4 Runge-Kutta methods

The Euler method, as well as the improved and modified Euler methods are all examples on *explicit Runge-Kutta methods* (ERK). Such schemes are given by

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f(t_n + c_2 h, y_n + h a_{21} k_1), \\
k_3 &= f\big(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)\big), \\
&\vdots \\
k_s &= f\Big(t_n + c_s h, y_n + h \sum_{j=1}^{s-1} a_{sj} k_j\Big), \\
y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i k_i,
\end{aligned} \tag{7}$$

where c_i, a_{ij} and b_i are coefficients defining the method. We always require $c_i = \sum_{j=1}^{s} a_{ij}$. Here, s is the number of *stages*, or the number of function evaluations needed for each step. The vectors k_i are called stage derivatives. The improved Euler method is then a two-stage RK-method, written as

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f(t_n + h, y_n + h k_1), \\
y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2).
\end{aligned}$$

Also implicit methods, like the trapezoidal rule,

$$y_{n+1} = y_n + \frac{h}{2}\big(f(t_n, y_n) + f(t_n + h, y_{n+1})\big)$$

can be written in a similar form,

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f\Big(t_n + h, y_n + \frac{h}{2}(k_1 + k_2)\Big), \\
y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2).
\end{aligned}$$

But, contrary to what is the case for explicit methods, a nonlinear system of equations has to be solved to find k_2.

Definition 4.1. *An s-stage Runge-Kutta method is given by*

$$\begin{aligned}
k_i &= f\Big(t_n + c_i h, y_n + h \sum_{j=1}^{s} a_{ij} k_j\Big), \qquad i = 1, 2, \cdots, s, \\
y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i k_i.
\end{aligned}$$

The method is defined by its coefficients, which is given in a Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}, \qquad \text{where } c_i = \sum_{i=1}^{s} a_{ij}, \quad i = 1, \cdots, s.$$

The method is explicit *if* $a_{ij} = 0$ *whenever* $j \geq i$, *otherwise* implicit.

Example 4.2. *The Butcher-tableaux for the methods presented so far are*

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

Euler — *improved Euler* — *modified Euler* — *trapezoidal rule*

When the method is explicit, the zeros on and above the diagonal is usually ignored. We conclude this section by presenting the maybe most popular among the RK-methods over times, *The* 4th order Runge-Kutta method (Kutta – 1901):

$$\begin{aligned} k_1 &= f(t_n, y_n) \\ k_2 &= f(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}k_1) \\ k_3 &= f(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}k_2) \\ k_4 &= f(t_n + h, y_n + hk_3) \\ y_{n+1} &= y_n + \tfrac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{aligned} \qquad \text{or} \qquad \begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}. \tag{8}$$

4.1 Order conditions for Runge-Kutta methods.

The following theorem were proved in Exercise 2, task 2:

Theorem 4.3. *Let*

$$y' = f(t, y), \qquad y(t_0) = y_0, \qquad t_0 \leq t \leq t_{end}$$

be solved by a onestep method

$$y_{n+1} = y_n + h\Phi(t_n, y_n; h), \tag{9}$$

with stepsize $h = (t_{end} - t_0)/Nstep$. *If*

1. *the increment function* Φ *is Lipschitz in* y, *and*
2. *the local truncation error* $d_{n+1} = \mathcal{O}(h^{p+1})$,

then the method is of order p, *that is, the global error at* t_{end} *satisfies*

$$e_{Nstep} = y(t_{end}) - y_{Nstep} = \mathcal{O}(h^p).$$

A RK method is a onestep method with increment function $\Phi(t_n, y_n; h) = \sum_{i=1}^{s} b_i k_i$. It is possible to show that Φ is Lipschitz in y whenever f is Lipschitz and $h \leq h_{max}$, where h_{max} is some predefined maximal stepsize. What remains is the order of the local truncation error. To find it, we take the Taylor-expansions of the exact and the numerical solutions and compare. The local truncation error is $\mathcal{O}(h^{p+1})$ if the two series matches for all terms corresponding to h^q with $q \leq p$. In principle, this is trivial. In practice, it becomes extremely tedious (give it a try). Fortunately, it is possible to express the two series very elegant by the use of *B-series* and *rooted trees*. Here, we present how this is done, but not why it works. A complete description can be found in the note *the B-series tutorial.*

B-series and rooted trees

We assume that the equation is rewritten in autonomous form

$$y(t)' = f(y(t)), \qquad y(t_0) = y_0. \tag{10}$$

The Taylor expansion of the exact solution of (10) is given by

$$y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{h}{2}y''(t_0) + \cdots + \frac{h^p}{p!}y^{(p)}(t_0) + \cdots . \tag{11}$$

From the ODE (10) and repeated use of the chain rule, we get $y' = f$, $y'' = f_y f$, $y''' = f_{yy}ff + f_y f_y f$, etc. Each higher derivative of y is split into several terms, denoted as *elementary differentials.* These can be represented by rooted trees. A node $\bullet$ represents f. A branch out from a bullet represent the derivative of f with respect to y. As the chain rule apply, this will always means that we multiply by $y' = f$, represented by a new node on the end of the branch. We get the following table:

Elementary differentials

$y' = f$

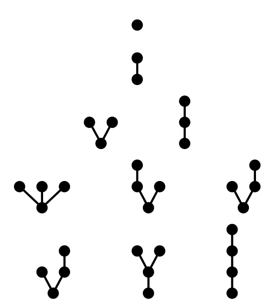
$y'' = f_y f$

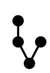
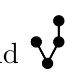
$y''' = f_{yy}ff + f_y f_y f$

