$

Order plots for RK methods of DAE of different index

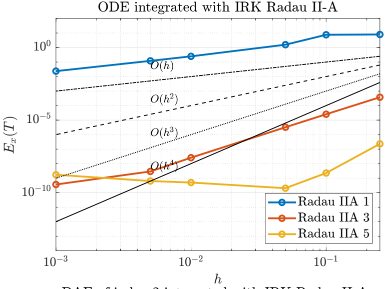
Integrate the pendulum model of different indexes with Radau IIA methods

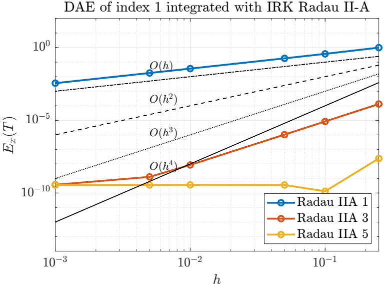


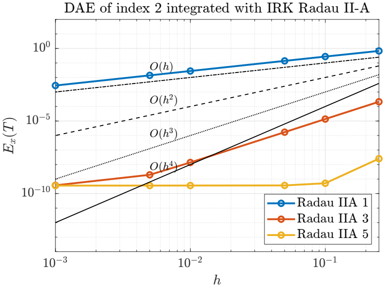


Order plots for RK methods of DAE of different index

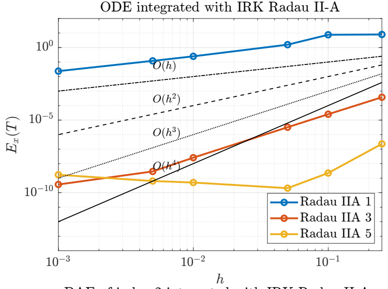
Integrate the pendulum model of different indexes with Radau IIA methods

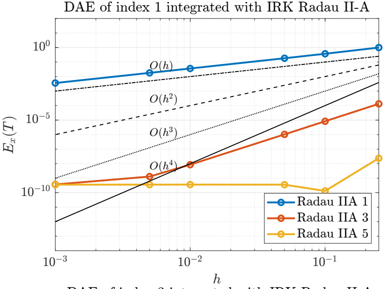


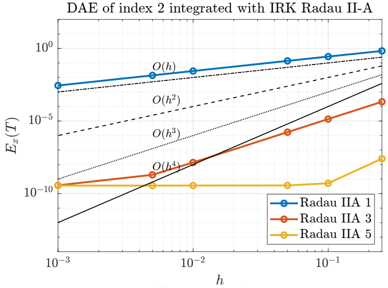


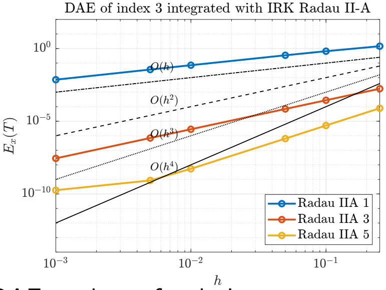


Integrate the pendulum model of different indexes with Radau IIA methods





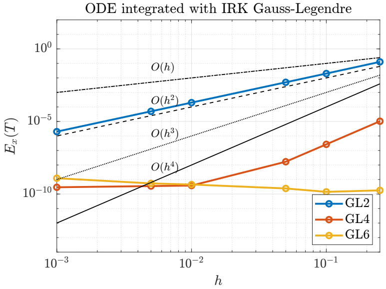


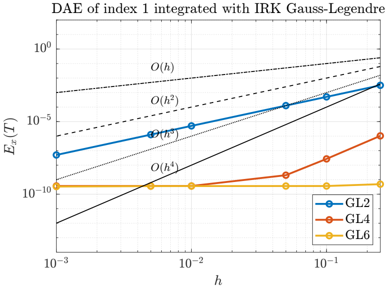


Direct discretization of higher index DAEs = loss of order!

