

Remark 2.6. Simplifying order conditions. The order conditions for an implicit Runge–Kutta scheme with s stages are the same as given in Theorems 1.26, 1.27, and Remark 1.28. These conditions lead to a nonlinear system of equations for computing the parameters of the scheme. These computations are generally quite complicated.

A useful tool for solving this problem are the so-called simplifying order conditions, introduced in Butcher (1964):

$$\begin{aligned} B(p) : \sum_{i=1}^s b_i c_i^{k-1} &= \frac{1}{k}, \quad k = 1, \dots, p, \\ C(l) : \sum_{j=1}^s a_{ij} c_j^{k-1} &= \frac{1}{k} c_i^k, \quad i = 1, \dots, s, \quad k = 1, \dots, l, \\ D(m) : \sum_{i=1}^s b_i c_i^{k-1} a_{ij} &= \frac{1}{k} b_j (1 - c_j^k), \quad j = 1, \dots, s, \quad k = 1, \dots, m, \end{aligned}$$

with $0^0 = 1$.

One can show that for sufficiently large values l and m , the conditions $C(l)$ and $D(m)$ can be reduced to $B(p)$ with appropriate p . \square

Remark 2.7. Interpretation of $B(p)$ and $C(l)$. Consider the initial value problem

$$y'(x) = f(x), \quad y(x_0) = 0.$$

With the fundamental theorem of differential calculus, one sees that this problem has the solution

$$y(x_0 + h) = \int_{x_0}^{x_0+h} f(\xi) d\xi = h \int_0^1 f(x_0 + h\theta) d\theta.$$

A Runge–Kutta method with s stages gives

$$y_1 = h \sum_{i=1}^s b_i f(x_0 + c_i h).$$

Consider in particular the case that $f(x)$ is a polynomial $f(x) = (x - x_0)^{k-1}$, $k \in \mathbb{N} \setminus \{0\}$. Then, the analytical solution has the form

$$y(x_0 + h) = h \int_0^1 (h\theta)^{k-1} d\theta = \frac{(h\theta)^k}{k} \Big|_{\theta=0}^{\theta=1} = \frac{h^k}{k}. \quad (2.2)$$

The Runge–Kutta scheme yields

$$y_1 = h \sum_{i=1}^s b_i (c_i h)^{k-1} = h^k \sum_{i=1}^s b_i c_i^{k-1}. \quad (2.3)$$

Comparing (2.2) and (2.3), one can observe that condition $B(p)$ means that the quadrature rule that is the basis of the Runge–Kutta method is exact for polynomials of degree $(p - 1)$.

Condition $C(1)$ is (1.13) with the upper limit s

$$c_i = \sum_{j=1}^s a_{ij}, \quad i = 1, \dots, s. \quad (2.4)$$

\square

Example 2.8. Classes of implicit Runge–Kutta schemes.

- *Gauss–Legendre schemes.* The nodes of the Gauss–Legendre quadrature are used. A method with s stages possesses the maximal possible order $2s$, where all nodes are in the interior of the intervals. To get the optimal order, one has to show that $B(2s)$, $C(s)$, $D(s)$ are satisfied, see (Strehmel *et al.*, 2012, Section 8.1.2), i.e.,

$$\begin{aligned} \sum_{i=1}^s b_i c_i^{k-1} &= \frac{1}{k}, \quad k = 1, \dots, 2s, \\ \sum_{j=1}^s a_{ij} c_j^{k-1} &= \frac{1}{k} c_i^k, \quad i = 1, \dots, s, \quad k = 1, \dots, s, \\ \sum_{i=1}^s b_i c_i^{k-1} a_{ij} &= \frac{1}{k} b_j (1 - c_j^k), \quad j = 1, \dots, s, \quad k = 1, \dots, s. \end{aligned} \tag{2.5}$$

An example is the implicit mid point rule, whose coefficients can be derived by setting $s = 1$ in (2.5). One obtains the following conditions

$$b_1 = 1, \quad b_1 c_1 = \frac{1}{2}, \quad a_{11} = c_1, \quad b_1 a_{11} = b_1 (1 - c_1).$$

