Simulation methods for differential equations

Rien Quirynen

August 6, 2014

Introduction

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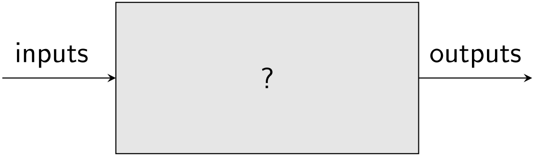

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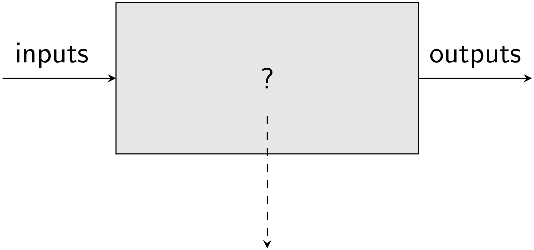

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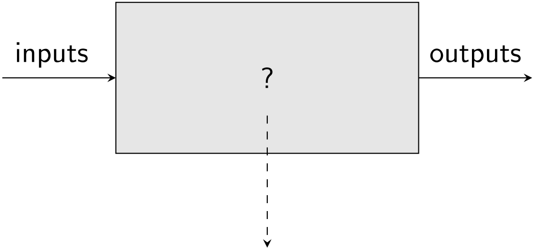

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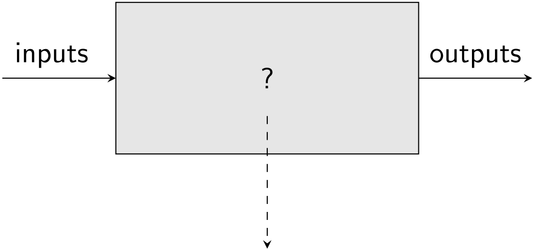

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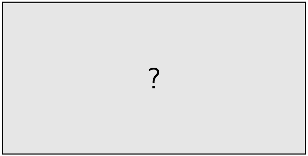

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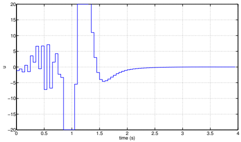

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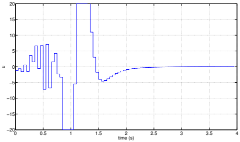

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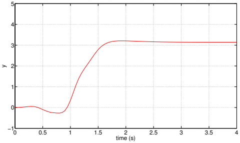

Introduction: IVP

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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- and Lipschitz continuous $f(t, x(t), u(t), p)$

has **unique** solution

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

Introduction: numerical simulation

Aim of numerical simulation:

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

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

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

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

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

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Global error or "transported error":

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$$\lim_{h \to 0} e(t_i) = O(h^{p+1})$$

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General Linear Methods

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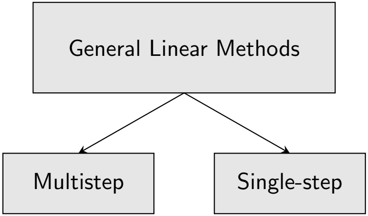

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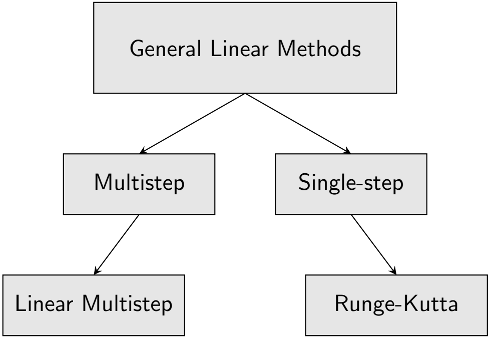