Order plots for RK methods of DAE of different index

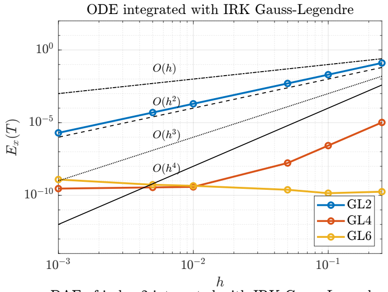
Integrate the pendulum model of different indexes with Gauss-Legendre methods

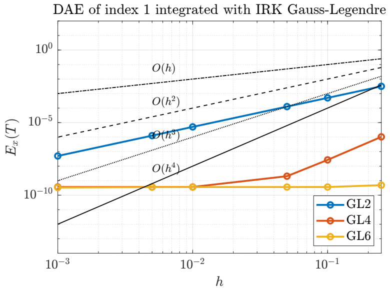


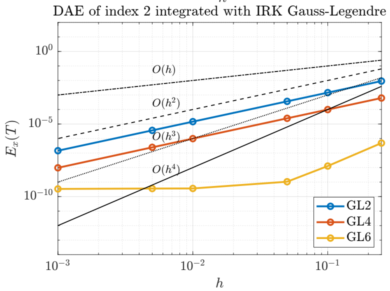


Order plots for RK methods of DAE of different index

Integrate the pendulum model of different indexes with Gauss-Legendre methods

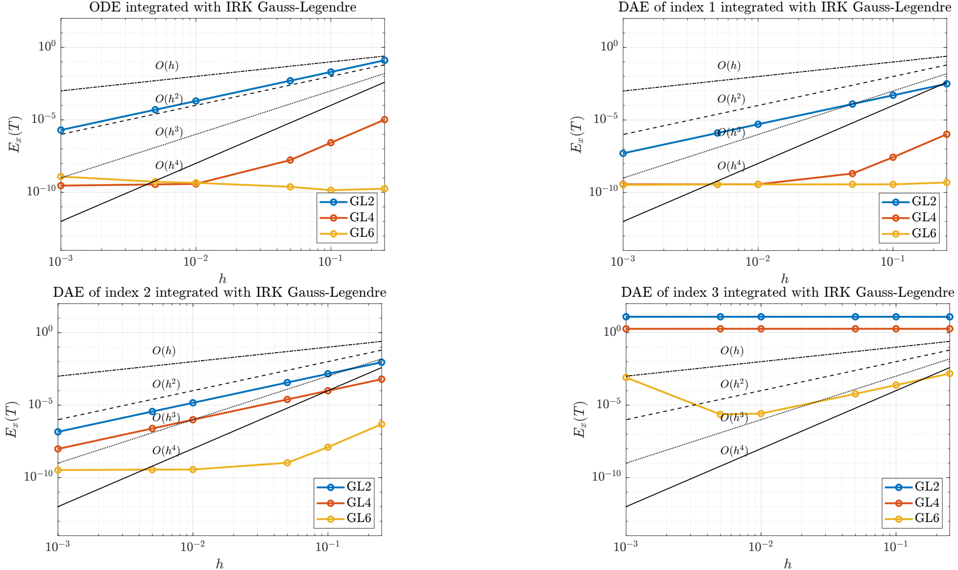






Order plots for RK methods of DAE of different index

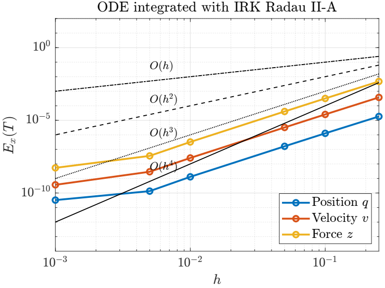
Integrate the pendulum model of different indexes with Gauss-Legendre methods

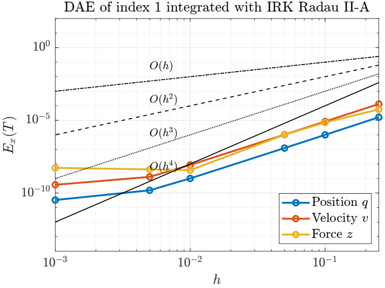


Direct discretization with GL of higher index DAEs = loss of order even more sever!

