Simulation methods for differential equations

Rien Quirynen

July 28, 2015

Introduction

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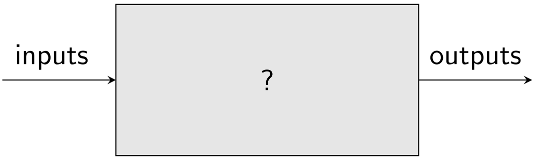

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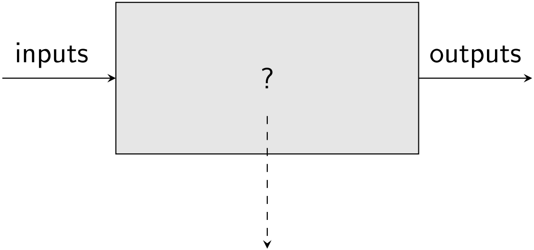

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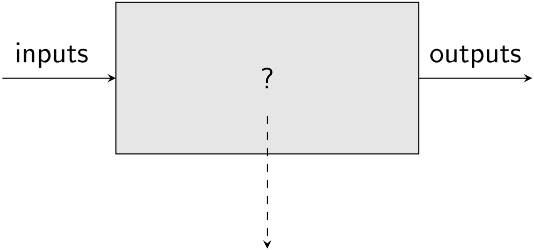

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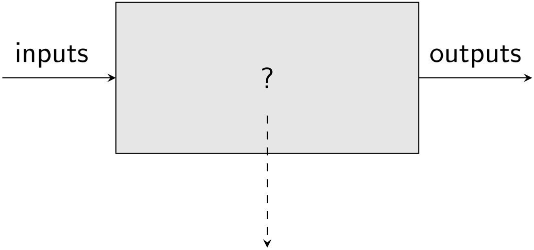

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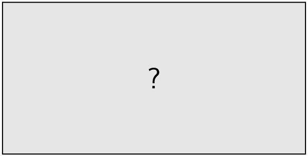

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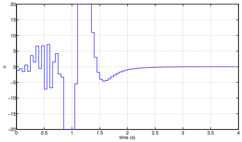

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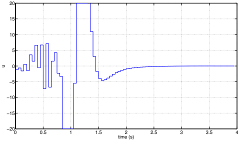

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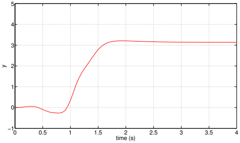

Introduction: IVP

THEOREM [Picard 1890, Lindelöf 1894]:

Initial value problem in ODE

$$\begin{aligned} \dot{x}(t) &= f(t, x(t), u(t), p), \quad t \in [t_0, t_{\mathrm{end}}], \\ x(t_0) &= x_0 \end{aligned}$$

- with given initial state x_0, parameters p, and controls $u(t)$,
- and Lipschitz continuous $f(t, x(t), u(t), p)$

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has **unique** solution

$$x(t), \ t \in [t_0, t_{\text{end}}]$$

Introduction: numerical simulation

Aim of numerical simulation:

Compute $x(t)$, $t \in [t_0, t_{\mathrm{end}}]$ which approximately satisfies

$$\begin{aligned} \dot{x}(t) &= f(t, x(t), u(t), p), \quad t \in [t_0, t_{\mathrm{end}}], \\ x(t_0) &= x_0, \end{aligned}$$

and $z(t)$ in case of index-1 DAE

$$\begin{aligned} \dot{x}(t) &= f(t, x(t), z(t), u(t), p), \\ 0 &= g(t, x(t), z(t), u(t), p), \quad t \in [t_0, t_{\mathrm{end}}], \\ x(t_0) &= x_0 \end{aligned}$$

NOTE: interested in values at discrete times $t_i \in [t_0, t_{\mathrm{end}}]$, especially $t = t_{\mathrm{end}}$

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Let us define the exact trajectory $x(t)$, $t \in [t_0, t_{\mathrm{end}}]$ and a set of discrete time steps $t_0, t_1, \dots$

