12.3. **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

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

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.

$$k_1(x_n, y_n) = h_n f(x_n, y_n), \qquad k_2(x_n, y_n) = h_n f(x_n + \alpha_2 h_n, y_n + \beta_{21} k_1(x_n, y_n)), \qquad , \cdots .$$

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 coeffients 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

$$y_{n+1} = y_n + w_1 k_1(x_n, y_n) + w_2 k_2(x_n, y_n), \qquad k_1(x_n, y_n) = hf(x_n, y_n),$$
$$k_2(x_n, y_n) = hf(x_n + ah, y_n + bk_1(x_n, y_n)).$$

To calculate the local truncation error, we expand $y(x_{n+1}) - y(x_n) - \sum_{i=0}^{m} w_i k_i(x_n, y(x_n))$ 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

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

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 $w_1k_1(x_n, y(x_n)) + w_2k_2(x_n, y(x_n))$. Now $w_1k_1(x_n, y(x_n)) = w_1hf(x_n, y(x_n))$, so it only remains to compute the expansion of the term

$$\begin{aligned} w_2k_2(x_n, y(x_n)) &= hw_2f(x_n + ah, y(x_n) + bk_1(x_n, y(x_n))) \\ &= hw_2f(x_n + ah, y(x_n) + bhf(x_n, y(x_n))). \end{aligned}$$

But

$$\begin{aligned} &f(x_n + ah, y(x_n) + bhf(x_n, y(x_n))) \\ &\qquad = f + ahf_x + bhf_yf + \frac{a^2h^2}{2}f_{xx} + abh^2f_{xy}f + \frac{1}{2}b^2h^2f_{yy}f^2 + O(h^3), \end{aligned}$$

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

$$\begin{aligned} w_1k_1(x_n, y(x_n)) + w_2k_2(x_n, y(x_n)) &= hf[w_1 + w_2] + h^2f_x[aw_2] + h^2f_yf[bw_2] \\ &\quad + h^3[(1/2)a^2w_2f_{xx} + abw_2f_{xy}f + (1/2)b^2w_2f_{yy}f^2] + O(h^4) \end{aligned}$$

Hence,

$$\begin{aligned} LTE &= hf[1 - w_1 - w_2] + h^2f_x[(1/2) - aw_2] + h^2f_yf[(1/2) - bw_2] \\ &+ \frac{h^3}{6}[f_{xx}(1 - 3a^2w_2) + 2f_{xy}f(1 - 3abw_2) + f_{yy}f^2(1 - 3b^2w_2) + f_y(f_x + f_yf)] + O(h^4). \end{aligned}$$

Choosing

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

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

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

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 $LTE = -(1/6)h^3y + O(h^4)$ 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

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

Example: Compute approximations to the solution of $y' = 2x - y$, $y(0) = 1$ at the points $x = 1/2$ and $x = 1$ using the modified Euler's method with $h = 1/2$. We have

$$\begin{aligned} y_1 &= y_0 + hf(x_0 + h/2, y_0 + (h/2)f(x_0, y_0)) = 1 + (1/2)f(0 + 1/4, 1 + (1/4)(2 \cdot 0 - 1)) \\ &= 1 + (1/2)f(1/4, 3/4) = 1 + (1/2)(-1/4) = 7/8. \\ y_2 &= y_1 + hf(x_1 + h/2, y_1 + (h/2)f(x_1, y_1)) = 7/8 + (1/2)f(1/2 + 1/4, 7/8 + (1/4)(1/8)) \\ &= 7/8 + (1/2)f(3/4, 29/32) = 7/8 + (1/2)(19/32) = 75/64. \end{aligned}$$

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

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

where

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

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

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

where

$$\mathcal{L} = L[|1 - 1/(2a)| + |1/(2a)| + |h_0 L/2|],$$

for all $h \le h_0$.

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

$$k_1 = h_n f(x_n, y_n), \qquad k_2 = h_n f(x_n + h_n/2, y_n + k_1/2),$$
$$k_3 = h_n f(x_n + h_n/2, y_n + k_2/2), \qquad k_4 = h_n f(x_n + h_n, y_n + k_3),$$

and

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

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

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

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

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 $K_i = (k_{i,1}, \dots, k_{i,n})$.

Example: Let $Y = \begin{pmatrix} w \\ z \end{pmatrix}$ and $F(x, Y) = \begin{pmatrix} f_1(x, w, z) \\ f_2(x, w, z) \end{pmatrix}$. The modified Euler's method for the system of differential equations $Y' = F(x, Y)$, with initial condition $Y(x_0) = Y_0$, is given by:

$$Y_{n+1} = Y_n + hF(x_n + h/2, Y_n + (h/2)F(x_n, y_n)).$$

Use this method to find approximations to $w(h)$ and $z(h)$ for the system

$$w' = z, \quad z' = -cw, \qquad w(0) = a, \quad z(0) = b,$$

where a, b, c are given constants.

In terms of w and z, we get:

$$w_{n+1} = w_n + hf_1(x_n + h/2, w_n + (h/2)f_1(x_n, w_n, z_n), z_n + (h/2)f_2(x_n, w_n, z_n)),$$
$$z_{n+1} = z_n + hf_2(x_n + h/2, w_n + (h/2)f_1(x_n, w_n, z_n), z_n + (h/2)f_2(x_n, w_n, z_n)).$$

Now

$$w' = f_1(x, w, z) = z, \qquad z' = f_2(x, w, z) = -cw, \qquad w(0) = a, \quad z(0) = b.$$

So

$$w(h) \approx w_1 = w_0 + h[z_0 + (h/2)f_2(x_0, w_0, z_0)] = w_0 + h(z_0 - (h/2)cw_0) = a + hb - ach^2/2.$$
$$z(h) \approx z_1 = z_0 - ch[w_0 + (h/2)f_1(x_0, y_0, z_0)] = z_0 - ch(w_0 + (h/2)z_0) = b - cha - cbh^2/2.$$