Order plots for the different variables of a DAE

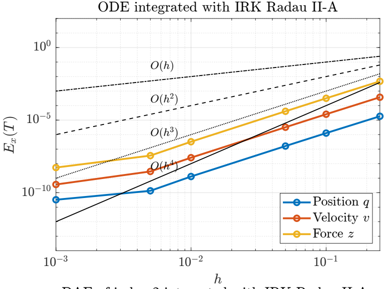
Integrate the pendulum model of with Radau IIA and $n_s = 2$

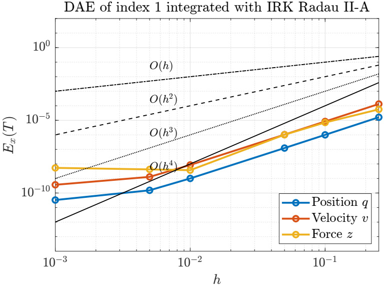


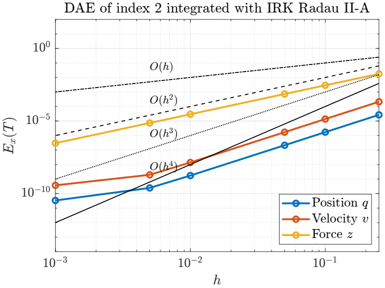


Order plots for the different variables of a DAE

Integrate the pendulum model of with Radau IIA and $n_s = 2$

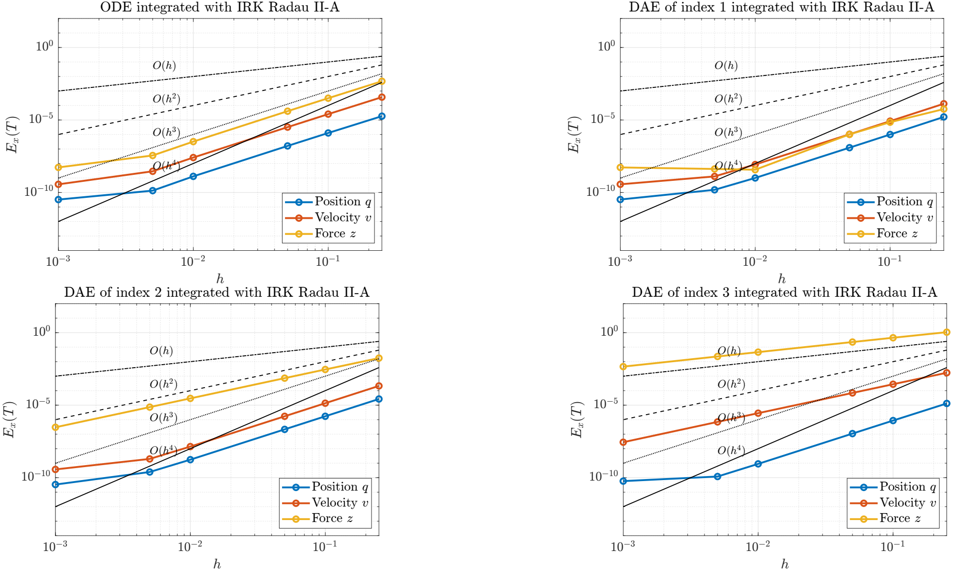






Order plots for the different variables of a DAE

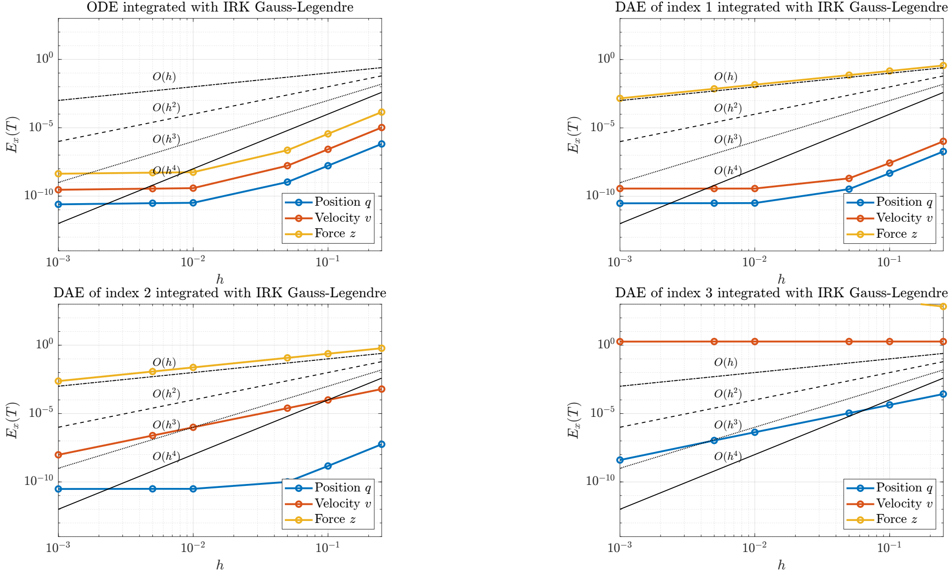
Integrate the pendulum model of with Radau IIA and $n_s = 2$



Depending on index, different components have different accuracy.

