Numerical Analysis Hilary Term 2023
Lecture 14: Runge–Kutta methods

Runge–Kutta methods: Runge–Kutta (RK) methods form a broad class of algorithms for the numerical solution of IVPs. The class includes both explicit and implicit schemes. When applications call for an integrator with some kind of stability or conservation property, there usually exists a suitable RK method. In particular, RK methods can be made arbitrarily high-order without the loss of stability.

Here we state some results without proof; they are nonexaminable. For a detailed discussion, we refer to the books

- Süli and Mayer, "Introduction to Numerical Analysis"
- Hairer, Norsett, and Wanner, "Solving Ordinary Differential Equations"
- Butcher, "Numerical Methods for Ordinary Differential Equations"

Definition 1. *The family of* s-stage Runge–Kutta methods *is defined by*

$$\mathbf{\Psi}(x, \mathbf{y}, h, \mathbf{f}) = \mathbf{y} + h \sum_{i=1}^{s} b_i \mathbf{k}_i \,, \tag{1}$$

where the stages $\mathbf{k}_i s$ *(recall that* $\mathbf{y} \in \mathbb{R}^d$*, and so do the* $\mathbf{k}_i s$*) are the solutions of the coupled system of (generally nonlinear) equations*

$$\mathbf{k}_i := \mathbf{f}\big(x + c_i h, \mathbf{y} + h \sum_{j=1}^{s} a_{ij} \mathbf{k}_j\big) \,, \quad i = 1, \ldots, s \,. \tag{2}$$

The coefficients $\{c_i\}_{i=1}^{s}$ *are always given by*

$$c_i := \sum_{j=1}^{s} a_{ij} \quad i = 1, \ldots, s \,.$$

Definition 2. *The coefficients of a Runge–Kutta method are commonly summarized in a* Butcher tableau[1]

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^\top \end{array} \,.$$

Example 3. *The explicit Euler method, the implicit Euler method, and the implicit midpoint rule are Runge–Kutta methods. Their Butcher tables are*

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}\,, \quad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}\,, \quad \textit{and} \quad \begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}\,, \quad \textit{respectively.}$$

[1] The use of this tableau was introduced by J. C. Butcher in 1963 with the article *Coefficients for the study of Runge–Kutta integration processes.*

It is convenient at this point to restrict our attention to autonomous IVPs. (Recall that a nonautonomous system can always be made autonomous by increasing its dimension.) The process of making an IVP autonomous commutes with Runge–Kutta discretisation if and only if

$$\sum_{i=1}^{s} b_i = 1, \quad c_k = \sum_{j=1}^{s} a_{kj} \quad k = 1, \ldots, s\,,$$

which we assume henceforth. (In other words, if these conditions hold, the RK discretisation of the autonomised system is the autonomisation of the RK discretisation of the original problem.)

By computing appropriate Taylor expansions, it is possible to derive algebraic conditions the Runge–Kutta coefficients must satisfy for the method to have a targeted consistency order. For example:

Lemma 4. *A Runge–Kutta method is consistent if and only if* $\sum_{i=1}^{s} b_i = 1$*. If the condition*

$$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}$$

is also satisfied, the Runge–Kutta method has consistency order 2, and if the conditions

$$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3} \quad \text{and} \quad \sum_{i=1}^{s} b_i \sum_{j=1}^{s} a_{ij} c_j = \frac{1}{6}$$

are also satisfied, the Runge–Kutta method has consistency order 3.

The following table indicates the number of conditions as described above that a Runge–Kutta method must satisfy to have order p:

p	1	2	3	4	5	6	7	8	9	10	20
#conditions	1	2	4	8	17	37	85	200	486	1205	20247374

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The number of stages of a Runge–Kutta method provides an interesting upper bound on its consistency order.

Lemma 5. *The (consistency) order p of an s-stage Runge–Kutta method is bounded by $p \leq 2s$. If the Runge–Kutta method is explicit, then $p \leq s$.*

To evolve a numerical solution from x_n to x_{n+1} with a Runge–Kutta method, one needs to compute the stages $\mathbf{k}_i$. If the Runge–Kutta method is explicit, these stages can be computed sequentially (and at a low-cost) starting from $\mathbf{k}_1$ (a Runge–Kutta method is explicit if $a_{ij} = 0$ whenever $j \geq i$, i.e. the matrix $\mathbf{A}$ is strictly lower-triangular). An example of this is the explicit Euler method. If $\mathbf{A}$ is lower-triangular (i.e. possibly $a_{ii} \neq 0$), then the scheme is said to be *diagonally-implicit*; one can compute the stages $\mathbf{k}_i$ sequentially, solving a sequence of nonlinear problems. The implicit Euler and implicit midpoint rules are examples of diagonally-implicit RK methods. Finally, if $\mathbf{A}$ enjoys neither of these structures, the RK method is said to be fully implicit; one must solve a large coupled nonlinear system for all stages simultaneously.

