Explicit and implicit Runge-Kutta methods: an overview

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30-01-2002

Introduction

Quadrature Problem:

$$\begin{aligned} y' &= f(x) \\ y(x_0) &= y_0 \end{aligned}$$

Midpoint rule

$$y_1 = y_0 + hf\left(x_0 + \frac{h}{2}\right)$$

Introduction

Initial Value Problem:

$$\begin{aligned} y' &= f(x, y) \\ y(x_0) &= y_0 \end{aligned}$$

Midpoint rule

$$y_1 = y_0 + hf\left(x_0 + \frac{h}{2}, y\left(x_0 + \frac{h}{2}\right)\right)$$

How do we compute $y\left(x_0 + \frac{h}{2}\right)$?

Use Euler for: $y\left(x_0 + \frac{h}{2}\right)$.

This results in:

$$\begin{aligned} k_1 &= f(x_0, y_0) \\ k_2 &= f\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2}k_1\right) \\ y_1 &= y_0 + hk_2 \end{aligned}$$

General definition

Let $b_1, \ldots, b_s$, $a_{ij} (i, j = 1, \ldots s)$ be real numbers. Let $c_i = \sum_j a_{ij}$. The method

$$\begin{aligned} k_i &= f\left(x_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j\right) \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i k_i \end{aligned}$$

is called an s-stage RK method.

Butcher tableau:

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \ldots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \ldots & a_{ss} \\ \hline & b_1 & \ldots & b_s \end{array}$$

Types

Explicit

$$\begin{array}{c|ccccc} 0 & 0 & & & \\ c_2 & a_{21} & 0 & & \\ \vdots & \vdots & \ddots & \ddots & \\ c_s & a_{s1} & \dots & a_{ss-1} & 0 \\ \hline & b_1 & \dots & b_{s-1} & b_s \end{array}$$

Examples:

Forward Euler:

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

Runge:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$

Types

Diagonal(DIRK)

$$\begin{array}{c|ccc} c_1 & a_{11} & & \\ \vdots & \vdots & \ddots & \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array}$$

Examples:

Implicit midpoint rule:

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

Modified Extended BDF 1:

$$\begin{array}{c|ccc} 1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ 1 & \frac{1}{2} & -\frac{1}{2} & 1 \\ \hline & \frac{1}{2} & -\frac{1}{2} & 1 \end{array}$$

Types

Implicit (IRK)

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array}$$

Example:

Hammer-Hollingsworth

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Order conditions

2 stage Explicit Runge-Kutta method

$$\begin{aligned} y_1 &= y_0 + hb_1 f(y_0) \\ &\quad + hb_2 f(y_0 + ha_{21} f(y_0)) \end{aligned}$$

Taylor

$$\begin{aligned} y_1 &= y_0 + hb_1 f(y_0) + hb_2 f(y_0) \\ &\quad + h^2 b_2 a_{21} f'(y_0) f(y_0) \\ &\quad + \frac{h^3}{2} b_2 a_{21}^2 f^{(2)}(y_0) f(y_0)^2 + O(h^4) \end{aligned}$$

Taylor of exact solution

$$\begin{aligned} y(x_1) &= y_0 + hf(y_0) + \frac{1}{2} h^2 f'(y_0) f(y_0) \\ &\quad + \frac{1}{6} h^3 \Big(f^{(2)}(y_0) f(y_0) f(y_0) \\ &\quad + f'(y_0) f'(y_0) f(y_0) \Big) + O(h^4) \end{aligned}$$

Order conditions

Error:

$$
\begin{aligned}
y_1 - y(x_1) &= h(b_1 + b_2 - 1)f(y_0) \\
&+ h^2(b_2 a_{21} - \frac{1}{2})f'(y_0)f(y_0) \\
&+ \frac{h^3}{2}\left(b_2 a_{21}^2 - \frac{1}{3}\right) f^{(2)}(y_0)f(y_0)^2 \\
&- \frac{1}{6}h^3 f'(y_0)f'(y_0)f(y_0) + O(h^4)
\end{aligned}
$$

Order conditions for order 2 approximation:

$$
\begin{aligned}
b_1 + b_2 &= 1 \\
b_2 a_{21} &= \frac{1}{2}
\end{aligned}
$$

Principal Error terms

$$
\frac{1}{2}\left(b_2 a_{21}^2 - \frac{1}{3}\right), \qquad -\frac{1}{6}
$$

Order conditions

order p	1	2	3	4	5	6	7	8
no. of conditions	1	2	4	8	17	37	85	200

Mathematica