

$$(I - ahJ) \mathbf{K}_2 = \mathbf{f} \left( \mathbf{y}_k + \frac{1}{2} h \mathbf{K}_1 \right) - ahJ \mathbf{K}_1, \quad (2.16)$$

$$\mathbf{y}_{k+1} = \mathbf{y}_k + h \mathbf{K}_2.$$

From the equation for the second increment, it follows that  $d_{21} = a$ . Then, one obtains with (2.15)  $a_{21} = 1/2 - d_{21} = 1/2 - a$ . Using the condition that the nodes are the sums of the rows of the matrix, it follows that the corresponding Butcher tableau looks like

$$\begin{array}{c|c} a & a \\ \hline 1/2 & 1/2 - a \quad a \\ \hline & 0 \quad 1 \end{array}$$

□

**Theorem 2.38. Consistency order of ode23s.** *The Rosenbrock method ode23s is of second order consistent if  $h \in (0, 1/(2a \|J\|_2))$ .*

*Proof.* Let  $h \in (0, 1/(2a \|J\|_2))$ , where  $\|\cdot\|_2$  denotes the spectral norm of  $J$ , which is induced by the Euclidean vector norm  $\|\cdot\|_2$ . It can be shown, see class Computer Mathematics, that the matrix  $(I - ahJ)$  is invertible if  $\|ahJ\|_2 < 1$ . This condition is satisfied for the choice of  $h$  from above.

Let  $\mathbf{K}$  be the solution of

$$(I - ahJ) \mathbf{K} = \mathbf{f}. \quad (2.17)$$

Then, one obtains with the triangle inequality, with the compatibility of the Euclidean vector norm and the spectral matrix norm, and with the choice of  $h$  that

$$\begin{aligned} \|(I - ahJ) \mathbf{K}\|_2 &\geq \|\mathbf{K}\|_2 - ah \|J \mathbf{K}\|_2 \geq \|\mathbf{K}\|_2 - ah \|J\|_2 \|\mathbf{K}\|_2 \\ &\geq \|\mathbf{K}\|_2 - \frac{a \|J\|_2}{2a \|J\|_2} \|\mathbf{K}\|_2 = \frac{1}{2} \|\mathbf{K}\|_2. \end{aligned}$$

It follows with (2.17) that

$$\frac{1}{2} \|\mathbf{K}\|_2 \leq \|(I - ahJ) \mathbf{K}\|_2 = \|\mathbf{f}\|_2 \implies \|\mathbf{K}\|_2 \leq 2 \|\mathbf{f}\|_2. \quad (2.18)$$

Thus, the solution of the linear system of equations is bounded by the right-hand side, independently of  $h$ . This result will be applied to (2.16). For  $\mathbf{K}_1$ , the right-hand side does not depend on  $h$ . Also the right-hand side of  $\mathbf{K}_2$  does not depend on negative powers of  $h$ , e.g., using the step length restriction, one obtains also for  $\mathbf{K}_2$  a bound that is independent of negative powers of  $h$

$$\begin{aligned} \left\| \mathbf{f} \left( \mathbf{y}_k + \frac{1}{2} h \mathbf{K}_1 \right) - ahJ \mathbf{K}_1 \right\|_2 &\leq \left\| \mathbf{f} \left( \mathbf{y}_k + \frac{1}{2} h \mathbf{K}_1 \right) \right\|_2 + ah \|J\|_2 \|\mathbf{K}_1\|_2 \\ &\leq \left\| \mathbf{f} \left( \mathbf{y}_k + \frac{1}{2} h \mathbf{K}_1 \right) \right\|_2 + \frac{1}{2} \|\mathbf{K}_1\|_2, \end{aligned}$$

and the first term on the right-hand side can be further estimated as in (2.20) below.

One obtains for the first increment of **ode23s** by recursive insertion, using (2.16),

$$\begin{aligned} \mathbf{K}_1 &= \mathbf{f}(\mathbf{y}_k) + ahJ \mathbf{K}_1 = \mathbf{f}(\mathbf{y}_k) + ahJ (\mathbf{f}(\mathbf{y}_k) + ahJ \mathbf{K}_1) \\ &= \mathbf{f}(\mathbf{y}_k) + ahJ \mathbf{f}(\mathbf{y}_k) + h^2 a^2 J^2 \mathbf{K}_1 \\ &= \mathbf{f}(\mathbf{y}_k) + ahJ \mathbf{f}(\mathbf{y}_k) + \mathcal{O}(h^2). \end{aligned} \quad (2.19)$$