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$$e(t_i) = x(t_i) - x(t_i;\ t_{i-1}, x(t_{i-1}))$$

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Global error or "transported error":

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Overview

Classes of numerical methods:

General Linear Methods

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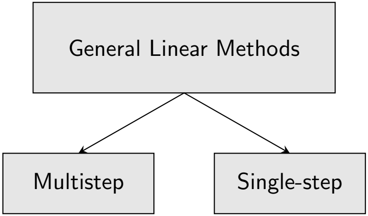

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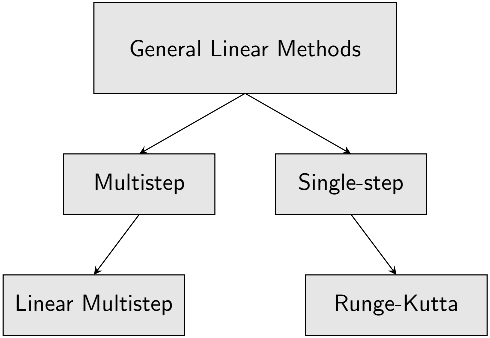

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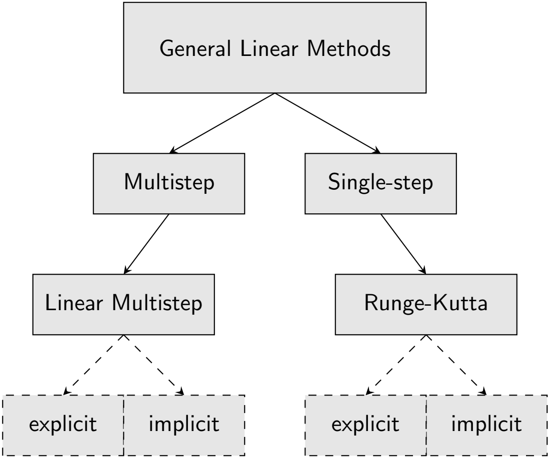

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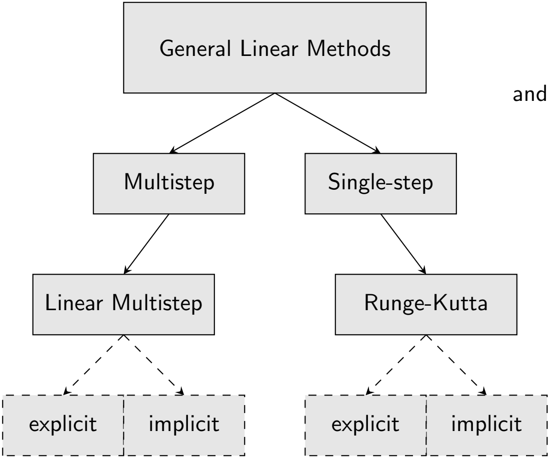

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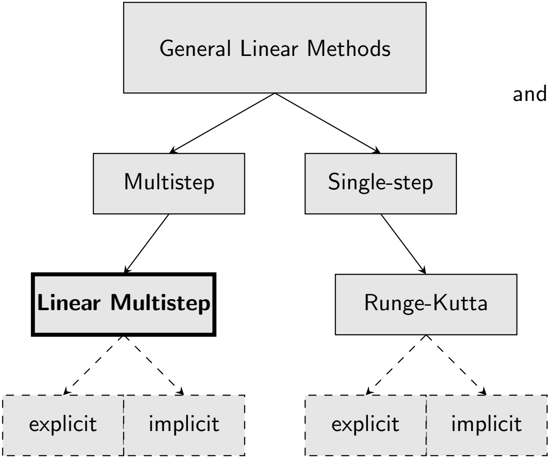

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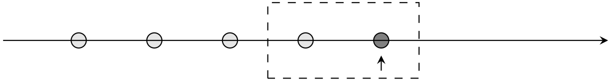

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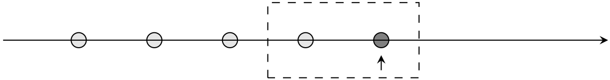