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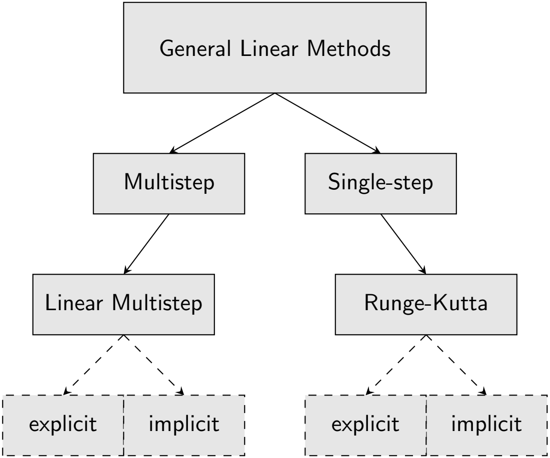

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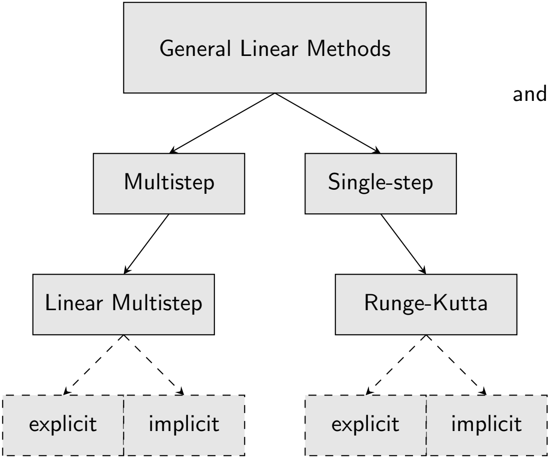

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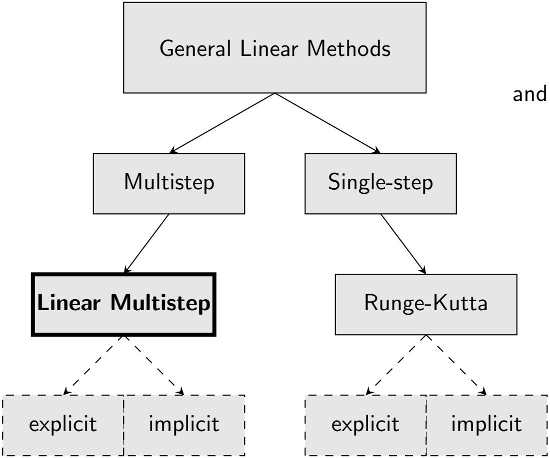

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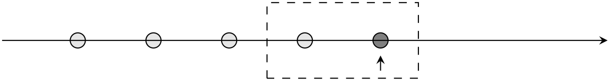

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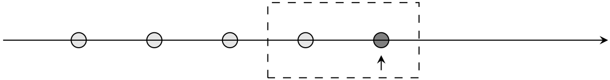

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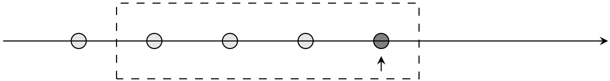

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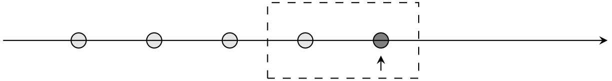

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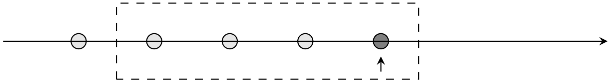

$\Rightarrow$ **good starting procedure needed!**

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 $x_n \approx x(t_n)$:

$$
\begin{aligned}
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)

Linear multistep methods: Adams

Let us consider the time step in integrated form

$$x(t_n) = x(t_{n-1}) + \int_{t_{n-1}}^{t_n} f(t, x(t))\, \mathrm{d}t$$

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Explicit examples:

- $s = 1: \quad x_n = x_{n-1} + h\, f_{n-1}$ (Euler)
- $s = 2: \quad x_n = x_{n-1} + h\, \left(\frac{3}{2} f_{n-1} - \frac{1}{2} f_{n-2}\right)$
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- $s = 2: \quad x_n = x_{n-1} + h\, \left(\frac{5}{12} f_n + \frac{8}{12} f_{n-1} - \frac{1}{12} f_{n-2}\right)$
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NOTE: implicit methods include $(x_n, f_n) \Rightarrow$ **nonlinear system**

Linear multistep methods: BDF

numerical integration $\quad \leftrightarrow \quad$ numerical differentiation

Let us again consider the interpolating polynomial $q(x)$ through (x_i, f_i) for $i = n - s, \ldots, \mathbf{n}$ (implicit!) on which we impose

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NOTE: widely used for stiff systems !!

