Simulation Tools

Unit 2: Implicit ODEs

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2.1 Classification

Explicit ODE:

$$\dot{x} = f(t, x) \;\; x(0) = x_0$$

Implicit ODE:

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

Initial conditions ?

Special cases:

Nonlinear equation system

$$F(t, x) = 0 \;\text{ or even }\quad F(x) = 0$$

Linearly implicit ODE

$$E(x)\dot{x} - f(t, x) = 0$$

2.2 Classification (Cont.)

Special cases:

Linear singularly implicit ODE

$$\det(E) = 0$$

$$\begin{aligned} M(x_1)\dot{x}_1 &= f_1(t, x_1, x_2) \\ 0 &= f_2(t, x_1, x_2) \end{aligned}$$

"differential algebraic equation (DAE)", "differential variables x_1", "algebraic variables x_2".

See also

$$F(t, x, \dot{x}) = 0 \quad \text{with} \quad \det(F_3'(t, x, \dot{x})) = 0$$

(derivative with respect to the "third slot")

2.3 Occurence

These types of equations occur

- in rigid body mechanics
- in chemical engineering
- in electrical engineering (circuit simulation)

See also the overdetermined case:

$$\begin{aligned} M(x_1)\dot{x}_1 &= f_1(t, x_1) \\ 0 &= f_2(t, x_1) \end{aligned}$$

for all cases of applications with invariants (i.e. conservation properties)

2.4 Example: Pendulum

$$\begin{aligned}
\dot{p}_1 &= v_1 \\
\dot{p}_2 &= v_2 \\
\dot{v}_1 &= -\lambda p_1 \\
\dot{v}_2 &= -g - \lambda p_2 \\
0 &= p_1^2 + p_2^2 - l^2
\end{aligned}$$

The last equation is a (position-) constraint.
It can be replaced by a velocity constraint:

$$0 = 2(v_1 p_1 + v_2 p_2)$$

or an acceleration constraint

$$0 = \dot{v}_1 p_1 + \dot{v}_2 p_2 + v_1^2 + v_2^2$$

2.5 Example: Pendulum (Cont.)

.... or an acceleration constraint

$$0 = \dot{v}_1 p_1 + \dot{v}_2 p_2 + v_1^2 + v_2^2$$

That is equivalent with

$$0 = -\lambda(p_1^2 + p_2^2) - g + v_1^2 + v_2^2$$

(by inserting the differential equation)

or

$$0 = -\lambda l^2 - g + v_1^2 + v_2^2$$

and after a further differentiation we get

$$\dot{\lambda} = ...$$

a differential equation for λ.

2.6 The (differention) index of an implicit ODE

The number of differentiations needed to transform a singularly implicit ODE
(in particular a differential algebraic equation)
into a regularly implicit ODE
(in particular an explicit ODE)
is called the differentiation index.

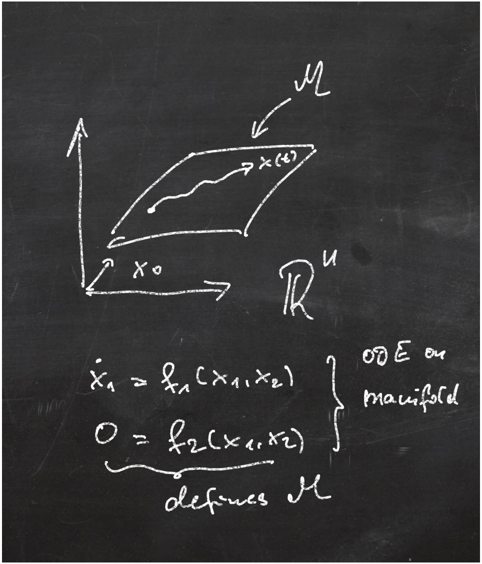
Mechanical systems with position constraints have index 3 (in general).

2.7 The index affects...

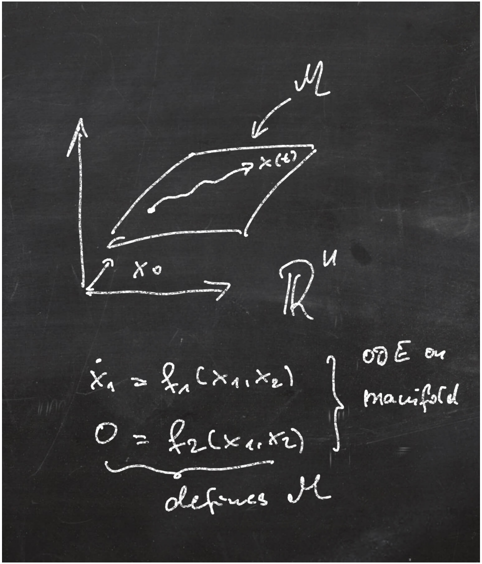
The index affects

- stabiity
- the freedom in choosing initial conditions
- the performance (and the success) of the numerical method
  - Newton's method might fail to converge
  - Linear systems might get ill-conditioned
  - Error estimation might be wrong
  - Step size control might fail

