# Runge-Kutta method.

One step method

use several $f$ evaluation to advance from

$$t_n \longrightarrow t_{n+1}$$

Ex. $\begin{cases} k_1 = f(u_n, t_n) \\ u_{n+1} = u_n + h k_1 \end{cases}$ forward Euler. $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$

Ex. $\begin{cases} k_1 = f(u_n, t_n) \\ k_2 = f(u_n + h k_1, t_n + h) \\ u_{n+1} = u_n + \frac{h}{2}(k_1 + k_2) \end{cases}$ 2nd order explicit. $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$

$$\tilde{u} = u_n + h f(u_n, t_n)$$

Modified Euler.

$$u_{n+1} = u_n + \frac{h}{2} f(u_n, t_n) + \frac{h}{2} f(\tilde{u}, t_{n+1})$$

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

Ex.
$$\begin{cases} k_1 = f(u_n, t_n) \\ k_2 = f\left(u_n + \frac{h}{2}(k_1 + k_2),\ t_n + h\right) \\ u_{n+1} = u_n + \frac{h}{2}(k_1 + k_2) \end{cases}$$

Trapezoidal

Ex.
$$\begin{cases} k_1 = f(u_n, t_n) \\ k_2 = f\left(u_n + \frac{h}{2} k_1,\ t_n + \frac{h}{2}\right) \\ k_3 = f\left(u_n + \frac{h}{2} k_2,\ t_n + \frac{h}{2}\right) \\ k_4 = f\left(u_n + h k_3,\ t_n + h\right) \\ u_{n+1} = u_n + h\left[\frac{1}{6} k_1 + \frac{1}{3} k_2 + \frac{1}{3} k_3 + \frac{1}{6} k_4\right] \end{cases}$$

"The" RK4.

explicit

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

General $r$-stage RK.

$$\begin{cases} k_1 = f\left(u_n + h(a_{11}k_1 + \cdots + a_{1r}k_r),\ t_n + c_1 h\right) \\ \vdots \\ k_r = f\left(u_n + h(a_{r1}k_1 + \cdots + a_{rr}k_r),\ t_n + c_r h\right) \\ u_{n+1} = u_n + h\left(b_1 k_1 + \cdots + b_r k_r\right) \end{cases}$$

$A \in \mathbb{R}^{r\times r}, \vec{b}, \vec{c} \in \mathbb{R}^r$.

Butcher array $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$

$$\vec{k} = (k_1, \cdots, k_r)^T, \quad \vec{e} = (1, \cdots, 1)^T$$

$$\vec{k} = f(u_n \vec{e} + hA\vec{k}, \; t_n \vec{e} + \vec{c}h)$$

$$u_{n+1} = u_n + h \vec{b}^T \vec{k}$$

explicit method: upper triangular part (diag. elements included) of $A \equiv 0$.

special case: upper tri. part (diag elements excluded) of $A \equiv 0$.

$$\begin{array}{c|ccc} c_1 & a_{11} & & 0 \\ \vdots & \vdots & \ddots & \\ c_r & a_{r1} & \cdots & a_{rr} \\ \hline & b_1 & \cdots & b_r \end{array}$$

diagonal implicit RK (DIRK)

Solve $r$ nonlinear systems sequentially.

Advantage:

① Easy to start

② adaptive stepsize control.

③ relatively good stability properties.

disadvantage:

① Do NOT reuse history.

② high order can be tricky.

autonomization (remove explicit time dependency).

$$\xi = \begin{pmatrix} u \\ t \end{pmatrix} \in \mathbb{R}^{d+1}$$

$$\begin{cases} \dot{\xi} = \begin{pmatrix} f(\xi) \\ 1 \end{pmatrix} \\ \xi(0) = \begin{pmatrix} u(0) \\ 0 \end{pmatrix} \end{cases}$$

Consistency for the time variable.

$$t_n + h \sum_{j=1}^{r} a_{ij} \cdot 1 = t_n + c_i h$$

$$\sum_{j=1}^{r} a_{ij} = c_i$$ Kutta's condition $$\begin{array}{c|c} & A \\ \hline & b^T \end{array}$$

2-stage explicit RK

$$\begin{array}{c|cc} & 0 & 0 \\ & a & 0 \\ \hline & b_1 & b_2 \end{array}$$

$$\begin{cases} k_1 = f(u_n) \\ k_2 = f(u_n + h a k_1) \\ u_{n+1} = u_n + h(b_1 k_1 + b_2 k_2) \end{cases}$$