Intermezzo: stiffness[1]

"... stiff equations are equations where certain implicit methods, in paricular BDF, perform better, usually tremendously better, than explicit ones."
- (Curtiss & Hirschfelder, 1952)

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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)

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Let us consider the following simple one-dimensional system

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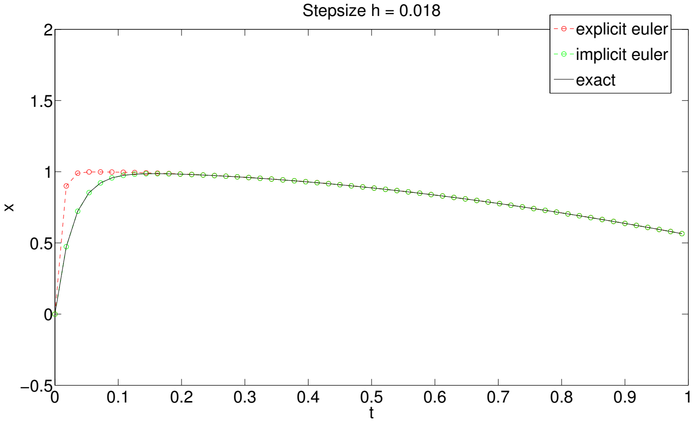

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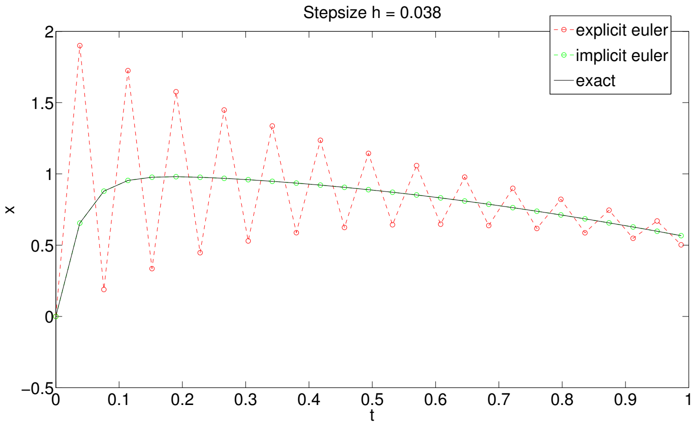

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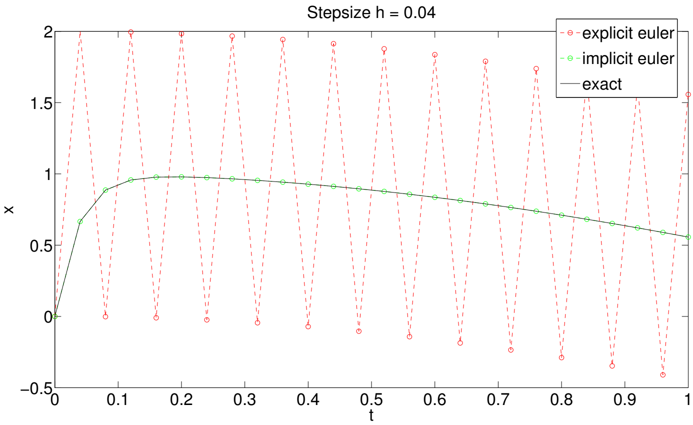

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Main message: stiff systems require (semi-)implicit methods!

Linear multistep 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 RK
- ...