It is possible to construct Runge–Kutta methods that achieve maximal order. So-called *Butcher barriers* quantify the minimal amount of stages that an explicit Runge–Kutta method of order p requires. The following table shows some of these minimal amount of stages:

p	1	2	3	4	5	6	7	8	≥ 9
minimal value of s	1	2	3	4	6	7	9	11	$\geq p+3$

This implies that a Runge–Kutta method that has maximal order must be implicit.

Construction of explicit RK methods: To construct explicit Runge–Kutta methods, we start by recalling that the analytic solution of

$$\mathbf{y}' = \mathbf{f}(x, \mathbf{y}), \qquad \mathbf{y}(x_0) = \mathbf{y}_0, \tag{3}$$

is given by the (implicit) formula

$$\mathbf{y}(x+h) = \mathbf{y}(x) + \int_x^{x+h} \mathbf{f}(\tau, \mathbf{y}(\tau))\,\mathrm{d}\tau = \mathbf{y}(x) + h\int_0^1 \mathbf{f}(x+h\tau, \mathbf{y}(x+h\tau))\,\mathrm{d}\tau\,.$$

Approximating the latter integral with a quadrature rule on $[0,1]$ with s nodes $c_1, \dots, c_s$ and weights $b_1, \dots, b_s$ returns

$$\mathbf{y}(x+h) \approx \mathbf{y}(x) + h\sum_{i=1}^{s} b_i \mathbf{f}(x + c_i h, \mathbf{y}(x + c_i h))\,. \tag{4}$$

Note that this approximation requires the values $\mathbf{y}(x + c_i h)$. To make the method explicit, we approximate the values $\mathbf{y}(x_0 + c_i h)$ with explicit Runge–Kutta methods we already know. This way, we can construct s-stage explicit Runge–Kutta methods by induction.

Example 6. *If we choose the 1-point Gauss quadrature rule, that is,*

$$\mathbf{y}(x+h) \approx \mathbf{y}(x) + h\mathbf{f}(x + h/2, \mathbf{y}(x + h/2)) \tag{5}$$

and approximate $\mathbf{y}(x + h/2)$ *with the explicit Euler method, the resulting scheme reads*

$$\mathbf{\Psi}(x, \mathbf{y}, h, \mathbf{f}) = \mathbf{y} + h\mathbf{f}\left(x + h/2, \mathbf{y} + \frac{h}{2}\mathbf{f}(x, \mathbf{y})\right)\,. \tag{6}$$

Example 7. *If we use the trapezium rule, that is,*

$$\mathbf{y}(x+h) \approx \mathbf{y}(x) + \frac{h}{2}\mathbf{f}(x, \mathbf{y}(x)) + \frac{h}{2}\mathbf{f}(x+h, \mathbf{y}(x+h))\,,$$

and approximate $\mathbf{y}(x+h)$ *with the explicit Euler method, the resulting scheme reads*

$$\mathbf{\Psi}(x, \mathbf{y}, h, \mathbf{f}) = \mathbf{y} + \frac{h}{2}\mathbf{f}(x, \mathbf{y}) + \frac{h}{2}\mathbf{f}\left(x + h, \mathbf{y} + h\mathbf{f}(x, \mathbf{y})\right)\,. \tag{7}$$

Both of these are 2nd-order Runge–Kutta methods. Their Butcher tables read

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array} \quad \text{and} \quad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array},$$

respectively.

A similar approach leads to the most famous explicit Runge–Kutta method *RK4*, a 4-stage 4th-order explicit Runge–Kutta method whose Butcher table reads

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array}.$$

We have seen that s-stage explicit Runge–Kutta methods have at most order s. Next, we construct s-stage implicit Runge–Kutta methods whose order is at least s.