Consequently, the implicit mid point rule is given by

$$\frac{1/2 \mid 1/2}{\mid 1}.$$

- *Gauss–Radau¹ methods.* These methods are characterized by the feature that one of the end points of the interval $[x_k, x_{k+1}]$ belongs to the nodes. A method of this class with s stages has at most order $2s - 1$. Examples ($s = 1$):

- $\frac{0 \mid 1}{\mid 1}$ $s = 1, p = 1$,
- $\frac{1 \mid 1}{\mid 1}$ $s = 1, p = 1$, implicit Euler scheme.

The first scheme does not satisfy condition (2.4).

- *Gauss–Lobatto² methods.* In these methods, both end points of the interval $[x_k, x_{k+1}]$ are nodes. A method of this kind with s stages cannot be of higher order than $(2s - 2)$.

Examples:

- trapezoidal rule, Crank³–Nicolson⁴ scheme

$$\frac{0 \mid 0 \quad 0}{1 \mid 1/2 \quad 1/2} \quad s = p = 2.$$

- other scheme

¹ Rodolphe Radau (1835 – 1911)

² Rehuel Lobatto (1797 – 1866)

³ John Crank (1916 – 2006)

⁴ Phyllis Nicolson (1917 – 1968)

$$\begin{array}{c|cc} 0 & 1/2 & 0 \\ 1 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \quad s = 2, \quad p = 2.$$

The second scheme does not satisfy condition (2.4). □

Remark 2.9. Diagonally implicit Runge–Kutta methods (DIRK methods). For an implicit Runge–Kutta method with s stages and a full matrix A , one has to solve a coupled nonlinear system for the increments $K_1(x, y), \dots, K_s(x, y)$. This step is expensive for a large number of stages s . A compromise is the use of so-called diagonally implicit Runge–Kutta (DIRK) methods

$$\begin{array}{c|cccc} c_1 & a_{11} & 0 & 0 & \cdots & 0 \\ c_2 & a_{21} & a_{22} & 0 & \cdots & 0 \\ c_3 & a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & a_{s2} & \cdots & & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

In DIRK methods, one has to solve s independent nonlinear equations for the increments. In the equation for $K_i(x, y)$, only the stages $K_1(x, y), \dots, K_i(x, y)$ appear, where $K_1(x, y), \dots, K_{i-1}(x, y)$ were already computed. □

2.3 Linear Stability Theory

Remark 2.10. On the stability theory. The stability theory studies numerical methods for solving the linear initial value problem

$$y'(x) = \lambda y(x), \quad y(0) = 1, \quad \lambda \in \mathbb{C}. \quad (2.6)$$

It will turn out the even at the simple initial value problem (2.6) the most important stability properties of numerical methods can be explored. The solution of (2.6) is

$$y(x) = e^{\lambda x}.$$

If the initial condition will be slightly perturbed to be $1 + \delta_0$, then the solution of the perturbed initial value problem is

$$\tilde{y}(x) = (1 + \delta_0)e^{\lambda x} = e^{\lambda x} + \delta_0 e^{\lambda x}.$$

If $\lambda = a + ib$ with $a = \operatorname{Re}(\lambda) > 0$, then the difference

$$|y(x) - \tilde{y}(x)| = \left| \delta_0 e^{\lambda x} \right| = |\delta_0| |e^{ax}| |e^{ibx}| = |\delta_0| |e^{ax}|$$

becomes for each $\delta_0 \neq 0$ arbitrarily large if x is sufficiently large. That means, the initial value problem (2.6) is not stable in this case. In this situation, one cannot expect that any numerical method is stable. Hence, this situation is not of interest for numerical simulations.

In contrast, if $\operatorname{Re}(\lambda) < 0$, then the difference $|y(x) - \tilde{y}(x)|$ becomes arbitrarily small and the initial value problem is stable, i.e., small changes of the data result only in small changes of the solution. For $\operatorname{Re}(\lambda) = 0$, the difference $|y(x) - \tilde{y}(x)|$ is at least bounded. These cases, in particular the first one, are of interest for the stability theory of methods for solving ordinary differential equations.