The last step is allowed since  $\mathbf{K}_1$  is bounded by the data of the problem (the right-hand side  $\mathbf{f}(\mathbf{y}_k)$ ) independently of  $h$ , see (2.18) where the constant in the estimate is 2. Using a Taylor series expansion and considering only first order terms explicitly, one obtains in a similar way for the second increment of **ode23s**

$$\begin{aligned} \mathbf{K}_2 &= \mathbf{f} \left( \mathbf{y}_k + \frac{1}{2} h \mathbf{K}_1 \right) - ahJ \mathbf{K}_1 + ahJ \mathbf{K}_2 \\ &= \mathbf{f}(\mathbf{y}_k) + \frac{1}{2} h \partial_{\mathbf{y}} \mathbf{f}(\mathbf{y}_k) \mathbf{K}_1 - ahJ \mathbf{K}_1 + ahJ \mathbf{K}_2 + \mathcal{O}(h^2) \\ &\stackrel{(2.19)}{=} \mathbf{f}(\mathbf{y}_k) + \frac{1}{2} h \partial_{\mathbf{y}} \mathbf{f}(\mathbf{y}_k) \mathbf{f}(\mathbf{y}_k) - ahJ \mathbf{f}(\mathbf{y}_k) + ahJ \mathbf{K}_2 + \mathcal{O}(h^2) \end{aligned} \quad (2.20)$$

$$\begin{aligned}
&\stackrel{(2.20)}{=} \mathbf{f}(\mathbf{y}_k) + \frac{1}{2}h\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)\mathbf{f}(\mathbf{y}_k) - ahJ\mathbf{f}(\mathbf{y}_k) + ahJ\mathbf{f}(\mathbf{y}_k) + \mathcal{O}(h^2) \\
&= \mathbf{f}(\mathbf{y}_k) + \frac{1}{2}h\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)\mathbf{f}(\mathbf{y}_k) + \mathcal{O}(h^2).
\end{aligned}$$

Inserting these results in (2.16) gives for one step of `ode23s`

$$\mathbf{y}_{k+1} = \mathbf{y}_k + h\mathbf{f}(\mathbf{y}_k) + \frac{1}{2}h^2\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)\mathbf{f}(\mathbf{y}_k) + \mathcal{O}(h^3). \quad (2.21)$$

The Taylor series expansion of the solution  $\mathbf{y}(x)$  of the system of differential equations in  $x_k$  has the form, using the differential equation and the chain rule,

$$\begin{aligned}
\mathbf{y}(x_{k+1}) &= \mathbf{y}(x_k) + h\mathbf{y}'(x_k) + \frac{h^2}{2}\mathbf{y}''(x_k) + \mathcal{O}(h^3) \\
&= \mathbf{y}(x_k) + h\mathbf{f}(\mathbf{y}_k) + \frac{h^2}{2}\frac{\partial\mathbf{f}(\mathbf{y})}{\partial x}(x_k) + \mathcal{O}(h^3) \\
&= \mathbf{y}(x_k) + h\mathbf{f}(\mathbf{y}_k) + \frac{h^2}{2}\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)\mathbf{y}'(x_k) + \mathcal{O}(h^3) \\
&= \mathbf{y}(x_k) + h\mathbf{f}(\mathbf{y}_k) + \frac{h^2}{2}\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)\mathbf{f}(\mathbf{y}_k) + \mathcal{O}(h^3).
\end{aligned}$$

Starting with the exact value at  $x_k$ , then the first three terms of (2.21) correspond to the Taylor series expansion of the solution  $\mathbf{y}(x)$  of the system of differential equations in  $x_k$ . Thus, it follows that the local error is of order  $\mathcal{O}(h^3)$ , from what follows that the consistency order of `ode23s` is two, see Definition 1.14.  $\blacksquare$

*Remark 2.39. To the proof of Theorem 2.38.* Note that it is not needed in the proof of Theorem 2.38 that  $J$  is the exact derivative  $\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)$ . The method `ode23s` remains a second order method if  $J$  is only an approximation of  $\partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)$  and even if  $J$  is an arbitrary matrix. However, the transfer of the stability properties from the original method to `ode23s` is only guaranteed for the choice  $J = \partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)$ , see Theorem 2.33.  $\square$

**Theorem 2.40. Stability function of `ode23s`.** Assume that  $J = \partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)$ , then the stability function of the Rosenbrock method `ode23s` has the form

$$R(z) = \frac{1 + (1 - 2a)z}{(1 - az)^2}. \quad (2.22)$$

*Proof.* The statement of the theorem follows from applying the method to the usual test equation, *exercise*.  $\blacksquare$

**Corollary 2.41. Stability of `ode23s`.** If  $J = \partial_{\mathbf{y}}\mathbf{f}(\mathbf{y}_k)$ , then the Rosenbrock method `ode23s` is L-stable.