$u \in \mathbb{R}$

LTE : $\tau_n = u(t_{n+1}) - u(t_n) - h\left[b_1 f(u(t_n)) + b_2 f(u(t_n) + h a f(u(t_n)))\right]$

$u \equiv u(t_n)$, $u' \equiv u'(t_n) = f(u(t_n))$, $f \equiv f(u(t_n))$

$f_u \equiv f_u(u(t_n))$

$$u'' = f' \leftarrow f_u(u(t_n))\, u'(t_n) \equiv f_u f$$

$$u''' = f_{uu} f^2 + f_u^2 f$$

$$\tau_n = hf + \frac{h^2}{2} f_u f + \frac{h^3}{6}\left(f_{uu} f^2 + f_u^2 f\right) + O(h^4)$$

$$- h(b_1+b_2) f - h^2 b_2 a f_u f - \frac{h^3}{2} b_2 a^2 f_{uu} f^2 + O(h^4)$$

$$= hf\left(1-(b_1+b_2)\right) + h^2 f_u f \left(\frac{1}{2} - b_2 a\right)$$

$$+ h^3 f_{uu} f^2 \left(\frac{1}{6} - \frac{1}{2} b_2 a^2\right) + \frac{h^3}{6} f_u^2 f + O(h^4)$$

second order method:

$$\begin{cases} 1 = b_1 + b_2 \\ \frac{1}{2} = b_2 a \end{cases} \longrightarrow \text{not unique.}$$

e.g.
$$\begin{array}{c|cc} & 0 & 0 \\ & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$
2nd order Runge.

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

additional effort.

$$\frac{1}{6} = \frac{1}{2} b_2 a^2$$

$$\begin{array}{c|cc} & 0 & 0 \\ & \frac{2}{3} & 0 \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$
Heun's method.

general 2nd RK

$$\begin{array}{c|cc} & a_{11} & a_{12} \\ & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array}$$

$$k_i = f\left(u_n + h \sum_j a_{ij} k_j\right) \qquad i = 1, 2$$

$$u_{n+1} = u_n + h \sum_i b_i k_i ,$$

$$\tau_n = h f + \frac{h^2}{2} f_u f + \frac{h^3}{6}\left(f_{uu} f^2 + f_u^2 f\right) + O(h^4)$$

$$- h\Big(\sum_i b_i f + \sum_i b_i h f_u \sum_j a_{ij} f$$

$$+ h^2 f_u \sum_{jk} a_{ij} a_{jk} f_u f + \frac{h^2}{2} f_{uu} \Big(\sum_j a_{ij} f\Big)^2 + O(h^4)\Big)$$

$$= h f \left(1 - \sum_i b_i\right) + h^2 f_u f \left(\frac{1}{2} - \sum_{ij} b_i a_{ij}\right)$$

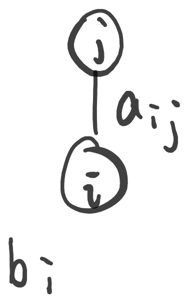
$$+ h^3 f_{uu} f^2 \left(\frac{1}{6} - \frac{1}{2} \sum_{ijk} b_i a_{ij} a_{ik}\right)$$

$$+ h^3 f_u^2 f \left(\frac{1}{6} - \sum_{ijk} b_i a_{ij} a_{jk}\right) + O(h^4)$$

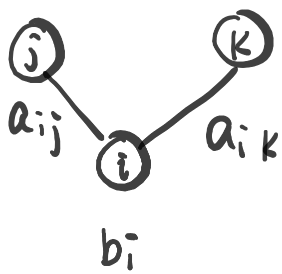
$$\left\{\begin{array}{ll}
\sum_i b_i = 1 & \longrightarrow 1 \\
\sum_{ij} b_i a_{ij} = \frac{1}{2} & \longrightarrow 2 \\
\left.\begin{array}{l}
\sum_{ijk} b_i a_{ij} a_{ik} = \frac{1}{3} \\
\sum_{ijk} b_i a_{ij} a_{jk} = \frac{1}{6}
\end{array}\right\} & \longrightarrow 3
\end{array}\right.$$