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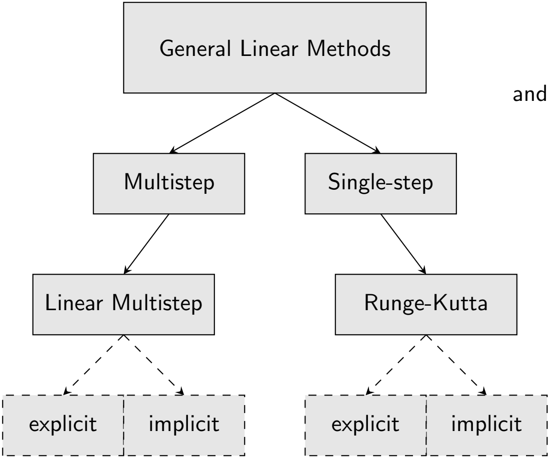

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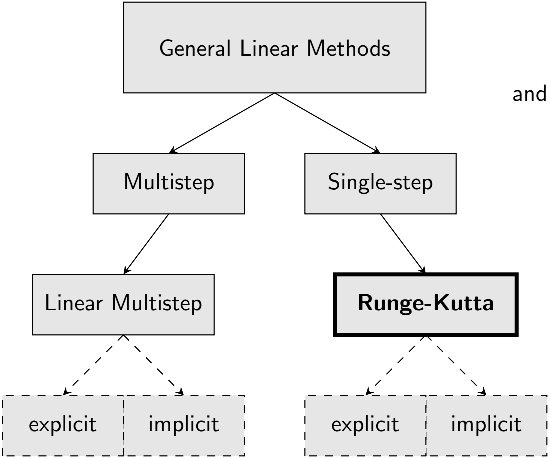

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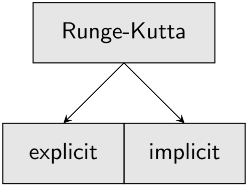

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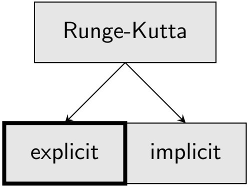

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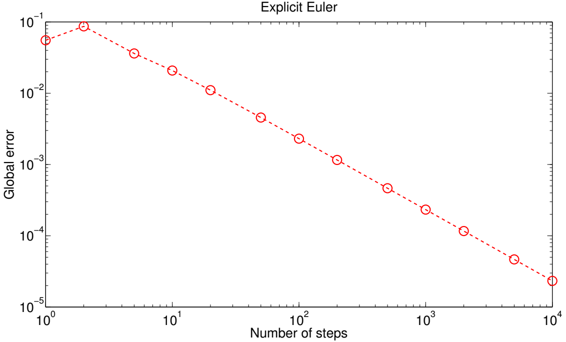
Higher order methods need much fewer steps for same accuracy!



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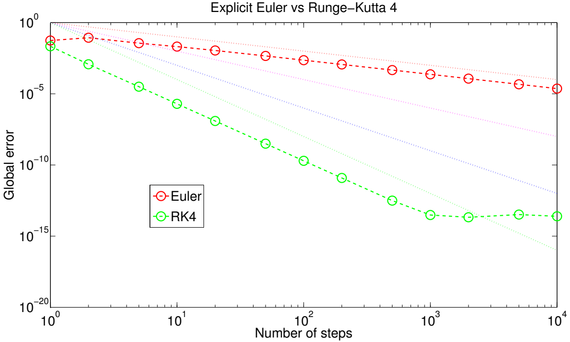
x_n &= x_{n-1} + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$



Explicit Runge-Kutta (ERK) methods

The RK4 method

$$
\begin{aligned}
k_1 &= f(t_{n-1}, x_{n-1}) \\
k_2 &= f(t_{n-1} + \frac{h}{2}, x_{n-1} + \frac{h}{2} k_1) \\
k_3 &= f(t_{n-1} + \frac{h}{2}, x_{n-1} + \frac{h}{2} k_2) \\
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\end{aligned}
$$