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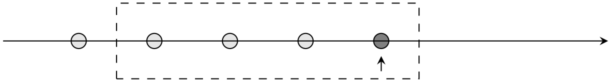

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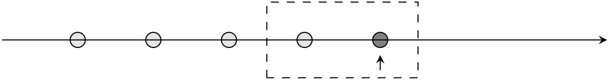

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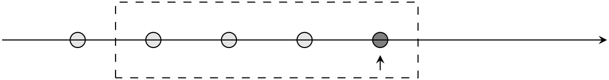

$\Rightarrow$ **good starting procedure needed!**

Linear multistep methods

Let us consider the simplified system $\dot{x}(t) = f(t, x(t))$.

A s-step LM method then uses x_i, $f_i = f(t_i, x_i)$ for $i = n - s, \ldots, n - 1$ to compute $x_n \approx x(t_n)$:

$$x_n + a_{s-1}x_{n-1} + \ldots + a_0 x_{n-s} = h\left(b_s f_n + b_{s-1} f_{n-1} + \ldots + b_0 f_{n-s}\right)$$

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Three main families:

- Adams-Bashforth (explicit)
- Adams-Moulton (implicit)
- Backward differentiation formulas (BDF)

Intermezzo: stiffness

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"... Around 1960, things became completely different and everyone became aware that the world was full of stiff problems."

- (G. Dahlquist, 1985)

Intermezzo: stiffness example

Let us consider the following simple one-dimensional system

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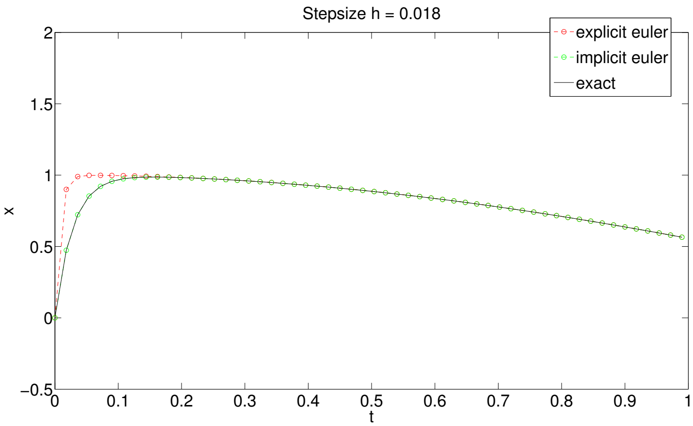

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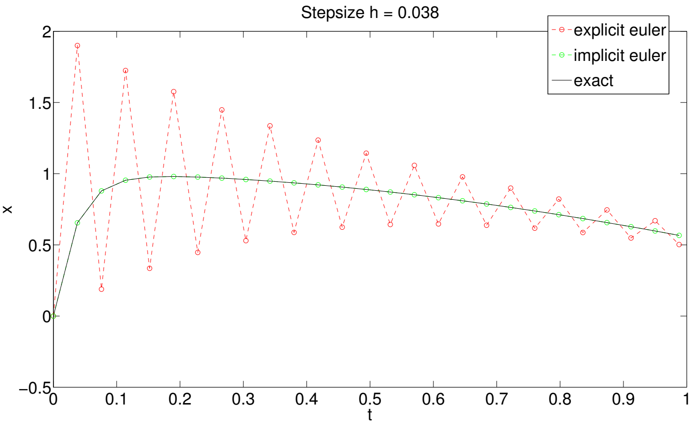