$y^{iv} = f_{yyy}fff + f_{yy}f_y ff + f_{yy}ff_y f$

$+ f_{yy}ff_y f + f_y f_{yy}ff + f_y f_y f_y f$

corresponding trees

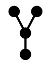


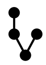
The elementary differentials corresponding to the trees  and  are equal, thus

$$y^{iv} = f_{yyy}fff + 3f_{yy}f_y ff + f_y f_{yy}ff + f_y f_y f_y f.$$

And we can go on like that. For each tree τ with p nodes we construct a set of total p new trees with $p+1$ nodes by adding one new node to an existing node in τ. This procedure might produce the same tree several times, and the total number of ways to construct a distinct tree is denoted by $\alpha(\tau)$. Let T be the set of all possible, distinct, rooted trees constructed this way, and let $\tau \in T$. A tree with p nodes corresponds to one of the terms in $y^{(p)}$, thus we call this *the order* of the tree and denote it $|\tau|$. The elementary differentials corresponding to a tree is denoted $F(\tau)(y)$.

Example 4.4.

For $\tau =$  *we have* $|\tau| = 4,$ $F(\tau)(y) = f_y f_{yy} f f,$ $\alpha(\tau) = 1.$

For $\tau =$  *we have* $|\tau| = 4,$ $F(\tau)(y) = f_{yy} f_y f f,$ $\alpha(\tau) = 3.$

Here, f *and its differentials are evaluated in* y*.*

Putting this together: If $y(t)$ is the solution of (10), then

$$y^{(p)}(t_n) = \sum_{\substack{\tau \in T \\ |\tau| = p}} \alpha(\tau) F(\tau)(y(t_n)).$$

Insert this into (11), and we can write the exact solution as a B-series:

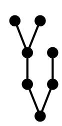
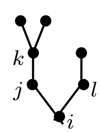
$$y(t_n + h) = y(t_n) + \sum_{\tau \in T} \frac{h^{|\tau|}}{|\tau|!} \alpha(\tau)\ F(\tau)(y(t_n)). \tag{12}$$

The numerical solution after one step can also be written as a B-series, but with some different coefficients

$$y_{n+1} = y_n + \sum_{\tau \in T} \frac{h^{|\tau|}}{|\tau|!} \gamma(\tau)\varphi(\tau)\ \alpha(\tau)\ F(\tau)(y_n). \tag{13}$$

where $\gamma(\tau)$ is an integer, and $\varphi(\tau)$ depends on the method coefficients, given in the Butcher tableau in Definition 4.1. Both can be found quite easily by the following procedure: Take a tree τ. Label the root with i, and all other non-terminal nodes by $j, k, l, \cdots$. The root correspond to b_i. A branch between a lower node j and an upper node k correspond to a_{jk}. A terminal node, connected to a node with label k corresponds to c_k. $\phi(\tau)$ is found by multiplying all these coefficients, and then take the sum over all the indices from 1 to s.

Example 4.5.

The tree $\tau =$  *can be labelled* 

so that $\varphi(\tau) = \sum_{i,j,k,l=1}^{s} b_i a_{ij} a_{jk} c_k^2 a_{il} c_l.$

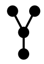
A tree τ can also be described by its subtrees. Let $\tau = [\tau_1, \tau_2, \cdots, \tau_l]$ be the tree composed by joining the root of the subtrees $\tau_1,\ \tau_2,\ \cdots,\ \tau_l$ to a joint new root. The term $\gamma(\tau)$ is defined recursively by

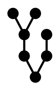
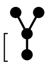
- $\gamma(\bullet) = 1.$
- $\gamma(\tau) = |\tau| \cdot \gamma(\tau_1) \cdots \gamma(\tau_l)$ for $\tau = [\tau_1, \tau_2, \cdots, \tau_l].$

Example 4.6.

$\tau =$  $= [\bullet]$, $\gamma(\tau) = 2 \cdot 1 = 2$

$\tau =$  $= [\bullet, \bullet]$, $\gamma(\tau) = 3 \cdot 1 \cdot 1 = 3$

$\tau =$  $=$ [], $\gamma(\tau) = 4 \cdot 3 = 12$

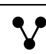
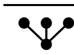
$\tau =$  $=$ [, ], $\gamma(\tau) = 7 \cdot 12 \cdot 2 = 168$

By comparing the two series (12) and (13) with $y(t_n) = y_n$ we can state the following theorem:

Theorem 4.7. *A Runge-Kutta method is of order p if and only if*

$$\varphi(\tau) = \frac{1}{\gamma(\tau)} \qquad \forall \tau \in T, \quad |\tau| \le p.$$

The order conditions up to order 4 are:

τ	$\lvert\tau\rvert$	$\varphi(\tau) = 1/\gamma(\tau)$
•	1	$\sum b_i = 1$
	2	$\sum b_i c_i = 1/2$
	3	$\sum b_i c_i^2 = 1/3$
		$\sum b_i a_{ij} c_j = 1/6$
	4	$\sum b_i c_i^3 = 1/4$
		$\sum b_i c_i a_{ij} c_j = 1/8$
		$\sum b_i a_{ij} c_j^2 = 1/12$
		$\sum b_i a_{ij} a_{jk} c_k = 1/24$