

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 9

9 Runge-Kutta methods

Revision 9.1 (Quadrature formulae) We may approximate the integral by the quadrature

$$\int_0^1 f(t) dt \approx \sum_{i=1}^s b_i f(c_i), \quad (9.1)$$

where – changing previous quadrature notations to match standard RK formulas below – for given knots c_i , the weights b_i are chosen to make this quadrature exact for all polynomials of degree $s-1$, that is $b_i = \int_0^1 \ell_i(t) dt$, where ℓ_i are fundamental Lagrange polynomials, i.e., $\ell_i(c_j) = \delta_{ij}$. If $\omega(t) = \prod_{i=1}^s (t - c_i)$ is orthogonal to all polynomials of degree $s-1$ on $[0, 1]$, then we obtain the Gaussian quadrature: the formula that is exact for all polynomials of degree $2s-1$.

Method 9.2 (Explicit Runge-Kutta methods) Suppose that we wish to solve the ODE $y' = f(t)$, with $y(0) = y_0$. The exact solution is $y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t) dt$ and we can approximate the integral by the quadrature (9.1) scaling it to the interval $[t_n, t_{n+1}]$. In that way, we obtain the time-stepping scheme

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i f(t_n + c_i h), \quad h = t_{n+1} - t_n.$$

Can we generalize this to genuine ODEs of the form $y' = f(t, y)$? Formally, $y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t, y(t)) dt$, and this can be approximated as before by

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i f(t_n + c_i h, y(t_n + c_i h)), \quad (9.2)$$

except that, of course, the vectors $y(t_n + c_i h)$ are unknown. But they can be approximated by another quadrature using approximate values of $y(t_n + c_j h)$ obtained earlier:

$$y(t_n + c_i h) = y(t_n) + \int_{t_n}^{t_n + c_i h} f(t, y(t)) dt \approx y(t_n) + h \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, y(t_n + c_j h)),$$

so that applying f to both sides of this formula we obtain

$$f(t_n + c_i h, y(t_n + c_i h)) \approx f\left(t_n + c_i h, y(t_n) + h \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, y(t_n + c_j h))\right). \quad (9.3)$$

Finally, from (9.2)-(9.3), letting $k_i \approx f(t_n + c_i h, y(t_n + c_i h))$, we arrive at the general form of an *s-stage explicit Runge-Kutta method* (RK):

$$\begin{aligned} k_i &= f(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j), & i = 1..s, \\ y_{n+1} &= y_n + h \sum_{i=1}^s b_i k_i. \end{aligned}$$

Here are the same formulas with more details:

$$\begin{aligned} k_1 &= f(t_n, y_n), & c_1 &= 0, \\ k_2 &= f(t_n + c_2 h, y_n + h a_{21} k_1), & c_2 &= a_{21}, \\ k_3 &= f(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)), & c_3 &= a_{31} + a_{32}, \\ &\vdots & &\vdots \\ k_s &= f(t_n + c_s h, y_n + h \sum_{j=1}^{s-1} a_{sj} k_j), & c_s &= \sum_{j=1}^{s-1} a_{sj}, \\ y_{n+1} &= y_n + h \sum_{i=1}^s b_i k_i, & \sum b_i &= 1. \end{aligned}$$

Here, equalities $c_i = \sum_{j=1}^{i-1} a_{ij}$ (as well as $\sum b_i = 1$) simply say that quadratures are exact on constants: a reasonable (although not necessary for a_{ij}) requirement. A more sophisticated choice of the RK coefficients a_{ij} is motivated at the first instance by order considerations.

9.1 Order of Runge-Kutta methods

Example 9.3 (Two-stage methods of order 2) Let us analyse the order of two-stage methods

$$\begin{aligned} \mathbf{k}_1 &= \mathbf{f}(t_n, \mathbf{y}_n), \\ \mathbf{k}_2 &= \mathbf{f}(t_n + c_2 h, \mathbf{y}_n + c_2 h \mathbf{k}_1), \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + h(b_1 \mathbf{k}_1 + b_2 \mathbf{k}_2). \end{aligned}$$

Taylor-expanding $\mathbf{k}_2$ about $(t_n, \mathbf{y}_n)$, and using $\mathbf{k}_1 = \mathbf{f}$, we obtain

$$\mathbf{k}_2 = \mathbf{f}(t_n + c_2 h, \mathbf{y}_n + c_2 h \mathbf{f}) = \mathbf{f} + c_2 h [\mathbf{f}_t + \mathbf{f}_y \mathbf{f}] + \mathcal{O}(h^2).$$

