Let the jth row of $\mathcal{A}$ be identical with $\boldsymbol{b}^T$. Then

$$\boldsymbol{b} = \boldsymbol{e}_j^T \mathcal{A},$$

where $\boldsymbol{e}_j$ denotes the jth unit vector. The conclusion

$$\lim_{z \to \infty} R(z) = 1 - \boldsymbol{e}_j^T \mathcal{A}\mathcal{A}^{-1}\boldsymbol{1} = 0$$

follows immediately. ■

At this point we believe to have given a sufficient introduction to the stability of ODEs and one-step methods. For a deeper study of this topic we refer the reader to the books [25] and [60]. In the last section of this chapter let us discuss the most sophisticated one-step ODE solvers: the higher-order implicit Runge–Kutta methods.

5.4 HIGHER-ORDER IRK METHODS

It was discovered in early 1970s that general (implicit) RK methods could be generated by combining classical collocation methods with higher-order numerical quadrature rules. Several RK methods derived via the traditional Taylor expansion techniques turned out to actually be collocation methods. A classical book on higher-order IRK methods is [60].

5.4.1 Collocation methods

Let us return to the (nonautonomous) ODE system (5.11), (5.12) resulting from the MOL,

$$\dot{\boldsymbol{Y}}(t) = \boldsymbol{\Phi}(\boldsymbol{Y}(t), t), \tag{5.79}$$

$$\boldsymbol{Y}(0) = \boldsymbol{Y}^0. \tag{5.80}$$

The collocation constructs the approximate solution $\boldsymbol{X}(t) \approx \boldsymbol{Y}(t)$ as a continuous (vector-valued) function which is a polynomial of degree s in every interval $[t_k, t_k + \Delta t_k]$, $k = 0, 1, \ldots, K-1$,

$$\boldsymbol{X}(t_k + \tau) = \mathcal{E}(\boldsymbol{Y}^k, t_k, \tau), \quad \tau \in [0, \Delta t_k].$$

In the interval $[t_k, t_k + \Delta t_k]$ the function $\boldsymbol{X}$ not only must fulfill the initial condition

$$\boldsymbol{X}(t_k) = \mathcal{E}(\boldsymbol{Y}^k, t_k, 0) = \boldsymbol{Y}^k, \tag{5.81}$$

but also it has to satisfy ("collocate") equation (5.79) at additional s internal points $t_k + c_1\Delta t_k, t_k + c_2\Delta t_k, \ldots, t_k + c_s\Delta t_k$ of the interval $[t_k, t_k + \Delta t_k]$,

$$\begin{aligned}
\dot{\boldsymbol{X}}(t_k + c_1\Delta t_k) &= \boldsymbol{\Phi}(\boldsymbol{X}(t_k + c_1\Delta t_k), t_k + c_1\Delta t_k), \qquad (5.82)\\
\dot{\boldsymbol{X}}(t_k + c_2\Delta t_k) &= \boldsymbol{\Phi}(\boldsymbol{X}(t_k + c_2\Delta t_k), t_k + c_2\Delta t_k),\\
&\vdots\\
\dot{\boldsymbol{X}}(t_k + c_s\Delta t_k) &= \boldsymbol{\Phi}(\boldsymbol{X}(t_k + c_s\Delta t_k), t_k + c_s\Delta t_k),
\end{aligned}$$

where $0 \le c_1 < c_2 < \ldots, < c_s \le 1$ are suitable constants. These s parameters fully determine the method (its consistency, convergence, stability, and all other aspects). With the approximate solution $\boldsymbol{X}(t)$ in hand, the approximate solution on the new time level is defined as

$$\boldsymbol{Y}^{k+1} = \boldsymbol{X}(t_k + \Delta t_k) = \mathcal{E}(\boldsymbol{Y}^k, t_k, \Delta t_k). \tag{5.83}$$

It is known that $\boldsymbol{X}(t)$ exists and is unique for sufficiently small time steps and a sufficiently regular right-hand side $\boldsymbol{\Phi}$. However, the proof is by no means trivial, and we refer the reader to [25] and [60]. In the following let us discuss the selection of the parameters c_i, $i = 1, 2, \ldots, s$.