Order plots for the different variables of a DAE

Integrate the pendulum model of with Gauss-Legendre and $n_s = 2$



Depending on index, different components have different accuracy.

Order reduction in higher index DAEs

- RK methods experience **order reduction** for higher index DAEs
- Different components of the solution may have different accuracy
- Index reduction requires consistent initialization and drift handling
- Condition number of Newton matrix $O(h^{-k})$ where k is the index

Order reduction in higher index DAEs

- RK methods experience **order reduction** for higher index DAEs
- Different components of the solution may have different accuracy
- Index reduction requires consistent initialization and drift handling
- Condition number of Newton matrix $O(h^{-k})$ where k is the index

Method	n_s	ODE	DAE index 1		DAE index 2	
		x	x	z	x	z
Gauss-Legendre	odd	$2n_s$	$2n_s$	n_s	n_s+1	n_s-1
	even	$2n_s$	$2n_s$	n_s+1	n_s	n_s-2
Radau IA	odd/even	$2n_s-1$	$2n_s-1$	n_s	n_s	n_s-1
Radau IIA	odd/even	$2n_s-1$	$2n_s-1$	$2n_s-1$	$2n_s-1$	n_s
Lobatto IIIA	odd	$2n_s-2$	$2n_s-2$	$2n_s-2$	$2n_s-2$	n_s-1
	even	$2n_s-2$	$2n_s-2$	$2n_s-2$	$2n_s-2$	n_s
Lobatto IIIC	odd/even	$2n_s-2$	$2n_s-2$	$2n_s-2$	$2n_s-2$	n_s-1

Table: Overview of accuracy orders for some IRK methods for ODEs, DAEs of index 1 and 2

Order reduction in higher index DAEs

- RK methods experience **order reduction** for higher index DAEs
- Different components of the solution may have different accuracy
- Index reduction requires consistent initialization and drift handling
- Condition number of Newton matrix $O(h^{-k})$ where k is the index

Method	n_s	x	y	z
Radau IA	$n_\mathrm{s} > 2$	n_s	$n_\mathrm{s} - 1$	$n_\mathrm{s} - 2$
Radau IIA	$n_\mathrm{s} > 1$	$2n_\mathrm{s} - 1$	n_s	$n_\mathrm{s} - 1$
Lobatto IIIC	$n_\mathrm{s} > 2$	$2n_\mathrm{s} - 3$	n_s	$n_\mathrm{s} - 1$

Table: Overview of accuracy orders for some IRK methods for DAEs of index 3

Summary of Runge-Kutta methods for DAEs

- Practical difference between ODEs and DAEs is that DAEs must be solved consistently with respect to all constraints (even the hidden ones)
- RK methods for higher index DAES may suffer from order reduction - but not index reduction needed, Radau IIA a good choice
- In particular, Gauss-Legendre suffer from severe order reduction if index $k > 1$
- Methods for higher index methods may be ill conditioned
- Nonsmooth ODEs switch between index 0, 1 and 2. Sometimes they have hidden index reduced DAEs (e.g. time-freezing)

References

- Moritz Diehl, Sébastien Gros. "Numerical optimal control (Draft)," Lecture notes, 2019.
- Gerhard Wanner, Ernst Hairer. "Solving ordinary differential equations II." Vol. 375. New York: Springer Berlin Heidelberg, 1996.
- Ernst Hairer, Christian Lubich, and Michel Roche. "The numerical solution of differential-algebraic systems by Runge-Kutta methods." Vol. 1409. Springer, 2006.
- Uri M. Ascher, Linda R. Petzold. "Computer methods for ordinary differential equations and differential-algebraic equations." Vol. 61. SIAM, 1998.
- Lorenz T. Biegler. "Nonlinear programming: concepts, algorithms, and applications to chemical processes." SIAM, 2010.