This section considers one-step methods with equidistant meshes with step size h . The solution of (2.6) in the node $x_{k+1} = (k + 1)h$ is

$$y(x_{k+1}) = e^{\lambda x_{k+1}} = e^{\lambda(x_k+h)} = e^{\lambda h} e^{\lambda x_k} = e^{\lambda h} y(x_k) =: e^z y(x_k),$$

with $z := \lambda h \in \mathbb{C}$, $\operatorname{Re}(z) \leq 0$. Now, it will be studied how the step from x_k to x_{k+1} looks like for different one-step methods. In particular, large steps are of interest, i.e., $|z| \rightarrow \infty$. \square

Example 2.11. Behavior of different one-step methods for one step of the model problem (2.6).

1. *Explicit Euler method.* The general form of this method is

$$y_{k+1} = y_k + hf(x_k, y_k).$$

In particular, one obtains for (2.6)

$$y_{k+1} = y_k + h\lambda y_k = (1+z)y_k =: R(z)y_k.$$

It holds, independently of $\operatorname{Re}(z)$, that $\lim_{|z| \rightarrow \infty} |R(z)| = \infty$.

2. *Implicit Euler method.* This method has the form

$$y_{k+1} = y_k + hf(x_{k+1}, y_{k+1}).$$

For applying it to (2.6), one can rewrite it as follows

$$\begin{aligned} y_{k+1} &= y_k + h\lambda y_{k+1} && \iff \\ (1-z)y_{k+1} &= y_k && \iff \\ y_{k+1} &= \frac{1}{1-z}y_k = \left(1 + \frac{z}{1-z}\right)y_k =: R(z)y_k. \end{aligned}$$

For this method, one has, independently of $\operatorname{Re}(z)$, that $\lim_{|z| \rightarrow \infty} |R(z)| = 0$.

3. *Trapezoidal rule.* The general form of this method is

$$y_{k+1} = y_k + \frac{h}{2}(f(x_k, y_k) + f(x_{k+1}, y_{k+1})),$$

which can be derived from the Butcher tableau given in Example 2.8. For the linear differential equation (2.6), one gets

$$\begin{aligned} y_{k+1} &= y_k + \frac{h}{2}(\lambda y_k + \lambda y_{k+1}) && \iff \\ \left(1 - \frac{z}{2}\right)y_{k+1} &= \left(1 + \frac{z}{2}\right)y_k && \iff \\ y_{k+1} &= \frac{1+z/2}{1-z/2}y_k = \left(1 + \frac{z}{1-z/2}\right)y_k =: R(z)y_k. \end{aligned}$$

Let $z = 2r(\cos(\phi) + i\sin(\phi))$. Inserting this expression gives

$$\begin{aligned} \lim_{|z| \rightarrow \infty} \left| \frac{1+z/2}{1-z/2} \right| &= \lim_{r \rightarrow \infty} \left| \frac{1+r(\cos(\phi) + i\sin(\phi))}{1-r(\cos(\phi) + i\sin(\phi))} \right| \\ &= \lim_{r \rightarrow \infty} \left| \frac{1/r + (\cos(\phi) + i\sin(\phi))}{1/r - (\cos(\phi) + i\sin(\phi))} \right| \\ &= \frac{|(\cos(\phi) + i\sin(\phi))|}{|-(\cos(\phi) + i\sin(\phi))|} = \frac{1}{1} = 1. \end{aligned}$$

Hence, one has that $\lim_{|z| \rightarrow \infty} |R(z)| = 1$ for the trapezoidal rule, independently of ϕ , and with that independently of $\operatorname{Re}(z)$.