Definition 8. *Let $c_1, \dots, c_s \in [0,1]$ be (pairwise distinct) collocation points. The corresponding collocation method is the one-step method defined by*

$$\mathbf{\Psi}(x, \mathbf{y}, h, \mathbf{f}) = \tilde{\mathbf{y}}(h)\,,$$

where $\tilde{\mathbf{y}}$ is the unique polynomial of degree s that satisfies

$$\tilde{\mathbf{y}}(0) = \mathbf{y} \quad \text{and} \quad \tilde{\mathbf{y}}'(c_i h) = \mathbf{f}(x + c_i h, \tilde{\mathbf{y}}(c_i h))\,, \quad \text{for } i = 1, \dots, s\,. \tag{8}$$

Lemma 9. *Let Q be the highest-order quadrature rule on $[0,1]$ that can be constructed using the nodes $c_1, \dots, c_s$, and let p_Q be its order (p_Q = 1 + the maximal degree of polynomials it integrates exactly). If $\mathbf{f}$ is sufficiently smooth and $h > 0$ is sufficiently small, the collocation method associated to $c_1, \dots, c_s$ has order p_Q.*

Corollary 10. *If $\mathbf{f}$ is sufficiently smooth and $h > 0$ is sufficiently small, the order of the collocation method associated to $c_1, \dots, c_s$ is at least s and at most $2s$ (Gauss quadrature).*

It is not obvious, but collocation methods are indeed Runge–Kutta methods.

Lemma 11. *Collocation methods are Runge–Kutta methods. Their coefficients are*

$$a_{ij} = \int_0^{c_i} L_j(\tau)\,\mathrm{d}\tau\,, \quad b_i = \int_0^1 L_i(\tau)\,\mathrm{d}\tau\,, \tag{9}$$

where $\{L_i\}_{i=1}^s$ are the Lagrange polynomials associated to $c_1, \dots, c_s$.

Stability of Runge–Kutta methods We have seen that numerical methods for IVPs may encounter stability issues. For simplicity, we only consider autonomous ODEs.

Definition 12. *A* fixed point *of* $\mathbf{y}' = \mathbf{f}(\mathbf{y})$ *is a point* $\mathbf{y}^*$ *such that* $\mathbf{f}(\mathbf{y}^*) = \mathbf{0}$. *A fixed point* $\mathbf{y}^*$ *is* asymptotically stable *(or attractive) if there exists a ball* $B_\delta(\mathbf{y}^*)$ *(of radius* $\delta > 0$ *and centered at* $\mathbf{y}^*$*) such that, whenever* $\mathbf{y}_0 \in B_\delta(\mathbf{y}^*)$*, the solution to* $\mathbf{y}' = \mathbf{f}(\mathbf{y})$*,* $\mathbf{y}(0) = \mathbf{y}_0$ *satisfies* $\lim_{x\to\infty} \mathbf{y}(x) = \mathbf{y}^*$.

Theorem 13. *A fixed point* $\mathbf{y}^*$ *of an autonomous ODE is asymptotically stable if*

$$\sigma\left(\mathbf{Df}(\mathbf{y}^*)\right) \subset \mathbb{C}^- := \{z \in \mathbb{C} : \mathrm{Re} z < 0\} ,$$

where $\sigma\left(\mathbf{Df}(\mathbf{y}^*)\right)$ *denotes the set of eigenvalues of the matrix* $\mathbf{Df}(\mathbf{y}^*)$.

This theorem implies that, to study the asymptotic stability of $\mathbf{y}^*$, we can restrict our considerations to the linearised ODE $\mathbf{y}' = \mathbf{Df}(\mathbf{y}^*)(\mathbf{y} - \mathbf{y}^*)$, that is, we can restrict our attention to linear ODEs. To further simplify the analysis, we restrict our attention to a single eigenvalue, yielding the *Dahlquist test equation*

$$y' = zy , \quad y(0) = 1 , \quad \text{and} \quad \mathrm{Re} z < 0 . \tag{10}$$

Clearly, the solution of the Dahlquist test equation is $y(x) = \exp(zx)$, which satisfies $\lim_{x\to\infty} y(x) = 0$. Therefore, $y^* = 0$ is an attractive fixed point.

The solution of the Dahlquist test equation obtained with a Runge–Kutta method has a special structure:

Definition 14. *Let* $\mathbf{\Psi}$ *be a Runge–Kutta method. The function*

$$S : \mathbb{C} \to \mathbb{C} , \quad z \mapsto S(z) := \mathbf{\Psi}(0, 1, 1, f : y \mapsto zy) ,$$

is called the stability function *of* $\mathbf{\Psi}$. *To shorten the notation, we henceforth write* $\mathbf{\Psi}(0, 1, 1, z)$ *instead of* $\mathbf{\Psi}(0, 1, 1, f : y \mapsto zy)$.