# Diagram.


$\sum_i b_i$ $\quad$ $f^i$




$\sum_{ij} b_i a_{ij}$ $\quad$ $\sum_j (Df)^i_j f^j$




$\sum_{ijk} b_i a_{ij} a_{ik}$ $\quad$ $\sum_{jk} (D^2 f)^i_{jk} f^j f^k$


$\sum_{ijk} b_i a_{ij} a_{jk}.$ $\quad$ $\sum_{jk} (Df)^i_j (Df)^j_k f^k$

Multivariable Taylor expansion.

$$f : \mathbb{R}^d \to \mathbb{R}.$$

$$f(\vec{x}) = f(\vec{x}_0) + \nabla f(\vec{x}_0)^T (\vec{x} - \vec{x}_0) + \frac{1}{2} (\vec{x} - \vec{x}_0)^T \nabla^2 f(\vec{x}_0)(\vec{x} - \vec{x}_0) + \dots$$

$$\nabla f(\vec{x}_0) = \left( \frac{\partial f}{\partial x_1}(\vec{x}_0), \cdots, \frac{\partial f}{\partial x_d}(\vec{x}_0) \right)^T$$ gradient

$$\nabla^2 f(\vec{x}_0) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2}(\vec{x}_0) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d}(\vec{x}_0) \\ & \vdots & \\ & & \frac{\partial^2 f}{\partial x_d^2}(\vec{x}_0) \end{pmatrix}$$ Hessian.

Component wise form.

$$f(\vec{x}) = f(\vec{x}_0) + \sum_{j=1}^{d} (Df)_j (\vec{x}_0) (\vec{x}-\vec{x}_0)_j$$

$$+ \frac{1}{2} \sum_{jk=1}^{d} (D^2 f)_{jk} (\vec{x}_0) \cdot (\vec{x}-\vec{x}_0)_j (\vec{x}-\vec{x}_0)_k$$

$$+ \frac{1}{6} \sum_{jkl=1}^{d} (D^3 f)_{jkl} (\vec{x}_0) (\vec{x}-\vec{x}_0)_j (\vec{x}-\vec{x}_0)_k (\vec{x}-\vec{x}_0)_l + \cdots$$

$$(Df)_j = (Df)_j \,, \quad (D^2 f)_{jk} = (D^2 f)_{jk}$$

$$(D^3 f)_{jkl} = \frac{\partial^3 f}{\partial x_j \partial x_k \partial x_l}$$

$$f : \mathbb{R}^d \to \mathbb{R}^d$$

$$f^i(\vec{x}) = f^i(\vec{x}_0) + \sum_j (Df)^i_j \, (\vec{x} - \vec{x}_0)_j$$

$$+ \frac{1}{2} \sum_{jk} (D^2 f)^i_{jk} \, (\vec{x} - \vec{x}_0)_j \, (\vec{x} - \vec{x}_0)_k + \cdots$$

$$(Df)^i_j = \frac{\partial f^i}{\partial x_j} \qquad (D^2 f)^i_{jk} = \frac{\partial^2 f^i}{\partial x_j \partial x_k}$$

Multivariable case ($\mathbb{R}^d$) 2nd order general RK.

$$\tau_n^p = hf^p + \frac{h^2}{2}\sum_q (Df)^p_q f^q$$

$$+ \frac{h^3}{6}\left[\sum_{qr} (D^2f)^p_{qr} f^q f^r + \sum_{qr} (Df)^p_q (Df)^q_r f^r\right]$$

$$- h\sum_i b_i \Big( f^p + h\sum_q (Df)^p_q \sum_j a_{ij} f^q$$

$$+ h^2 \sum_{qr} (Df)^p_q \sum_{jk} a_{ij} a_{jk} (Df)^q_r f^r$$

$$+ \frac{h^2}{2} \sum_{qr} (D^2f)^p_{qr} \sum_{jk} a_{ij} a_{ik} f^q f^r \Big] + O(h^4)$$

$$= h f^p \left(1 - \sum_i b_i\right) + \frac{h^2}{2}\left(\sum_q (Df)^p_q f^q\right)\left(\frac{1}{2} - \sum_{ij} b_i a_{ij}\right)$$

$$+ h^3\left(\sum_{qr} (Df)^p_q (Df)^q_r f^r\right)\left(\frac{1}{6} - \sum_{ijk} b_i a_{ij} a_{jk}\right)$$

$$+ \frac{h^3}{2}\left(\sum_{qr} (D^2 f)^p_{qr} f^q f^r\right)\left(\frac{1}{3} - \sum_{ijk} b_i a_{ij} a_{ik}\right) + O(h^4)$$

$p, q, r \longleftrightarrow i, j, k$.