The collocation procedure Consider a set of collocation points $0 \le c_1 < c_2 < \ldots, < c_s \le 1$, along with the standard Lagrange nodal basis $\theta_1, \theta_2, \ldots, \theta_s$ of the polynomial space

$$P = P^{s-1}(0, 1),$$

satisfying the condition

$$\theta_i(c_j) = \delta_{ij}.$$

For brevity, by z_i denote the derivative of $\boldsymbol{X}(t)$ at the collocation point c_i,

$$\boldsymbol{z}_i = \dot{\boldsymbol{X}}(t_k + c_i \Delta t_k) \qquad \text{for all } 1 \le i \le s.$$

Exploiting the Lagrange interpolation polynomial (A.75), the derivative $\dot{\boldsymbol{X}}(t)$ in the interval $[t_k, t_k + \Delta t_k]$ can be written as

$$\dot{\boldsymbol{X}}(t_k + \xi \Delta t_k) = \sum_{j=1}^{s} \boldsymbol{z}_j \theta_j(\xi), \quad \xi \in [0, 1]. \tag{5.84}$$

Integrating (5.84) and using the initial condition (5.81), we find that

$$\boldsymbol{X}(t_k + c_i \Delta t_k) = \boldsymbol{Y}^k + \Delta t_k \int_0^{c_i} \dot{\boldsymbol{X}}(t_k + \xi \Delta t_k)\, \mathrm{d}\xi = \boldsymbol{Y}^k + \Delta t_k \sum_{j=1}^{s} a_{ij} \boldsymbol{z}_j, \tag{5.85}$$

where

$$a_{ij} = \int_0^{c_i} \theta_j(\xi)\, \mathrm{d}\xi, \quad i, j = 1, 2, \ldots, s. \tag{5.86}$$

Substituting these values into the collocation condition (5.82), one obtains

$$\boldsymbol{z}_i = \boldsymbol{\Phi}\left(\boldsymbol{Y}^k + \Delta t_k \sum_{j=1}^{s} a_{ij} \boldsymbol{z}_j, t_k + c_i \Delta t_k\right), \quad i = 1, 2, \ldots, s.$$

By (5.83) and (5.85) the approximation at the $(k+1)$th time level has the form

$$\boldsymbol{Y}^{k+1} = \boldsymbol{X}(t_k + \Delta t_k) = \boldsymbol{Y}^k + \Delta t_k \int_0^1 \dot{\boldsymbol{X}}(t_k + \xi \Delta t_k)\, \mathrm{d}\xi = \boldsymbol{Y}^k + \Delta t_k \sum_{j=1}^{s} b_j \boldsymbol{z}_j, \tag{5.87}$$

where

$$b_j = \int_0^1 \theta_j(\xi)\,\mathrm{d}\xi, \quad j = 1, 2, \ldots, s. \tag{5.88}$$

Let us see that the points $\boldsymbol{c}$ and weights $\boldsymbol{b}$ represent a quadrature rule that is exact for polynomials of the degree $s-1$: Every such polynomial φ can be written in terms of the Lagrange basis,

$$\varphi(\xi) = \sum_{j=1}^{s} \varphi(c_j)\theta_j(\xi),$$

and for its integral one obtains

$$\int_0^1 \varphi(\xi)\,\mathrm{d}\xi = \int_0^1 \sum_{j=1}^{s} \varphi(c_j)\theta_j(\xi)\,\mathrm{d}\xi = \sum_{j=1}^{s} \varphi(c_j) \int_0^1 \theta_j(\xi)\,\mathrm{d}\xi = \sum_{j=1}^{s} \varphi(c_j) b_j.$$

