4.1 Order conditions for Runge-Kutta methods.

Theorem 4.2. *Let*

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

be solved by a one-step method

$$y_{n+1} = y_n + h\Phi(t_n, y_n; h), \tag{10}$$

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

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

The proof is left as an exercise.

A RK method is a one-step 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 practise, 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.*

B–series and rooted trees

B–series in different forms, and under different names, is essential the main tool for constructing order theory for time-dependent problems, like ODEs, DAEs and SDEs. In this note, with a B–series we mean a formal series of the form

$$B(\varphi, x_0; h) = x_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \varphi(\tau)(h) \cdot F(\tau)(\mathbf{x}_0). \tag{11}$$

Here, T is a set of rooted trees, $\bar{T} = T \backslash \emptyset$ where $\emptyset$ refer to the initial value term, $F(\tau)(x_0)$ the elementary differentials, $\varphi(\tau)(h)$ some integral, and $\alpha(\tau)$ is a symmetry factor. The idea is to express the solutions of the exact and the numerical solution after one step as B–series. For instance, consider the automomous ODE $y' = f(y), y(t_0) = y_0$, and let us solve this by the Euler method. Thus we have

$$\begin{aligned} B(e, y_0; h) &= y(t_0 + h) = y(t_0) + hf(y_0) + \frac{1}{2}h^2 f'f + \cdots \\ B(\phi, y_0; h) &= y_1 = y(t_0) + hf(y_0). \end{aligned}$$

So, if the these solution can be expressed as B–series, which we still have to prove, the first terms will be

τ	α	e	ϕ	F
	1	h	h	f .
	1	$\frac{1}{2}h^2$	0	$f'f$

But at the moment, we do not know how the rest of the terms looks like.

Before a more formal derivation of the series, let present a few definitions and results:

Definition 4.3. *Let* $y = [y_1, y_2, \cdots, y_m]^T \in \mathbb{R}^m$ *and* $f(y) = [f_1(y), f_2(y), \cdots, f_m(y)]^T \in \mathbb{R}^m$. *The* κ*'th Frechet derivative of* f*, denoted by* $f^{(\kappa)}(y)$ *is a* κ*-linear operator* $\mathbb{R}^m \times \mathbb{R}^m \times \cdots \times \mathbb{R}^m$ *(*κ *times)* $\to \mathbb{R}^m$*. Evaluation of component* i *of this operator working on the* m *operands* $v_1, v_2, \cdots v_\kappa \in \mathbb{R}^m$ *is given by*

$$\left[f^{(\kappa)}(y)(v_1, v_2, \cdots, v_\kappa)\right]_i = \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \cdots \sum_{j_\kappa=1}^{m} \frac{\partial^\kappa f_i(y)}{\partial y_{j_1} \partial y_{j_2} \cdots \partial y_{j_\kappa}} v_{1,j_1} v_{2,j_2} \cdots v_{\kappa,j_\kappa}$$

where $v_l = [v_{l,1}, v_{l,2}, \cdots v_{l,m}] \in \mathbb{R}^m$ *for* $l = 1, 2, \cdots, \kappa$.

Note that the κ'th Frechet derivative is independent of permutations of its operands, thus e.g. $f'''(y)(v_1, v_2, v_3) = f'''(y)(v_3, v_1, v_2)$.

The multivariable Taylor expansion is, for $y, v \in \mathbb{R}^m$:

$$f(y + v) = f(y) + \sum_{\kappa=1}^{\infty} \frac{1}{\kappa!} f^{(\kappa)}(y)(v, v, \ldots, v) = \sum_{\kappa=1}^{\infty} \frac{1}{\kappa!} f^{(\kappa)}(y)(v^\kappa), \tag{12}$$

the expression to the right is only a convenient way to write the expression in the middle.

Finally, the multinomial theorem states:

$$(v_1 + v_2 + \ldots + v_q)^\kappa = \sum_{r_1+\cdots+r_q=\kappa} \frac{\kappa!}{r_1! \cdots r_q!} v_1^{r_1} \cdots v_q^{r_q}$$

A similar argument applied to the Frechet derivative gives

$$f^{(\kappa)}(y)(a_1 v_1 + a_2 v_2 + \ldots + a_q v_q)^\kappa = \sum_{r_1+\cdots+r_q=\kappa} \frac{\kappa!}{r_1! \cdots r_q!} \cdot \prod_{k=1}^{\kappa} a_k \cdot f^{(\kappa)}(y)(v_1^{r_1}, \ldots, v_q^{r_q}) \tag{13}$$

where $\alpha_k \in \mathbb{R}$ and $v_k \in \mathbb{R}^m$.