Diagram.

rooted tree $\phi$

# derivatives on $f$ = # children of a vertex.

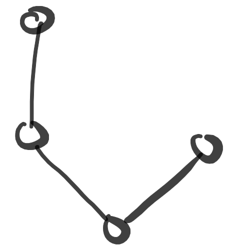
order of $\phi$ = # vertices.

$$\sum_i b_i \, \Phi_i(\phi) = \frac{1}{\gamma(\phi)}$$ $\leftarrow$ desired equality.

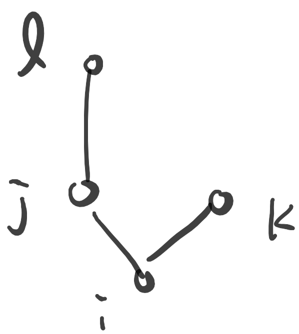
$\Phi_i(\phi)$ : sum of all non-rooted vertices of products of $a_{jk}$ corresponding to edges.

$\gamma(\phi)$ : integer. product of the order of $\phi$ and the order of all possible trees after successively removing roots.

Ex.

| $\phi$ |  |   |  |
|---|---|---|---|
| order | 4 | $2\cdot 1$ | 1 |

$$\gamma(\phi) = 4\cdot(2\cdot 1)\cdot 1 = 8$$




$$\sum_{ijkl} b_i\, a_{ij}\, a_{jl}\, a_{ik} = \frac{1}{8}$$

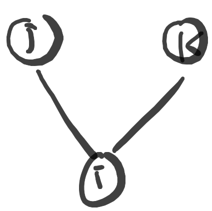
Thm. Assuming Kutta's condition. RK $r$-stage method is of order (at least) $p$ if

$$\sum_{i=1}^{r} b_i \, \Phi_i(\phi) = \frac{1}{\gamma(\phi)}, \quad \forall \phi \text{ of order} \le p.$$

Ref: [Hai] II.2. [Wil] pp 95-107.

Ex. 2-stage ERK.

$$\begin{array}{c|cc} & 0 & 0 \\ & a & 0 \\ \hline & b_1 & b_2 \end{array}$$

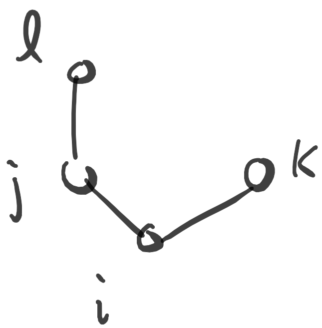
| tree | $\gamma$ | condition |
|---|---|---|
|  | 1 | $\sum_{i=1}^{2} b_i = b_1 + b_2 = 1$ |
|  | 2 | $\sum_{ij} b_i a_{ij} = b_2 a = \frac{1}{2}$ |
|  | 3 | $\sum_{ijk} b_i a_{ij} a_{ik} = b_2 a^2 = \frac{1}{3}$ |
|  | 6 | $\sum_{ijk} b_i a_{ij} a_{jk} = 0 \neq \frac{1}{6}$ |

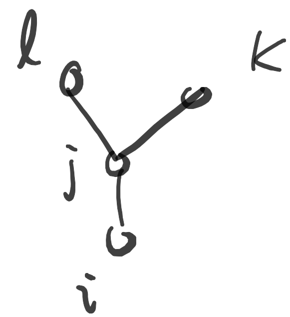
2nd order method.

# Butcher's theory of attainable orders

1. All RK of order $p \leq 4$ have the same order of accuracy independent of scalar/vector.

Ex.




vector $\displaystyle\sum_{jkl} (D^2 f)^i_{jk} (Df)^j_l f^k f^l$ $\qquad$ $\displaystyle\sum_{jkl} (Df)^i_j (D^2 f)^j_{lk} f^l f^k$

scalar $f_{uu} f_u f^2$ $\qquad$ $f_u f_{uu} f^2$

2. any $r$-stage ERK has order $p \le r$.

3. An ERK of order $p$ must have

$p+1$ stages if $p = 5, 6$

$p+2$ " " $p = 7$

$p+3$ " " $p > 7$.

Zero stability.

"Thm". RK methods always zero stable.

$\longrightarrow$ RK LTE $O(h^{p+1})$

$\Rightarrow$ converge w. $O(h^{p})$.