Finally let us define

$$\mathcal{A} = \{a_{ij}\}_{i,j=1}^{s}, \quad \boldsymbol{b} = (b_1, b_2, \ldots, b_s)^T, \quad \boldsymbol{c} = (c_1, c_2, \ldots, c_s)^T.$$

The relation (5.87) represents the implicit RK method $(\boldsymbol{b}, \boldsymbol{c}, \mathcal{A})$ defined in (5.44). The consistency condition for explicit RK methods (5.41),

$$\sum_{j=1}^{s} b_j = 1,$$

extends naturally to implicit RK methods via (5.88),

$$\sum_{j=1}^{s} b_j = \sum_{j=1}^{s} \int_0^1 \theta_j(\xi)\,\mathrm{d}\xi = \int_0^1 \sum_{j=1}^{s} \theta_j(\xi) \cdot 1\,\mathrm{d}\xi = \int_0^1 1\,\mathrm{d}\xi = 1. \tag{5.89}$$

Moreover, we have the following lemma:

Lemma 5.9 *The coefficients of an implicit RK method $(\boldsymbol{b}, \boldsymbol{c}, \mathcal{A})$ defined by collocation satisfy the conditions*

$$\sum_{j=1}^{s} b_j c_j^{q-1} = \frac{1}{q}, \quad q = 1, 2, \ldots, s, \tag{5.90}$$

and

$$\sum_{j=1}^{s} a_{ij} c_j^{q-1} = \frac{1}{q} c_i^q, \quad q = 1, 2, \ldots, s \tag{5.91}$$

(with the convention $0^0 = 1$). In particular, the method is consistent and invariant under autonomization.

Proof: It follows from (5.88) that

$$\sum_{j=1}^{s} b_j c_j^{q-1} = \sum_{j=1}^{s} \int_0^1 c_j^{q-1}\theta_j(\xi)\,\mathrm{d}\xi = \int_0^1 \sum_{j=1}^{s} c_j^{q-1}\theta_j(\xi)\,\mathrm{d}\xi.$$

Looking at the integrand in more detail, we discover that at each collocation point c_r it achieves the value c_r^{q-1}, $r = 1, 2, \ldots, s$. Thus necessarily

$$\sum_{j=1}^{s} c_j^{q-1} \theta_j(\xi) = \xi^{q-1},$$

and (5.90) follows,

$$\sum_{j=1}^{s} b_j c_j^{q-1} = \int_0^1 \xi^{q-1} \, \mathrm{d}\xi = \frac{1}{q}.$$

Using the same technique for (5.86), one easily obtains (5.91). The consistency follows from (5.89) which is a special case of (5.90), and the invariance under autonomization follows immediately from Lemma 5.4. ■

The formula (5.90) states that the quadrature rule

$$\sum_{j=1}^{s} b_j \varphi(c_j) \approx \int_0^1 \varphi(\xi) \, \mathrm{d}\xi$$

is exact for all polynomials $\varphi \in P^{s-1}(0, 1)$.

The following result, which relates the consistency order of an implicit RK method constructed via collocation to the order of accuracy of the underlying quadrature rule, was first proved under slightly simplified assumptions by J. C. Butcher in 1964. A different idea of the proof was presented by S.P. Norsett and G. Wanner [89] in 1979.

Theorem 5.5 *An implicit RK method $(\boldsymbol{b}, \boldsymbol{c}, \mathcal{A})$ generated by collocation has for a p-times continuously differentiable right-hand side $\boldsymbol{\Phi}$ the consistency order p if and only if the quadrature formula defined by the nodes $\mathbf{c}$ and weights $\mathbf{b}$ has the order of accuracy p.*

Proof: See, e.g., [59]. ■

5.4.2 Gauss and Radau IRK methods

Theorem 5.5 suggests an efficient strategy for the design of s-stage implicit RK schemes of the consistency order $1 \le p \le 2s$:

1. Choose a quadrature rule $(\boldsymbol{c}, \boldsymbol{b})$ that is exact for polynomials of order $p - 1$.

2. Use (5.86) to define the Butcher's array $(\boldsymbol{b}, \boldsymbol{c}, \mathcal{A})$.

Gauss IRK methods From Section 2.3 we know that every Gaussian quadrature rule $(\boldsymbol{c}, \boldsymbol{b})$ with s quadrature points is exact for polynomials of the degree up to $2s - 1$.