A *list* of trees, denoted by $\{\tau_1, \tau_2, \cdots, \tau_\kappa\}$, $\tau_i \in T$, $i = 1, \cdots, \kappa$ is an ordered set of trees, where each tree might appear more than once. If $\tau_1, \tau_2 \in T$ then $\{\tau_1, \tau_2, \tau_1\}$ and $\{\tau_2, \tau_1, \tau_1\}$ are two different lists. If a tree appear k times in the list, the tree has multiplicity k. A *multiset* of trees, denoted by $(\tau_1, \tau_2, \cdots, \tau_\kappa)$ is a set of trees where multiplicity is allowed and order does not matter. So $(\tau_1, \tau_2, \tau_1) = (\tau_2, \tau_1, \tau_1)$. A tree with multiplicity k will sometimes be denoted by τ^k, so $(\tau_1, \tau_2, \tau_1) = (\tau_1^2, \tau_2)$. The set of all possible lists of trees is denoted $\tilde{U}$, and the set of all possible multisets is denoted U:

$$\begin{aligned} \tilde{U} &= \{\{\tau_1, \tau_2, \cdots, \tau_\kappa\} : \tau_i \in T, \quad i = 1, \cdots, \kappa, \quad \kappa = 0, 1, 2, \cdots\}, \\ U &= \{(\tau_1, \tau_2, \cdots, \tau_\kappa) : \tau_i \in T, \quad i = 1, \cdots, \kappa, \quad \kappa = 0, 1, 2, \cdots\}. \end{aligned}$$

In the lemma below, U_f is the set of trees formed by taking a multiset from U and include a root f.

Lemma 4.1. *If $X(h) = B(\phi, x_0; h)$ is some B-series and $f \in C^\infty(\mathbb{R}^m, \mathbb{R}^m)$ then $f(X(h))$ can be written as a formal series of the form*

$$f(X(h)) = \sum_{u \in U_f} \beta(u) \cdot \psi_\phi(u)(h) \cdot G(u)(x_0) \tag{14}$$

where U_f is a set of trees derived from T, by

a) $[\emptyset]_f \in U_f$*, and if* $\tau_1, \tau_2, \cdots, \tau_\kappa \in T$ *then* $[\tau_1, \tau_2, \cdots, \tau_\kappa]_f \in U_f$.

b) $G([\emptyset]_f)(x_0) = f(x_0)$ *and*
$G(u = [\tau_1, \cdots, \tau_\kappa]_f)(x_0) = f^{(\kappa)}(x_0)\big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\big)$.

c) $\beta([\emptyset]_f) = 1$ *and* $\beta(u = [\tau_1, \cdots, \tau_\kappa]_f) = \dfrac{1}{r_1! r_2! \cdots r_q!} \prod_{k=1}^{\kappa} \alpha(\tau_k)$,
where $r_1, r_2, \cdots, r_q$ *count equal trees among* $\tau_1, \tau_2, \cdots, \tau_\kappa$.

d) $\psi_\phi([\emptyset]_f)(h) \equiv 1$ *and* $\psi_\phi(u = [\tau_1, \cdots, \tau_\kappa]_f)(h) = \prod_{k=1}^{\kappa} \phi(\tau_k)(h)$.

Proof. Writing $X(h)$ as a B-series, we have

$$\begin{aligned} f(X(h)) &= f\left(x_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(x_0)\right) \\ &\overset{(12)}{=} \sum_{\kappa=0}^{\infty} \frac{1}{\kappa!} f^{(\kappa)}(x_0) \left(\sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(x_0)\right)^{\kappa} \\ &\overset{(13)}{=} f(x_0) + \sum_{\kappa=1}^{\infty} \frac{1}{\kappa!} \sum_{(\tau_1, \tau_2, \cdots \tau_\kappa) \in U} \frac{\kappa!}{r_1! r_2! \cdots r_q!} \\ &\cdot \left(\prod_{k=1}^{\kappa} \alpha(\tau_k) \cdot \phi(\tau_k)(h)\right) f^{(\kappa)}(x_0)\big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\big). \end{aligned}$$

The number above the equal sign refer to the equation used. The last sum is taken over all possible unordered combinations of κ trees in T. For each set of trees $\tau_1, \tau_2, \cdots, \tau_\kappa \in T$ we assign a $u = [\tau_1, \tau_2, \cdots, \tau_\kappa]_f \in U_f$. The theorem is now proved by comparing term by term with (14). □

To find the B–series of the exact solution, write the ODE in integral form:

$$y(t_0 + h) = y_0 + \int_0^h f(y(t_0 + s))ds. \tag{15}$$

Assume that the exact solution can be written as a B-series

$$y(t_0 + h) = B(e, y_0; h). \tag{16}$$

Plug this into (15), apply Theorem 4.1 to get

$$y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot e(\tau)(h) \cdot F(\tau)(y_0) = y_0 + \sum_{u \in U_f} \beta(u) \cdot \int_0^h \psi_e(u)(s)ds \cdot G(u)(y_0).$$

For each term on the left hand side, there has to be a corresponding term on the right. Or for each $\tau = [\tau_1, \ldots, \tau_\kappa] \in T$ there is a corresponding $u = [\tau_1, \ldots, \tau_\kappa]_f \in U_f$, and $\alpha(\tau) = \beta(u)$, $F(\tau)(y_0) = G(u)(y_0)$ and finally $e(\tau)(h) = \int_0^h \psi_e(s)ds$.

