

13.3. Runge-Kutta methods. We now consider a class of methods, called Runge-Kutta methods, that achieve the same accuracy as Taylor series methods, without calculating derivatives of f . The basic idea is to use a linear combination of several evaluations of $f(x, y)$ to achieve high order accuracy. The simplest case of such methods is again Euler's method.

The basic idea of these methods is to write

$$y_{n+1} - y_n = \sum_{i=1}^m w_i k_i(x_n, y_n),$$

where the w_i 's are constants and

$$k_i(x, y) = h_n f\left(x + \alpha_i h_n, y + \sum_{j=1}^{i-1} \beta_{ij} k_j\right),$$

where $h_n = x_{n+1} - x_n$ (allowing for variable step-size), $\alpha_1 = 0$, and α_i and β_{ij} are constants.

Observe that if the w_i 's, α_i 's, and β_{ij} 's are given, then this is a self-starting method.

$$k_1(x_n, y_n) = h_n f(x_n, y_n), \quad k_2(x_n, y_n) = h_n f(x_n + \alpha_2 h_n, y_n + \beta_{21} k_1(x_n, y_n)), \quad \dots$$

Note that k_1 has already been computed when it is used to compute k_2 and this is true for all the k_i .

The coefficients in the method are determined by several criteria. The first is to achieve a desired order of accuracy in the local truncation error in the method, defined in a similar manner as above for one-step methods as:

$$LTE = y(x_{n+1}) - y(x_n) - \sum_{i=1}^m w_i k_i(x_n, y(x_n)).$$

Rather than consider the general case, for which the computations can get complicated, we illustrate the main idea for the case $m = 2$. To simplify notation, we set $h_n = h$, $\alpha_2 = a$ and $\beta_{21} = b$. Thus, we are considering the method

$$\begin{aligned} y_{n+1} &= y_n + w_1 k_1(x_n, y_n) + w_2 k_2(x_n, y_n), & k_1(x_n, y_n) &= h f(x_n, y_n), \\ k_2(x_n, y_n) &= h f(x_n + ah, y_n + bk_1(x_n, y_n)). \end{aligned}$$

To calculate the local truncation error, we expand $y(x_{n+1}) - y(x_n) - \sum_{i=1}^m w_i k_i(x_n, y(x_n))$ is a Taylor series about x_n . First, we note that

$$y(x_{n+1}) - y(x_n) = hy'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{6} y'''(x_n) + O(h^4).$$

Now for y a solution of the IVP, we have

$$\begin{aligned} y' &= f(x, y), & y'' &= f_x + f_y y' = f_x + f_y f, \\ y''' &= (f_{xx} + f_{xy} f) + [f_y (f_x + f_y f) + f(f_{yx} + f_{yy} f)] = f_{xx} + 2f_{xy} f + f_{yy} f^2 + f_y (f_x + f_y f). \end{aligned}$$

Hence,

$$y(x_{n+1}) - y(x_n) = hf + \frac{h^2}{2}(f_x + f_y f) + \frac{h^3}{6}[f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y(f_x + f_y f)] + O(h^4).$$

We next compute the Taylor series expansion of $w_1 k_1(x_n, y(x_n)) + w_2 k_2(x_n, y(x_n))$. Now $w_1 k_1(x_n, y(x_n)) = w_1 h f(x_n, y(x_n))$, so it only remains to compute the expansion of the term

$$\begin{aligned} w_2 k_2(x_n, y(x_n)) &= h w_2 f(x_n + ah, y(x_n) + b k_1(x_n, y(x_n))) \\ &= h w_2 f(x_n + ah, y(x_n) + b h f(x_n, y(x_n))). \end{aligned}$$

But

$$\begin{aligned} f(x_n + ah, y(x_n) + b h f(x_n, y(x_n))) \\ = f + ah f_x + bh f_y f + \frac{a^2 h^2}{2} f_{xx} + ab h^2 f_{xy} f + \frac{1}{2} b^2 h^2 f_{yy} f^2 + O(h^3), \end{aligned}$$

where all functions on the right side of the equation are evaluated at $(x_n, y(x_n))$. Adding these results, we get

$$\begin{aligned} w_1 k_1(x_n, y(x_n)) + w_2 k_2(x_n, y(x_n)) &= hf[w_1 + w_2] + h^2 f_x [aw_2] + h^2 f_y f [bw_2] \\ &\quad + h^3 [(1/2)a^2 w_2 f_{xx} + ab w_2 f_{xy} f + (1/2)b^2 w_2 f_{yy} f^2] + O(h^4) \end{aligned}$$