But $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$, hence $\mathbf{y}'' = \mathbf{f}_t + \mathbf{f}_y \mathbf{y}' = \mathbf{f}_t + \mathbf{f}_y \mathbf{f}$, therefore, substituting the exact solution $\mathbf{y} = \mathbf{y}(t_n)$ instead of $\mathbf{y}_n$ into the scheme, we obtain $\mathbf{k}_1 = \mathbf{y}'$ and $\mathbf{k}_2 = \mathbf{y}' + c_2 h \mathbf{y}'' + \mathcal{O}(h^2)$. Consequently, the RK method produces

$$\mathbf{y}(t_{n+1}) = \mathbf{y} + (b_1 + b_2)h\mathbf{y}' + b_2 c_2 h^2 \mathbf{y}'' + \mathcal{O}(h^3),$$

and we deduce that it is of order 2 if

$$b_1 + b_2 = 1, \quad b_2 c_2 = \frac{1}{2}.$$

It is easy to demonstrate that no such method may be of order ≥ 3 (e.g. by applying it to $y' = y$).

Method 9.4 (General Runge-Kutta method) A general s -stage Runge-Kutta method is

$$\begin{aligned} \mathbf{k}_i &= \mathbf{f}(t_n + c_i h, \mathbf{y}_n + h \sum_{j=1}^s a_{ij} \mathbf{k}_j), \quad i = 1..s, \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i. \end{aligned}$$

The explicit RK method corresponds to the case when $a_{ij} = 0$ for $i \leq j$. Otherwise, an RK method is *implicit*.

Example 9.5 Consider the 2-stage implicit method

$$\begin{aligned} \mathbf{k}_1 &= \mathbf{f}\left(t_n, \mathbf{y}_n + \frac{1}{4}h(\mathbf{k}_1 - \mathbf{k}_2)\right), \\ \mathbf{k}_2 &= \mathbf{f}\left(t_n + \frac{2}{3}h, \mathbf{y}_n + \frac{1}{12}h(3\mathbf{k}_1 + 5\mathbf{k}_2)\right), \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + \frac{1}{4}h(\mathbf{k}_1 + 3\mathbf{k}_2). \end{aligned}$$

We analyse its order with respect to scalar *autonomous* equations of the form $y' = f(y)$. For brevity, we use the convention that all functions are evaluated at $y = y(t_n)$. Thus,

$$\begin{aligned} k_1 &= f + \frac{1}{4}h f_y(k_1 - k_2) + \frac{1}{32}h^2 f_{yy}(k_1 - k_2)^2 + \mathcal{O}(h^3), \\ k_2 &= f + \frac{1}{12}h f_y(3k_1 + 5k_2) + \frac{1}{288}h^2 f_{yy}(3k_1 + 5k_2)^2 + \mathcal{O}(h^3). \end{aligned}$$

Substitution $k_1 = f + \mathcal{O}(h)$, $k_2 = f + \mathcal{O}(h)$ in the above equations (h -terms) yields

$$\begin{aligned} k_1 &= f + \mathcal{O}(h^2), \\ k_2 &= f + \frac{2}{3}h f_y f + \mathcal{O}(h^2). \end{aligned}$$

Substituting again, we obtain

$$\begin{aligned} k_1 &= f - \frac{1}{6}h^2 f_y^2 f + \mathcal{O}(h^3), \\ k_2 &= f + \frac{2}{3}h f_y f + h^2 \left(\frac{5}{18}f_y^2 f + \frac{2}{9}f_{yy} f^2 \right) + \mathcal{O}(h^3), \\ y(t_{n+1}) &= y + hf + \frac{1}{2}h^2 f_y f + \frac{1}{6}h^3 (f_y^2 f + f_{yy} f^2) + \mathcal{O}(h^4). \end{aligned}$$

But $y' = f$ implies $y'' = f_y f$ and $y''' = f_y^2 f + f_{yy} f^2$ and we deduce from Taylor's theorem that the method is at least of order 3. (It is easy to verify that it isn't of order 4, for example applying it to the equation $y' = y$.)

Theorem 9.6 (High-order RK methods) Let $\omega(t) = \prod_{i=1}^s (t - c_i)$ be orthogonal on the interval $[0, 1]$ to all polynomials of degree $r - 1 \leq s - 1$, let ℓ_i be the fundamental Lagrange polynomials of degree $s - 1$ for the knots c_i , and let

$$a_{ij} = \int_0^{c_i} \ell_j(t) dt, \quad b_i = \int_0^1 \ell_i(t) dt \quad (9.4)$$

Then the (highly implicit) s -stage RK method with parameters (9.4) is of order $s + r$.

Thus, the highest order of an s -stage implicit RK method is $2s$, it corresponds to collocation at zeros of Legendre polynomial (Gauss-Legendre RK method). Construction of explicit methods with high order is a kind of art.