*Proof.* The statement is obtained by applying the definition of L-stability to the stability function (2.22).  $\blacksquare$

*Remark 2.42. On the order of `ode23s`.* It remains the question whether an appropriate choice of  $J$  might even increase the order of the method. However, for the model problem of the linear stability analysis, a series expansion of the stability function shows that the exponential function is reproduced exactly only up to the quadratic term. From this observation, it follows that one does not obtain a third order method even with exact Jacobian. In practice, there is no important reason from the point of view of accuracy to compute a new Jacobian in each step. Often, it is sufficient to update  $J$  every now and then.  $\square$

## Chapter 3

# Multi-Step Methods

### 3.1 Definition

*Remark 3.1. Multi-step methods.* The characteristic feature of one-step methods is that they need for computing  $y_{k+1}$  only the value from the previous approximation  $y_k$  of the solution. A straightforward extension consists in constructing methods that use for computing  $y_{k+1}$  more than one of the previous approximations  $y_k, y_{k-1}, \dots$ . Such methods are called multi-step methods.  $\square$

**Definition 3.2.  $q$ -step method, linear  $q$ -step method.** A  $q$ -step method with  $q \geq 1$  is a numerical method for approximately solving

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \quad (3.1)$$

where  $y_{k+1}$  depends on  $y_{k+1-q}$  but not on  $y_i$  with  $i < k + 1 - q$ .

A  $q$ -step method is called linear, if it has the form

$$y_{k+1} = \sum_{j=0}^{q-1} a_j y_{k-j} + h \sum_{j=0}^{q-1} b_j f(x_{k-j}, y_{k-j}) + hb_{-1} f(x_{k+1}, y_{k+1}), \quad (3.2)$$

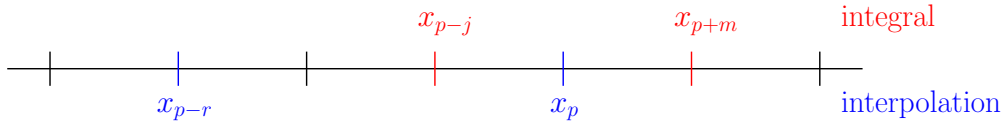
$k = q - 1, q, \dots$ , with  $q \geq 1$ ,  $a_0, \dots, a_{q-1}, b_{-1}, \dots, b_{q-1} \in \mathbb{R}$ ,  $a_{q-1} \neq 0$  or  $b_{q-1} \neq 0$ . For  $q = 1$ , the method is called a one-step method. If  $b_{-1} \neq 0$ , then the linear  $q$ -step method is an implicit method, otherwise it is an explicit method.  $\square$

*Remark 3.3. Initial values for a  $q$ -step method.* A  $q$ -step method needs  $q$  initial values. However, the initial value problem (3.1) provides only the initial value  $y_0$ . The second initial value  $y_1$  can be computed with a one-step method, the next initial value  $y_2$  with a one-step method or with a two-step method and so on. It follows that all initial values  $y_i$ ,  $i > 0$ , are already numerical approximations. This aspect has to be taken into account in the error analysis of multi-step methods, see Remark 3.23.  $\square$

### 3.2 Predictor-Corrector Methods

*Remark 3.4. Construction.* Starting point of the construction of predictor-corrector methods is the equivalent integral form of the initial value problem (3.1)

$$y(x) = y_0 + \int_{x_0}^x f(t, y(t)) dt. \quad (3.3)$$



**Fig. 3.1** Parameters in the derivation of predictor-corrector schemes.

Denote the solution at  $\tilde{x}$  by  $y(\tilde{x})$ , then it holds that

$$y(x) = y(\tilde{x}) + \int_{\tilde{x}}^x f(t, y(t)) dt. \quad (3.4)$$

The main idea of predictor-corrector methods consists in approximating the integral on the right-hand side of (3.4) in an appropriate way. There are two principal difficulties:

- The dependency of the term in the integral on  $t$  is generally not known since the function  $y(t)$  is unknown.
- Even if the dependency of the function in the integral on  $t$  is known, generally it will be impossible to find an analytic expression of the solution.

Consider an equidistant grid with nodes

$$x_i = x_0 + ih, \quad i = 0, 1, \dots$$

For the derivation of the methods, assume that the term in the integral is known. Then, the derivation is similar to the derivation of the Newton<sup>1</sup>–Cotes<sup>2</sup> formulas for numerical quadrature. In this approach, the term in the integral of (3.4) is replaced by a polynomial interpolant. Let the boundaries of the integral be the nodes

$$\begin{aligned} \tilde{x} &= x_{p-j}, & \text{starting point with parameter } j, \\ x &= x_{p+m} & \text{end point with parameter } m, \end{aligned} \quad (3.5)$$

with parameters  $j, m \in \mathbb{N}_0$  that need yet to be determined. It will be required that the interpolation polynomial  $p_r(x)$  satisfies the following properties:

- the degree of  $p_r(x)$  is lower than or equal to  $r$ ,
- $p_r(x_i) = f(x_i, y(x_i))$  for  $i = p, p-1, \dots, p-r$ .