The function $R(z)$ describes for each method the step from x_k to x_{k+1} . Thus, this function is an approximation of e^z , which has for different methods different properties, e.g., the limit for $|z| \rightarrow \infty$. \square

Definition 2.12. Stability function. Let $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^s$, $\hat{\mathbb{C}} = \mathbb{C} \cup \infty$, where ∞ has to be understood as in function theory (Riemann sphere), and consider a Runge–Kutta method with s stages and with the parameters $(A, \mathbf{b}, \mathbf{c})$. Then, the function

$$R : \hat{\mathbb{C}} \rightarrow \hat{\mathbb{C}}, \quad z \mapsto 1 + z\mathbf{b}^T(I - zA)^{-1}\mathbf{1} \quad (2.7)$$

is called stability function of the Runge–Kutta method. \square

Remark 2.13. Stability functions from Example 2.11. All stability functions from Example 2.11 can be written in the form (2.7). One obtains, e.g., for the trapezoidal rule

$$\mathbf{b} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}, \quad I - zA = \begin{pmatrix} 1 & 0 \\ -\frac{z}{2} & 1 - \frac{z}{2} \end{pmatrix}, \quad (I - zA)^{-1} = \frac{1}{1 - \frac{z}{2}} \begin{pmatrix} 1 - \frac{z}{2} & 0 \\ \frac{z}{2} & 1 \end{pmatrix},$$

from what follows that

$$1 + z\mathbf{b}^T(I - zA)^{-1}\mathbf{1} = 1 + \frac{z}{1 - z/2} \left(\frac{1}{2} - \frac{z}{4} + \frac{z}{4} + \frac{1}{2} \right) = 1 + \frac{z}{1 - z/2}.$$

\square

Theorem 2.14. Form of the stability function of Runge–Kutta methods. *Given a Runge–Kutta scheme with s stages and with the parameters $(A, \mathbf{b}, \mathbf{c})$, then the stability function $R(z)$ is a rational function defined on $\hat{\mathbb{C}}$, whose polynomial order in the numerator and in the denominator is at most s . The poles of this functions might be only at values that correspond to the inverse of an eigenvalue of A . For an explicit Runge–Kutta scheme, $R(z)$ is a polynomial.*

Proof. Consider first an explicit Runge–Kutta scheme. In this case, the matrix A is a strictly lower triangular matrix. Hence, $I - zA$ is a triangular matrix with the values one at its main diagonal. This matrix is invertible and it is

$$(I - zA)^{-1} = I + zA + \dots + z^{s-1}A^{s-1}, \quad (2.8)$$

which can be checked easily by multiplication with $(I - zA)$ and using that $A^s = 0$ since A is strictly lower triangular. It follows from (2.7) and (2.8) that $R(z)$ is a polynomial in z of degree at most s .

Now, the general case will be considered. The expression $(I - zA)^{-1}\mathbf{1}$ can be interpreted as the solution of the linear system of equations $(I - zA)\underline{\zeta} = \mathbf{1}$. Using the Cramer rule, one finds that the i -th component of the solution has the form

$$\zeta_i = \frac{\det A_i}{\det(I - zA)},$$

where A_i is the matrix that is obtained by replacing the i -th column of $(I - zA)$ by the right-hand side, i.e., by $\mathbf{1}$. The numerator of ζ_i is a polynomial in z of order at most $(s - 1)$ since there is one column where z does not appear. The denominator is a polynomial of degree at most s . Multiplying with $z\mathbf{b}^T$ from the left-hand side gives just a rational function with polynomials of at most degree s both in the numerator and in the denominator.

There is only one case where this approach does not work, namely if

$$\det(I - zA) = \det(z(I/z - A)) = z^s \det(I/z - A) = 0,$$

i.e., if $1/z$ is an eigenvalue of A . \blacksquare

Theorem 2.15. Solution of the initial value problem (2.6) obtained with a Runge–Kutta scheme. *Consider a Runge–Kutta method with s stages and with the parameters $(A, \mathbf{b}, \mathbf{c})$. If $z^{-1} = (\lambda h)^{-1}$ is not an eigenvalue of A , then the Runge–Kutta scheme is well-defined for the initial value problem (2.6). In this case, it is*

$$y_k = (R(h\lambda))^k, \quad k = 0, 1, 2, \dots$$

Proof. The statement of the theorem follows directly if one writes the Runge–Kutta scheme for (2.6) and applies induction. \blacksquare
exercise