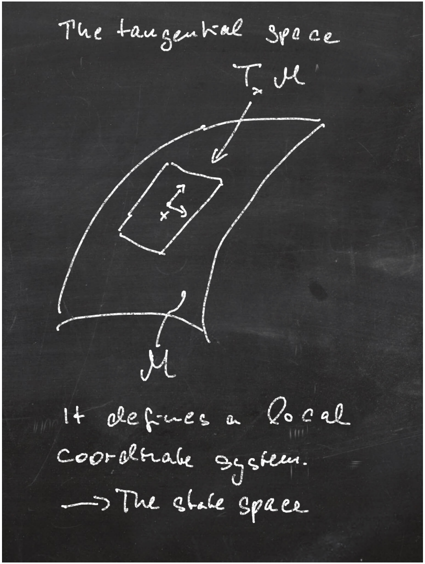
2.8 Differential Equations on Manifolds



2.9 Higher Index Systems have hidden manifolds



2.10 The state space



Minimal coordinate formulation ← state space formulation.

2.11 Initial Values - 2 examples

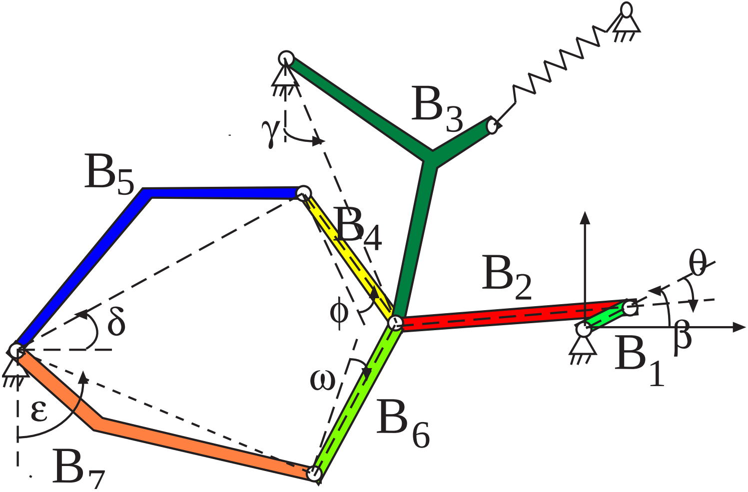
$$\begin{aligned}\dot{x}_2 &= x_1\\ 0 &= x_1 - f_2\end{aligned}$$

and

$$\begin{aligned}\dot{x}_2 &= x_1 - f_1\\ 0 &= x_2 - f_2\end{aligned}$$

Discuss the options to choose initial conditions. Determine the index first.

2.12 Example



7 position states, 14 differential eqs., 6 constraints
$\rightarrow$ 1 degree of freedom

2.13 Example (Cont.)

$$\begin{aligned} M(p)\ddot{p} &= f(t,p,\dot{p}) - G^{\mathrm{T}}(p)\lambda \\ 0 &= g(t,p) \quad \text{with} \quad G = \partial g/\partial p \end{aligned}$$

With $x^{\mathrm{T}} = \left(p, \dot{p}, \lambda\right)$ we write this in first order *residual form*:

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

see Assimulo problem class
`assimulo.problem.Implicit_Problem`.

2.14 Example (Cont.)

Initial conditions?

$$g(0, \cdot) : \mathbb{R}^7 \to \mathbb{R}^6$$

Solving $g(0, p) = 0$ gives consistent initial conditions.

Underdetermined nonlinear system.

2.15 Numerical Methods (explicit/ implicit Euler)

Let's solve

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

at a typical step $t_n \rightarrow t_{n+1} = t_n + h$.

Let's try the "two Eulers":

$$\dot{x}(t_n) \approx \frac{x(t_{n+1}) - x(t_n)}{h} \quad \text{Forward (Explicit) Euler}$$

and

$$\dot{x}(t_{n+1}) \approx \frac{x(t_{n+1}) - x(t_n)}{h} \quad \text{Backward (Implicit) Euler}$$

Observations?

2.16 BDF Methods for DAEs

Consider first the explicit problem case

$$\sum_{i=0}^{k} \alpha_{k-i} x_{n+1-i} - h_n \sum_{i=0}^{k} \beta_{k-i} f(t_{n+1-i}, x_{n+1-i}) = 0.$$

Thus,

$$\dot{x}(t_{n+1}) \approx \frac{\sum_{i=0}^{k} \alpha_{k-i} x_{n+1-i}}{h_n \beta_n}$$

Results in,

$$F(t_{n+1}, x_{n+1}, \frac{\sum_{i=0}^{k} \alpha_{k-i} x_{n+1-i}}{h_n \beta_n}) \stackrel{!}{=} 0$$

2.17 Multistep methods for DAEs

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

$$\begin{aligned} \dot{x} &= w \\ F(t, x, w) &= 0 \end{aligned}$$

This gives,

$$\begin{aligned} \sum_{i=0}^{k} \alpha_{k-i} x_{n+1-i} - h_n \sum_{i=0}^{k} \beta_{k-i} w_{n+1-i}) &= 0 \\ F(t_{n+1}, x_{n+1}, w_{n+1} &= 0 \end{aligned}$$