This gives us the following theorem:

Theorem 4.4. *The exact solution of* (4) *can be written as a formal series of the form* (16) *with*

i) $\emptyset \in T$, $\bullet = [\emptyset] \in T$, *and if* $\tau_1, \ldots, \tau_\kappa \in T$ *then* $\tau = [\tau_1, \ldots, \tau_\kappa] \in T$.
ii) $F(\emptyset)(y_0) = y_0$, $F(\bullet) = f(y_0)$, *and* $F(\tau)(y_0) = f^{(\kappa)}(y_0)\big(F(\tau_1)(y_0), \ldots, F(\tau_\kappa)(y_0)\big)$.
iii) $\alpha(\emptyset) = 1$, $\alpha(\bullet) = 1$ *and* $\alpha(\tau) = \frac{1}{r_1! r_2! \cdots r_q!} \prod_{k=1}^{\kappa} \alpha(\tau_k)$, *where* $r_1, \ldots, r_q$ *counts equal trees among the subtrees* $\tau_1, \ldots, \tau_\kappa$.
iv) $e(\emptyset)(h) = 1$, $e(\bullet)(h) = h$ *and* $e(\tau)(h) = \int_0^h \prod_{k=1}^{\kappa} e(\tau_k)(s)ds$.

Notice that $e(\tau)(h) = \frac{1}{\gamma(\tau)} h^{\rho(\tau)}$, where $\gamma(\tau)$ is an integer and $\rho(\tau)$ is the number of nodes. This is called *the order* of the tree τ.

To find the B–series of the numerical solution, write one stop of the RK–method in the form

$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(Y_j), \qquad i = 1, \ldots, s \tag{17}$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i f(Y_j). \tag{18}$$

and assume that both the stage values Y_i and the numerical solutions can be written as

$$Y_i = B(\phi_i, y_0; h), \qquad i = 1, \ldots, s, \quad \text{and} \quad y_1 = B(\phi, y_0; h).$$

It is straighforward to see that $\phi_i(\emptyset)(h) = \phi(\emptyset)(h) = 1$ and

$$\phi_i(\bullet) = \sum_{j=1}^{s} a_{ij} h = c_i h, \qquad \phi(\bullet)(h) = \sum_{i=1}^{s} b_i h.$$

For a general tree $\tau \in T$, insert the B–series for Y_i and y_1 into (18), apply Lemma 4.1 and compare equal terms. This results in the following reccurence formula for the weight functions $\phi_i(\tau)$ and $\phi(\tau)$ for a given $\tau = [\tau_1, \ldots, \tau_\kappa]$:

$$\phi_i(\tau)(h) = \sum_{j=1}^{s} a_{ij} \prod_{k=1}^{\kappa} \phi_j(\tau_k)(h), \qquad \phi(\tau)(h) = \sum_{i=1}^{s} b_i \prod_{k=1}^{\kappa} \phi_i(\tau_k)(h) \tag{19}$$

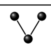
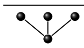
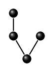
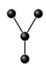
Notice again that $\phi(\tau)(h) = \hat{\phi}(\tau) \cdot h^{\rho(\tau)}$, where $\hat{\phi}(\tau)$ is a constant depending of the method coefficients. Similar, we can write $\phi_i(\tau)(h) = \hat{\phi}_i(\tau) \cdot h^{\rho(\tau)}$.

Comparing the series for the exact and the numerical solutions and applying Theorem 4.2 gives the following fundamental theorem:

Theorem 4.5. *A Runge-Kutta method is of order p if and only if*

$$\hat{\phi}(\tau) = \frac{1}{\gamma(\tau)}, \qquad \forall \tau \in T, \quad \rho(\tau) \leq p.$$

All trees up to and including order 4 and their corresponding terms are listed below:

τ	$\rho(\tau)$	$\hat{\phi}(\tau) = 1/\gamma(\tau)$
	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	$\sum b_i c_i^3 = 1/4$
		$\sum b_i c_i a_{ij} c_j = 1/8$
		$\sum b_i a_{ij} c_j^2 = 1/12$
		$\sum b_i a_{ij} a_{jk} c_k = 1/24$