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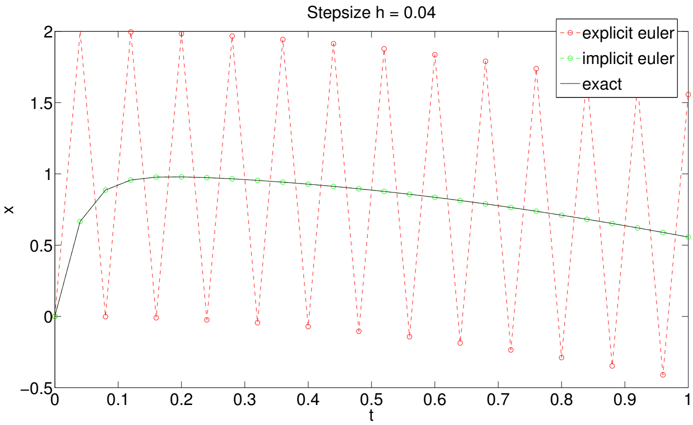

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Main message: stiff systems require (semi-)implicit methods!

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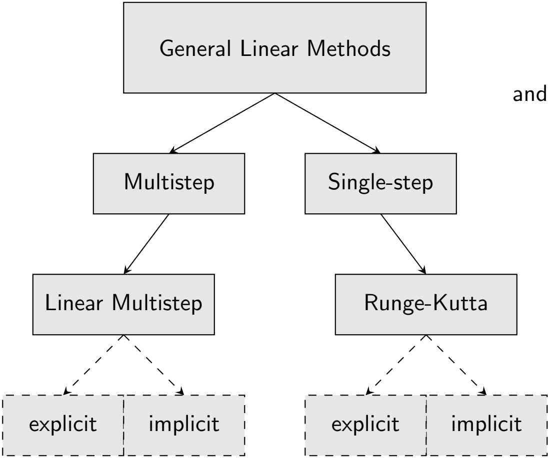

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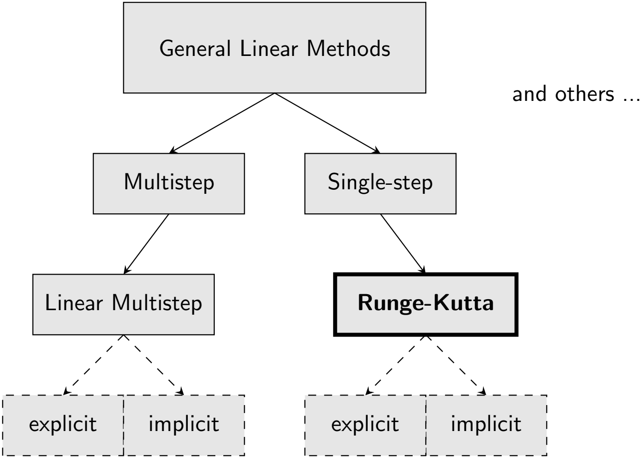

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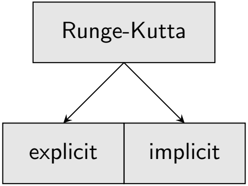

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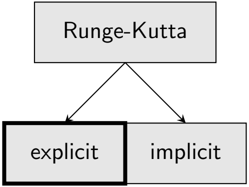

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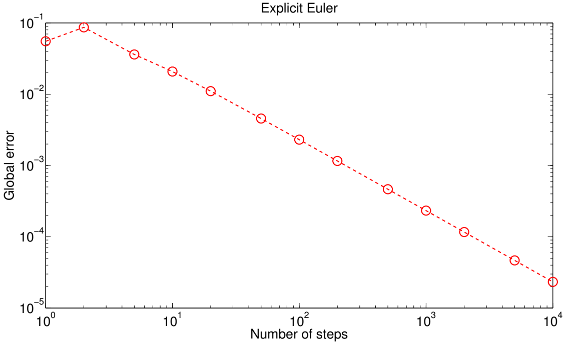
BUT: it is typically not a practical method... Why?
Higher order methods need much fewer steps for same accuracy!