Explicit Runge-Kutta (ERK) methods

So a general s-stage ERK method

$$
\begin{aligned}
k_1 &= f(t_{n-1}, x_{n-1}) \\
k_2 &= f(t_{n-1} + c_2\, h, x_{n-1} + a_{21}\, h\, k_1) \\
k_3 &= f(t_{n-1} + c_3\, h, x_{n-1} + a_{31}\, h\, k_1 + a_{32}\, h\, k_2) \\
&\vdots \\
k_s &= f(t_{n-1} + c_s\, h, x_{n-1} + a_{s1}\, h\, k_1 + a_{s2}\, h\, k_2 + \ldots + a_{s,s-1}\, h\, k_{s-1}) \\
x_n &= x_{n-1} + h \sum_{i=1}^{s} b_i\, k_i
\end{aligned}
$$

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\end{aligned}
$$

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & a_{32} & & \\
\vdots & \vdots & & \ddots & \\
c_s & a_{s1} & a_{s2} & \cdots & \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
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\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
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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

Typically:

no constant step size but suitable error control

Intermezzo: Step size control

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no constant step size but suitable error control

based on a local error estimate:

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

Intermezzo: Step size control

Example:

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

Intermezzo: Step size control

Example:

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

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

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

Intermezzo: Step size control

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

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

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

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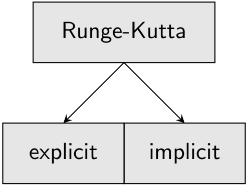
Embedded methods: Fehlberg (e.g. RKF45), Dormand-Prince, ...

Overview

Runge-Kutta methods:



Overview

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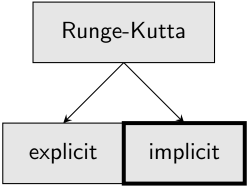

Implicit Runge-Kutta (IRK) methods

IRK as the natural generalization from ERK methods:

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & a_{32} & & \\
\vdots & \vdots & & \ddots & \\
c_s & a_{s1} & a_{s2} & \cdots & \\
\hline
 & b_1 & b_2 & \cdots & b_s
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$$

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\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
\quad \Rightarrow \quad
\begin{array}{c|ccc}
c_1 & a_{11} & \cdots & a_{1s} \\
c_2 & a_{21} & \cdots & a_{2s} \\
\vdots & \vdots & & \vdots \\
c_s & a_{s1} & \cdots & a_{ss} \\
\hline
 & b_1 & \cdots & b_s
\end{array}
$$

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

$$\vdots$$

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$$\begin{array}{c|ccc}
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$$

pro: nice properties (order, stability)

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pro: nice properties (order, stability)

con: large nonlinear system

Implicit Runge-Kutta (IRK) methods

Explicit ODE system:

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

$$
\begin{aligned}
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$$

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$$\vdots$$

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Implicit ODE/DAE (index 1):

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

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

$$\vdots$$

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$$x_n = x_{n-1} + h \sum_{i=1}^{s} b_i\, k_i$$

Collocation methods

Important family of IRK methods:

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

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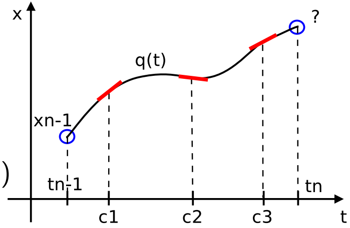

$$
\begin{aligned}
q(t_{n-1}) &= x_{n-1} \\
\dot{q}(t_{n-1} + c_1 h) &= f(t_{n-1} + c_1 h, q(t_{n-1} + c_1 h)) \\
&\vdots \\
\dot{q}(t_{n-1} + c_s h) &= f(t_{n-1} + c_s h, q(t_{n-1} + c_s h))
\end{aligned}
$$

continuous approximation

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

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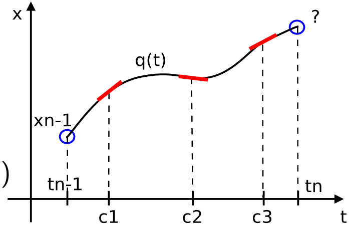

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&\vdots \\
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\end{aligned}
$$

continuous approximation

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

NOTE: this is very popular in direct optimal control!

Collocation methods

How to implement a collocation method?