Hence,

$$\begin{aligned} LTE &= hf[1 - w_1 - w_2] + h^2 f_x [(1/2) - aw_2] + h^2 f_y f [(1/2) - bw_2] \\ &\quad + \frac{h^3}{6} [f_{xx}(1 - 3a^2 w_2) + 2f_{xy} f (1 - 3ab w_2) + f_{yy} f^2 (1 - 3b^2 w_2) + f_y (f_x + f_y f)] + O(h^4). \end{aligned}$$

Choosing

$$w_1 + w_2 = 1, \quad aw_2 = 1/2, \quad bw_2 = 1/2,$$

we can make the local truncation error $O(h^3)$. Thus, we get a family of methods in which $b = a$, $w_1 = 1 - 1/(2a)$, and $w_2 = 1/(2a)$, i.e, methods of the form:

$$y_{n+1} = y_n + [1 - 1/(2a)]hf(x_n, y_n) + 1/(2a)hf(x_n + ah, y_n + ahf(x_n, y_n)).$$

For these choices, the local truncation becomes

$$\begin{aligned} LTE &= \frac{h^3}{12} [(2 - 3a)(f_{xx} + 2f_{xy}f + f_{yy}f^2) + 2f_y(f_x + f_y f)] + O(h^4) \\ &= \frac{h^3}{12} [(2 - 3a)y''' + 3af_y y'']. \end{aligned}$$

Clearly, there are no choices that will also make all the $O(h^3)$ terms zero, and in fact, there is not even a “best choice” to minimize the error. For example, one can show that for the equation $y' = y^q$ that if $q = 1$, then $LTE = -(1/6)h^3 y + O(h^4)$ for all a and for $q \neq 1$, $LTE = O(h^4)$ if $a = (4q - 2)/(3q - 3)$, i.e., the best choice of a depends on the equation.

The family of formulas

$$y_{n+1} = y_n + [1 - 1/(2a)]hf(x_n, y_n) + [1/(2a)]hf(x_n + ah, y_n + ahf(x_n, y_n))$$

are called simplified Runge-Kutta methods. Two special cases of interest are $a = 1$, called Heun's method

$$y_{n+1} = y_n + (h/2)f(x_n, y_n) + (h/2)f(x_n + h, y_n + hf(x_n, y_n))$$

and $a = 1/2$, called the modified Euler's method

$$y_{n+1} = y_n + hf(x_n + h/2, y_n + (h/2)f(x_n, y_n)).$$

To apply the convergence theorem for one-step methods, we only need to determine the Lipschitz constant

$$|\Phi(x, u) - \Phi(x, v)| \leq \mathcal{L}|u - v|,$$

where

$$\Phi(x, y) = [1 - 1/(2a)]f(x, y) + [1/(2a)]f(x + ah, y + ahf(x, y)).$$

If we assume that $|f(x, u) - f(x, v)| \leq L|u - v|$, then

$$\begin{aligned} |\Phi(x, u) - \Phi(x, v)| &\leq |1 - 1/(2a)||f(x, u) - f(x, v)| \\ &\quad + |1/(2a)||f(x + ah, u + ahf(x, u)) - f(x + ah, v + ahf(x, v))| \\ &\leq |1 - 1/(2a)|L|u - v| + |1/(2a)|L|u + ahf(x, u) - v - ahf(x, v)| \\ &\leq |1 - 1/(2a)|L|u - v| + |1/(2a)|L[|u - v| + ah|f(x, u) - f(x, v)|] \\ &\leq |1 - 1/(2a)|L|u - v| + |1/(2a)|L[|u - v| + ahL|u - v|] \\ &= L|u - v|[|1 - 1/(2a)| + |1/(2a)| + |hL/2|] \leq \mathcal{L}|u - v|, \end{aligned}$$

where

$$\mathcal{L} = L[|1 - 1/(2a)| + |1/(2a)| + |h_0L/2|],$$

for all $h \leq h_0$.

The classical 4th order Runge Kutta method (requiring 4 function evaluations per step) is given by:

$$\begin{aligned} k_1 &= h_n f(x_n, y_n), & k_2 &= h_n f(x_n + h_n/2, y_n + k_1/2), \\ k_3 &= h_n f(x_n + h_n/2, y_n + k_2/2), & k_4 &= h_n f(x_n + h_n, y_n + k_3), \end{aligned}$$

and

$$y_{n+1} = y_n + (k_1 + 2k_2 + 2k_3 + k_4)/6.$$

If f and y are vectors, i.e., we wish to solve

$$Y' = F(x, Y), \quad Y(x_0) = Y_0$$

where $Y = (y_1, \dots, y_n)^T$ and

$$F(x, Y) = (f_1(x, y_1, \dots, y_n), \dots, f_n(x, y_1, \dots, y_n))^T.$$

We then replace k_i by the vector $K_i = (k_{i,1}, \dots, k_{i,n})$.

Remark: For $m = 1, 2, 3, 4$, m th order formulas can be constructed using only m function evaluations per step. For $m = 5$, we require $> m$ function evaluations.