Lemma 5.10 *Every s-stage Gauss IRK method has the consistency order $p = 2s$ for all $2s$-times continuously differentiable right-hand sides $\boldsymbol{\Phi}$.*

Proof: Immediate consequence of Theorem 5.5. ■

Thus the Gauss IRK methods attain the maximum consistency order $p = 2s$ of s-stage IRK methods, derived in Paragraph 5.3.5. In contrast to this result, the maximum order of s-stage explicit RK methods is an open problem (see Table 5.1). The Gauss IRK method for $s = 1$ is the "implicit midpoint rule" that we are familiar with from Paragraph 5.2.6

and from Example 5.1. Another Gauss IRK method with the consistency order $p = 4$, corresponding to the stage count $s = 2$, is

$$\begin{array}{c|cc} 1/2 - \sqrt{3}/6 & 1/4 & 1/4 - \sqrt{3}/6 \\ 1/2 + \sqrt{3}/6 & 1/4 + \sqrt{3}/6 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}$$

Lemma 5.11 *All Gauss IRK methods are A-stable. Moreover, their stability domain $\mathcal{S}_R$ exactly coincides with the negative complex half plane $\mathcal{S}_{exp}$ (5.60).*

Proof: See, e.g., [60]. ■

Let us mention that $\mathcal{S}_R = \mathcal{S}_{exp}$ means that Gauss IRK methods preserve isometry. Moreover it is known that these methods are reversible. Both these properties are positive for the performance of the methods, as the reader may expect. These and more interesting aspects of IRK methods are thoroughly discussed in [60].

One of the few drawbacks of Gauss IRK methods is that generally they are not L-stable. This is a consequence of the fact that the Gaussian quadrature points do not lie at interval endpoints, and therefore the approximate solution obtained via collocation has jumps in the temporal derivative at all times t_k, $k = 1, 2, \ldots$.

Radau IRK methods The above-mentioned lack of L-stability is eliminated via collocation methods based on Radau quadrature rules, that place collocation points at the interval endpoints (see, e.g., [111] for details on this numerical quadrature and for a CD-ROM with Radau quadrature data).

Lemma 5.12 *Every s-stage Radau IRK method has the consistency order $p = 2s - 1$ for all $(2s - 1)$-times continuously differentiable right-hand sides $\mathbf{\Phi}$. All Radau IRK methods are A-stable and also L-stable.*

Proof: The consistency order follows from the fact that a Lobatto-Radau quadrature rule with s nodes has the order of accuracy $p = 2s - 1$, and from Theorem 5.5. For the rest see, e.g., [60]. ■

The reader already encountered the 1-stage Radau method (implicit Euler scheme) and the 2-stage third-order Radau method in Example 5.1. Let us present the 3-stage fifth-order Radau method,

$$\begin{array}{c|ccc} (4 - \sqrt{6})/10 & (88 - 7\sqrt{6})/360 & (296 - 169\sqrt{6})/1800 & (-2 + 3\sqrt{6})/225 \\ (4 + \sqrt{6})/10 & (296 + 169\sqrt{6})/1800 & (88 + 7\sqrt{6})/360 & (-2 - 3\sqrt{6})/225 \\ 1 & (16 - \sqrt{6})/36 & (16 + \sqrt{6})/36 & 1/9 \\ \hline & (16 - \sqrt{6})/36 & (16 + \sqrt{6})/36 & 1/9 \end{array}$$

The L-stability of this method follows from Theorem 5.4 immediately. For an implementation of this method, enhanced with a step size control based on an embedded third-order method, see code RADAU5 in [60].