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

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.

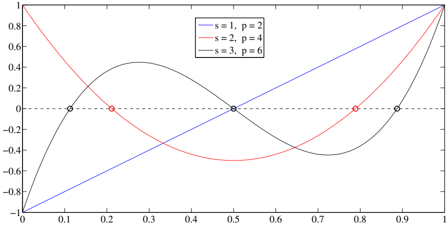
Collocation methods

Example: The Gauss methods

Collocation methods

Example: The Gauss methods

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



Collocation methods

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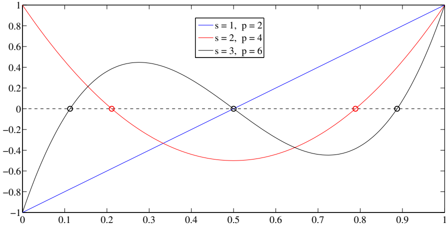
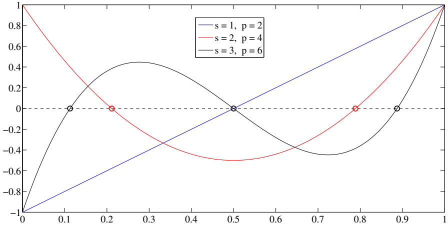


$$
\begin{aligned}
c_1 &= \frac{1}{2}, && s = 1, \quad p = 2,\\
c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6},\ c_2 &= \frac{1}{2} + \frac{\sqrt{3}}{6}, && s = 2, \quad p = 4,\\
c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10},\ c_2 = \frac{1}{2},\ c_3 &= \frac{1}{2} + \frac{\sqrt{15}}{10}, && s = 3, \quad p = 6.
\end{aligned}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

Collocation methods

Example: The Gauss methods

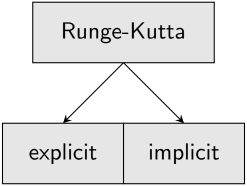
- roots of Legendre polynomials
- A-stable
- optimal order ($p = 2s$)

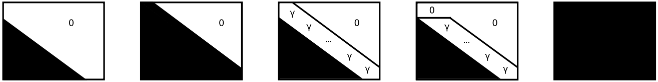


At least as popular:
Radau IIA methods ($p = 2s - 1$, stiffly accurate, L-stable)

Overview

Runge-Kutta methods:

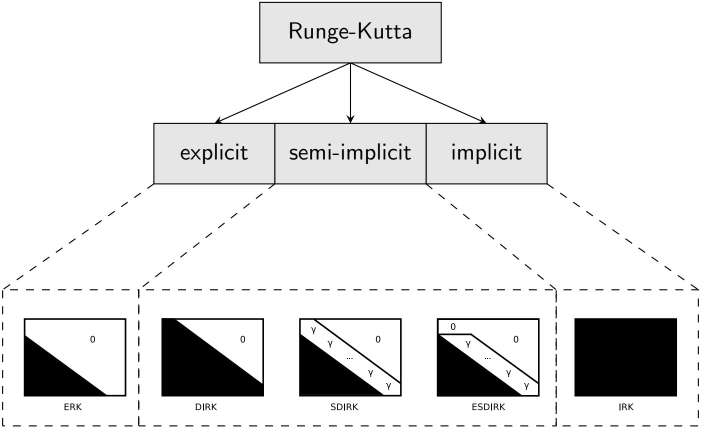




ERK DIRK SDIRK ESDIRK IRK

Overview

Runge-Kutta methods:



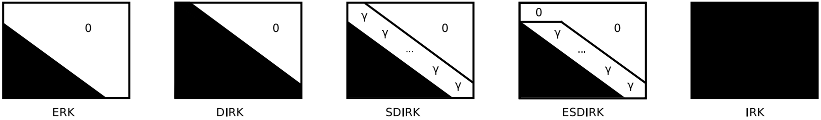
Semi-implicit Runge-Kutta methods

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)



Summary

- High order schemes preferable for smooth problems

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- Explicit methods are good for non-stiff systems

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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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