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k_1 &= f(t_{n-1}, x_{n-1}) \\
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k_3 &= f(t_{n-1} + \frac{h}{2}, x_{n-1} + \frac{h}{2} k_2) \\
k_4 &= f(t_{n-1} + h, x_{n-1} + h\, k_3) \\
x_n &= x_{n-1} + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4)
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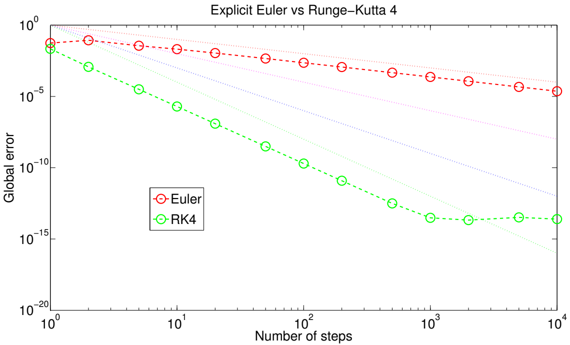

Explicit Runge-Kutta (ERK) methods

The RK4 method

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\begin{aligned}
k_1 &= f(t_{n-1}, x_{n-1}) \\
k_2 &= f(t_{n-1} + c_2\, h, x_{n-1} + a_{21}\, h\, k_1) \\
k_3 &= f(t_{n-1} + c_3\, h, x_{n-1} + a_{31}\, h\, k_1 + a_{32}\, h\, k_2) \\
&\vdots \\
k_s &= f(t_{n-1} + c_s\, h, x_{n-1} + a_{s1}\, h\, k_1 + a_{s2}\, h\, k_2 + \ldots + a_{s,s-1}\, h\, k_{s-1}) \\
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NOTE: each Runge-Kutta method is defined by its Butcher table!
other examples are e.g. the methods of Runge and Heun, ...

Intermezzo: Step size control

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no constant step size but suitable error control

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based on a local error estimate:

$$e_i \approx \|x(t_i) - x(t_i;\, t_{i-1}, x(t_{i-1}))\|$$

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Example:

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Euler: $x_n = x_{n-1} + h\, f_{n-1}$

Let us create a reference solution using 2 steps with $h/2$:

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\begin{aligned}
x_{n-1/2} &= x_{n-1} + \frac{h}{2}\, f_{n-1} \\
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$$\tilde{x}_n = x_{n-1/2} + \frac{h}{2}\, f_{n-1/2}$$

$e_n = \tilde{x}_n - x_n \quad \Rightarrow \quad$ accept/reject

and update the step size: $h_n = 0.9\, h_{n-1} \sqrt[p+1]{\frac{TOL}{E}}$

Intermezzo: Step size control

Example:

Euler: $x_n = x_{n-1} + h\, f_{n-1}$

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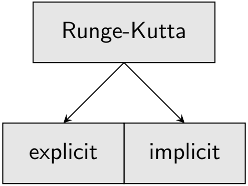
Embedded methods: Fehlberg (e.g. RKF45), Dormand-Prince, ...

Overview

Runge-Kutta methods:



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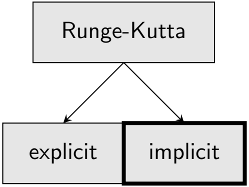

Implicit Runge-Kutta (IRK) methods

IRK as the natural generalization from ERK methods:

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & a_{32} & & \\
\vdots & \vdots & & \ddots & \\
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\hline
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e.g.

$x_n = x_{n-1} + h\, f_{n-1}$

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con: large nonlinear system $\Rightarrow$ Newton's method

Implicit Runge-Kutta (IRK) methods

Explicit ODE system:

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

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$$0 = f\left(t_{n-1} + c_1\, h, k_1, x_{n-1} + h \sum_{j=1}^{s} a_{1j}\, k_j, Z_1\right)$$

$$\vdots$$

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Collocation methods

Important family of IRK methods:

- distinct c_i's (nonconfluent)
- polynomial $q(t)$ of degree s

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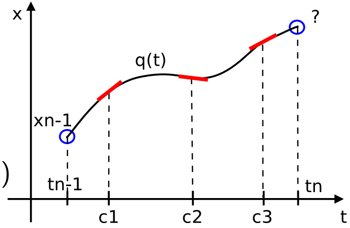

$$
\begin{aligned}
q(t_{n-1}) &= x_{n-1} \\
\dot{q}(t_{n-1} + c_1 h) &= f(t_{n-1} + c_1 h, q(t_{n-1} + c_1 h)) \\
&\vdots \\
\dot{q}(t_{n-1} + c_s h) &= f(t_{n-1} + c_s h, q(t_{n-1} + c_s h))
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$$

continuous approximation

$\Rightarrow \quad x_n = q(t_{n-1} + h)$

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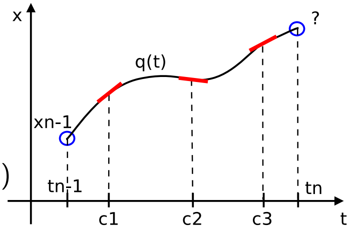

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NOTE: this is very popular in direct optimal control!

Collocation methods

How to implement a collocation method?

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$$

This is nothing else than ...

$$
\begin{aligned}
k_1 &= f(t_{n-1} + c_1\, h, x_{n-1} + h \sum_{j=1}^{s} a_{1j}\, k_j) \\
&\vdots \\
k_s &= f(t_{n-1} + c_s\, h, x_{n-1} + h \sum_{j=1}^{s} a_{sj}\, k_j) \\
x_n &= x_{n-1} + h \sum_{i=1}^{s} b_i\, k_i
\end{aligned}
$$

where the Butcher table is defined by the collocation nodes c_i.

Collocation methods

Example: The Gauss methods

Collocation methods

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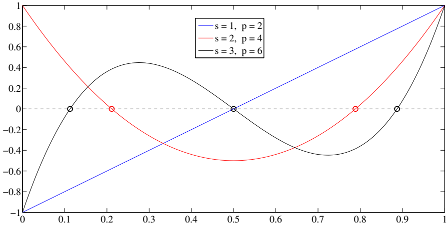
- roots of Legendre polynomials
- A-stable
- optimal order ($p = 2s$)



Collocation methods

Example: The Gauss methods

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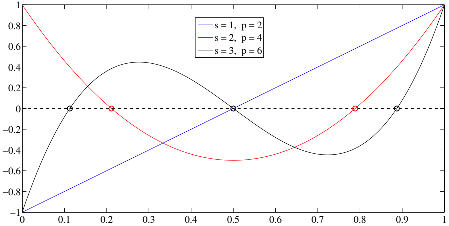

$$
\begin{aligned}
c_1 &= \frac{1}{2}, & s &= 1, \quad p = 2,\\
c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6},\ c_2 &= \frac{1}{2} + \frac{\sqrt{3}}{6}, & s &= 2, \quad p = 4,\\
c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10},\ c_2 = \frac{1}{2},\ c_3 &= \frac{1}{2} + \frac{\sqrt{15}}{10}, & s &= 3, \quad p = 6.
\end{aligned}
$$

Collocation methods

Example: The Gauss methods

- roots of Legendre polynomials
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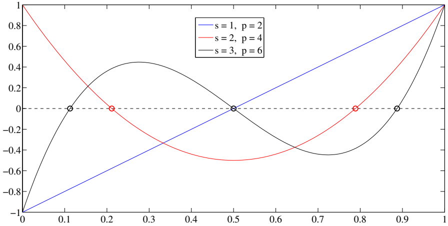
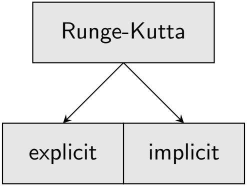
- optimal order ($p = 2s$)

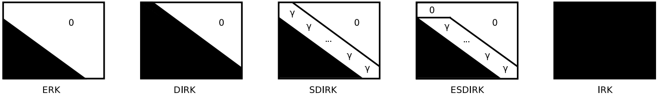


At least as popular:
Radau IIA methods ($p = 2s - 1$, stiffly accurate, L-stable)

Overview

Runge-Kutta methods:





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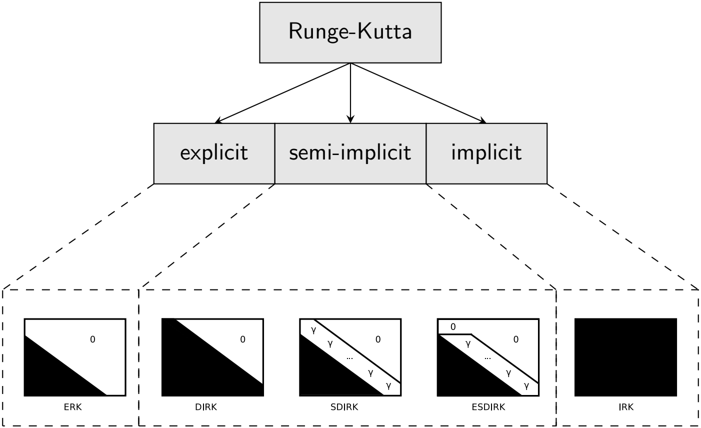


Semi-implicit Runge-Kutta methods

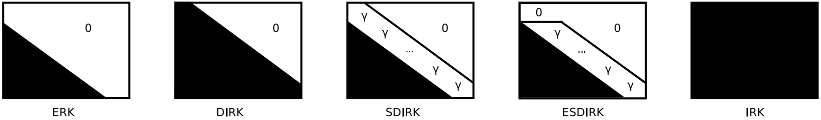
The matrix A is not strictly lower triangular . . .

Semi-implicit Runge-Kutta methods

The matrix A is not strictly lower triangular ...

but there is a specific structure!

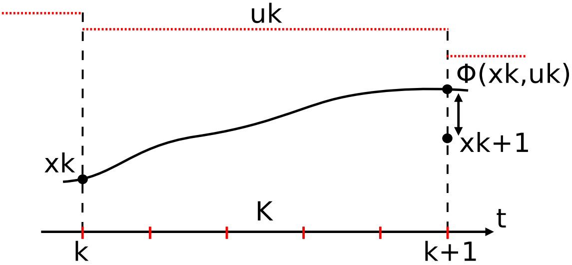
- Diagonal IRK (DIRK)
- Singly DIRK (SDIRK)
- Explicit SDIRK (ESDIRK)



Intermezzo: sensitivity propagation

Task of the integrator in nonlinear optimal control

- $x_{k+1} = \Phi_k(x_k, u_k)$
- nonlinear equality constraint



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Task of the integrator in nonlinear optimal control

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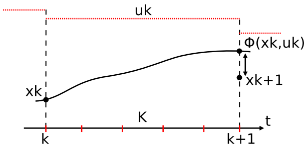
$$\downarrow$$

- linearization at $\bar{w}_k = (\bar{x}_k, \bar{u}_k)$



$$0 = \boldsymbol{\Phi_k(\bar{w}_k)} - x_{k+1} + \frac{\partial \boldsymbol{\Phi_k}}{\partial \mathbf{w}}\boldsymbol{(\bar{w}_k)}(w_k - \bar{w}_k)$$

- integration and sensitivity generation is typically a major computational step

Intermezzo: sensitivity propagation

"integrate-then-differentiate"

- derivatives of result
- Internal Numerical Differentiation (IND)
- direct IFT approach

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$\Rightarrow$ They are different

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$$\dot{x} = f(x)$$

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$$\Downarrow \text{ integrate}$$

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Variational Differential Equations
"differentiate-then-integrate"

Solve additional matrix differential equation

$$\dot{x} = f(x) \qquad\qquad x(0) = x_0\,,\; x(t_N) = x_N$$

$$\dot{S} = \frac{\partial f}{\partial x} S \qquad\qquad S(0) = d\,,\;\; S(t_N) = \frac{\partial x_N}{\partial x_0} d$$

Intermezzo: sensitivity propagation

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\end{aligned}
$$

Very accurate at reasonable costs, but:

- Have to get expressions for $\frac{\partial f}{\partial x}(\cdot)$.
- Computed sensitivity is not 100 % identical with derivative of (discretized) integrator result $\Phi(\cdot)$.
- What about implicit integration schemes?