Lemma 15. *If* $\mathbf{\Psi}$ *is a Runge–Kutta method, then* $\mathbf{\Psi}(0, \ell, h, z) = \mathbf{\Psi}(0, 1, 1, zh)\ell$.

Theorem 16. *Let* $\{y_k\}_{k\in\mathbb{N}}$ *be the Runge–Kutta solution to the Dahlquist test equation obtained with a time step* $h > 0$. *Then,* $y_k = S(zh)^k$.

Proof. By direct computation, we can see that

$$y_1 = \mathbf{\Psi}(0, 1, h, z) = \mathbf{\Psi}(0, 1, 1, zh) = S(zh)$$

and that

$$y_2 = \mathbf{\Psi}(0, y_1, h, z) = \mathbf{\Psi}(0, 1, 1, zh)y_1 = S(zh)y_1 = S(zh)^2 .$$

Therefore, we conclude that $y_k = S(h\lambda)^k$. □

It is desirable that the discrete solution $\{y_k\}_{k\in\mathbb{N}}$ satisfies $\lim_{k\to\infty} y_k = 0$, mimicking the behavior of the exact solution to the Dahlquist test equation. When this happens, we say that $\{y_k\}_{k\in\mathbb{N}}$ is *asymptotically stable.*

Definition 17. *The region in the complex plane*

$$S_{\boldsymbol{\Psi}} := \{z \in \mathbb{C} : |S(z)| < 1\}$$

is called the stability region *of the Runge–Kutta method. Clearly, $\{y_k\}_{k\in\mathbb{N}}$ is asymptotically stable if $zh \in S_{\Psi}$.*

It is not so difficult to see that the stability function of an explicit Runge–Kutta method is a polynomial, which implies that $S_{\boldsymbol{\Psi}}$ is bounded. Therefore, the numerical approximation computed with an explicit Runge–Kutta method cannot be asymptotically stable if the time step h is too large. This is what we saw in our previous numerical experiments. However, the stability function of an implicit Runge–Kutta method is a rational function, and hence may not suffer from this limitation.

Definition 18. *A Runge–Kutta method is said to be A-*stable[2] *if $\mathbb{C}^- \subset S_{\boldsymbol{\Psi}}$.*

The Gauss collocation methods form a family of arbitrarily high-order A-stable methods whose stability region is exactly $\mathbb{C}^-$.

A-stability guarantees that $\{y_k\}_{k\in\mathbb{N}}$ will eventually converge to zero. However, the decay can be very slow compared to that of the exact solution.

Example 19. *Let $\{y_k\}$ be the approximate solution to the Dalhquist test equation obtained with the implicit midpoint rule and a fixed step size h. By direct computation, we can see that stability function of the implicit midpoint rule is*

$$S(z) = \frac{1 + z/2}{1 - z/2}.$$

The exact solution converges exponentially to zero with rate $\mathrm{Re} z$. *In particular, the smaller (more negative) the* $\mathrm{Re} z$, *the quicker the convergence. On the other hand, $\{y_k\}$ is a geometric sequence with ratio $S(zh)$. This also converges to zero, but the more negative the* $\mathrm{Re} z$, *the closer $|S(zh)|$ to 1, and the slower the decay of $\{y_k\}$. This implies that, if* $\mathrm{Re} z \ll 0$, *the qualitative behavior of $\{y_k\}$ can be very different from the one of the exact solution.*

Therefore, if the initial value problem has a strongly attractive fixed point, it is advisable to further ensure that $\lim_{\mathrm{Re} z \to -\infty} |S(z)| = 0$.

Definition 20. *An A-stable method that further satisfies $\lim_{\mathrm{Re} z \to -\infty} |S(z)| = 0$ is said to be L-*stable *(or stiffly accurate).*

One can verify that the implicit Euler method is L-stable, but it is not the only one. An example of a family of L-stable RK methods is the Gauss–Radau family. This is a family of collocation methods where the final quadrature point is fixed to $c_s = 1$ and the remaining points $c_1, \dots, c_{s-1}$ are chosen to obtain an associated quadrature rule of maximal order $2s - 1$.

[2] This concept was introduced by G. Dahlquist in 1963 with the article *A special stability problem for linear multistep methods.*