Thus,  $x_p$  is the most right-hand side node for computing the interpolation polynomial. The value  $r$  is a third parameter, compare Figure 3.1. Note that two sets of nodes are involved in the construction, namely the nodes that determine the boundaries of the integral and the nodes that are used to define the interpolation polynomial. The solution of this interpolation problem is given by the Lagrange<sup>3</sup> interpolation polynomial

$$p_r(x) = \sum_{i=0}^r f(x_{p-i}, y(x_{p-i})) L_i(x)$$

with

$$L_i(x) = \prod_{l=0, l \neq i}^r \frac{x - x_{p-l}}{x_{p-i} - x_{p-l}}, \quad i = 0, 1, \dots, r. \quad (3.6)$$

It follows by using (3.4), (3.5), (3.6), and by replacing the unknown values  $y(x_{p-i})$  by their computed approximations  $y_{p-i}$  that

<sup>1</sup> Isaac Newton (1642 – 1727)

<sup>2</sup> Roger Cotes (1682 – 1716)

<sup>3</sup> Joseph Louis Lagrange (1736 – 1813)

$$\begin{aligned}
y_{p+m} &\approx y_{p-j} + \sum_{i=0}^r f(x_{p-i}, y_{p-i}) \int_{x_{p-j}}^{x_{p+m}} L_i(t) dt \\
&= y_{p-j} + h \sum_{i=0}^r \beta_i f(x_{p-i}, y_{p-i})
\end{aligned} \tag{3.7}$$

with

$$\beta_i = \frac{1}{h} \int_{x_{p-j}}^{x_{p+m}} L_i(t) dt = \frac{1}{h} \int_{x_{p-j}}^{x_{p+m}} \left( \prod_{l=0, l \neq i}^r \frac{t - x_{p-l}}{x_{p-i} - x_{p-l}} \right) dt.$$

The constructed method is in particular linear. Note that so far the assumption of having an equidistant grid was not used.

Finally, the formula for  $\beta_i$  should be simplified. To this end, note that all fixed values from the interval are nodes of the equidistant grid, such that, e.g.,  $x_p = x_0 + ph$ . Replacing these values and using the substitution

$$t = x_p + sh \implies dt = hds,$$

yields

$$\begin{aligned}
\beta_i &= \frac{1}{h} \int_{-j}^m \left( \prod_{l=0, l \neq i}^r \frac{x_p + sh - x_{p-l}}{x_{p-i} - x_{p-l}} \right) h ds \\
&= \int_{-j}^m \left( \prod_{l=0, l \neq i}^r \frac{x_0 + ph + sh - x_0 - ph + lh}{x_0 + ph - ih - x_0 - ph + lh} \right) ds \\
&= \int_{-j}^m \left( \prod_{l=0, l \neq i}^r \frac{s+l}{-i+l} \right) ds.
\end{aligned} \tag{3.8}$$

Now, different methods can be obtained depending on the choice of  $m$ ,  $j$ , and  $r$ . There are four important classes of methods.  $\square$

*Example 3.5. Adams<sup>4</sup>–Bashforth<sup>5</sup> methods.* The class of  $q$ -step Adams–Bashforth methods is given by  $m = 1$ ,  $j = 0$ , and  $r = q - 1$ . It follows that the  $q$ -step Adams–Bashforth method uses the nodes  $x_{k+1-q}, \dots, x_k$  for computing the Lagrangian interpolation polynomial. These are  $q$  nodes and  $p_q(x)$  is at most of degree  $q - 1$ . Adams–Bashforth methods are explicit methods. They have the general form

$$y_{k+1} = y_k + h \sum_{i=0}^{q-1} \beta_i f(x_{k-i}, y_{k-i}), \tag{3.9}$$

see (3.7), with

$$\beta_i = \int_0^1 \left( \prod_{l=0, l \neq i}^{q-1} \frac{s+l}{-i+l} \right) ds, \tag{3.10}$$

compare (3.8).

In the case  $q = 1$ , the term in the integral in (3.4) is replaced by a constant interpolation polynomial with the node  $(x_k, f(x_k, y_k))$ . Using the convention that the product is 1 if there is formally no factor in (3.10), this approach yields

<sup>4</sup> John Couch Adams (1819 – 1892)

<sup>5</sup> Francis Bashforth (1819 – 1912)