Intermezzo: sensitivity propagation

External Numerical Differentiation (END)
"integrate-then-differentiate"

Finite differences: perturb x_0 and call integrator several times

$$\frac{x(t_N; x_0 + \epsilon\, e_i) - x(t_N; x_0)}{\epsilon}$$

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Very easy to implement, but several problems:

- Relatively expensive with overhead of error control.
- How to choose perturbation stepsize? Rule of thumb: $\epsilon = \sqrt{\mathrm{TOL}}$ where TOL is integrator tolerance.
- Loss of half the digits of accuracy: if integrator accuracy has value of $\mathrm{TOL} = 10^{-4}$, derivative has only two valid digits!

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- Loss of half the digits of accuracy: if integrator accuracy has value of $\mathrm{TOL} = 10^{-4}$, derivative has only two valid digits!
- Due to adaptivity, each call might have different discretization grids: output $x(t_N; x_0)$ is not differentiable!

Intermezzo: sensitivity propagation

Internal Numerical Differentiation (IND)
"integrate-then-differentiate"

Like END, but evaluate simultaneously all perturbed trajectories x_i with frozen discretization grid.

Up to round-off and linearization errors identical with derivative of numerical solution $\Phi(\cdot)$, but:

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- How to choose perturbation stepsize? Rule of thumb: $\epsilon = \sqrt{\mathrm{PREC}}$ where PREC is **machine precision**.

Intermezzo: sensitivity propagation

Internal Numerical Differentiation (IND)
"integrate-then-differentiate"

Like END, but evaluate simultaneously all perturbed trajectories x_i with frozen discretization grid.

Up to round-off and linearization errors identical with derivative of numerical solution $\Phi(\cdot)$, but:

- How to choose perturbation stepsize? Rule of thumb: $\epsilon = \sqrt{\mathrm{PREC}}$ where PREC is **machine precision**.

Note: adaptivity of nominal trajectory only, reuse of matrix factorization in implicit methods, so not only more accurate, but also cheaper than END!

Intermezzo: sensitivity propagation

Algorithmic Differentiation (AD)
"integrate-then-differentiate"

Use Algorithmic Differentiation (AD) to differentiate each step of the integration scheme.

Intermezzo: sensitivity propagation

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Use Algorithmic Differentiation (AD) to differentiate each step of the integration scheme. Illustration: AD for Euler

$$\dot{x} = f(x)$$

Intermezzo: sensitivity propagation

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"integrate-then-differentiate"

Use Algorithmic Differentiation (AD) to differentiate each step of the integration scheme. Illustration: AD for Euler

$$\dot{x} = f(x)$$
$$\Downarrow \text{ integrate}$$
$$x_{k+1} = x_k + h\, f(x_k)$$

Intermezzo: sensitivity propagation

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"integrate-then-differentiate"

Use Algorithmic Differentiation (AD) to differentiate each step of the integration scheme. Illustration: AD for Euler

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$$S_{k+1} = S_k + h\,\frac{\partial f(x_k)}{\partial x} S_k$$

Up to machine precision 100 % identical with derivative of numerical solution $\Phi(\cdot)$, but:

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Up to machine precision 100 % identical with derivative of numerical solution $\Phi(\cdot)$, but:

- tailored implementations needed (e.g. ACADO) ...
- or integrator and right-hand side $f(\cdot)$ need to be compatible codes (e.g. C++ when using ADOL-C)

Simulation methods: software

Simulation for optimization:

- *SUNDIALS*: BDF and Adams in CVODE(S) + BDF in IDA(S)
- *SolvIND*: BDF in DAESOL-II + RK in RKFSWT
- *ACADO Toolkit*: BDF and (I)RK methods
- ...

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- High order schemes preferable for smooth problems
- Explicit methods are good for non-stiff systems
- For stiff and/or implicit models, the use of implicit methods (BDF, IRK, ...) is highly recommended

References

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