$$K_3 = hf(t_j + c_3 h,\ u_j + a_{31} K_1 + a_{32} K_2)$$

$$\cdots \quad \cdots \quad \cdots \quad \cdots \quad \cdots$$

$$K_v = hf(t_j + c_v h,\ u_j + a_{v1} K_1 + a_{v2} K_2 + \cdots + a_{v,\, v-1} K_{v-1}) \tag{6.94}$$

As mentioned earlier, the methods defined by (6.90), (6.91) or (6.93), (6.91) or (6.94), (6.91) should compare with the Taylor series method. Hence, to determine the parameters c_i's, a_i's and W_i's in the Runge-Kutta methods, we expand u_{j+1} and f's in powers of h such that it agrees with the Taylor series expansion of the solution of the differential equation upto a certain number of terms.

We shall first consider the derivation of explicit Runge-Kutta methods.

Explicit Runge-Kutta Methods

Second Order Methods

Consider the following Runge-Kutta method with two slopes

$$K_1 = hf(t_j, u_j)$$

$$K_2 = hf(t_j + c_2 h,\ u_j + a_{21} K_1)$$

$$u_{j+1} = u_j + W_1 K_1 + W_2 K_2 \tag{6.95}$$

where the parameters c_2, a_{21}, W_1 and W_2 are chosen to make u_{j+1} closer to $u(t_{j+1})$. There are four parameters to be determined. Now, Taylor series expansion about t_j gives

$$u(t_{j+1}) = u(t_j) + hu'(t_j) + \frac{h^2}{2!} u''(t_j) + \frac{h^3}{3!} u'''(t_j) + \cdots$$

$$= u(t_j) + hf(t_j, u(t_j)) + \frac{h^2}{2!} (f_t + ff_u)_{t_j}$$

$$+ \frac{h^3}{3!} [f_{tt} + 2ff_{tu} + f^2 f_{uu} + f_u(f_t + ff_u)]_{t_j} + \cdots \tag{6.96}$$

We also have

$$K_1 = hf_j$$

$$K_2 = hf(t_j + c_2 h,\ u_j + a_{21} hf_j)$$

$$= h[f_j + h(c_2 f_t + a_{21} ff_u)_{t_j}$$

$$+ \frac{h^2}{2} (c_2^2 f_{tt} + 2c_2 a_{21} ff_{tu} + a_{21}^2 f^2 f_{uu})_{t_j} + \cdots]$$

Substituting the values of K_1 and K_2 in (6.95), we get

$$u_{j+1} = u_j + (W_1 + W_2)hf_j + h^2(W_2 c_2 f_t + W_2 a_{21} ff_u)_{t_j}$$

$$+ \frac{h^3}{2} W_2(c_2^2 f_{tt} + 2c_2 a_{21} ff_{tu} + a_{21}^2 f^2 f_{uu})_{t_j} + \cdots \tag{6.97}$$

Comparing the coefficients of h and h^2 in (6.96) and (6.97), we obtain

$$W_1 + W_2 = 1$$

$$c_2 W_2 = 1/2$$

$$a_{21} W_2 = 1/2.$$

The solution of this system is

$$a_{21} = c_2,\ W_2 = \frac{1}{2c_2},\ W_1 = 1 - \frac{1}{2c_2} \tag{6.98}$$

where $c_2 \neq 0$, is arbitrary. It is not possible to compare the coefficients of h^3, as there are five terms in (6.96) and only three terms in (6.97). Therefore, the Runge-Kutta method using two evaluations of f is

$$u_{j+1} = u_j + \left(1 - \frac{1}{2c_2}\right) K_1 + \frac{1}{2c_2} K_2 \tag{6.99}$$

where $K_1 = hf(t_j, u_j)$,

$$K_2 = hf(t_j + c_2 h,\ u_j + c_2 K_1).$$

Substituting (6.98) in (6.97), we get

$$u_{j+1} = u_j + hf_j + \frac{h^2}{2}(f_t + ff_u)_{t_j}$$

$$+ \frac{h^3 c_2}{4}(f_{tt} + 2ff_{tu} + f^2 f_{uu})_{t_j} + \cdots \tag{6.100}$$

The local truncation error is given by

$$T_{j+1} = u(t_{j+1}) - u_{j+1}$$

$$= h^3 \left[\left(\frac{1}{6} - \frac{c_2}{4}\right)(f_{tt} + 2ff_{tu} + f^2 f_{uu})_{t_j} + \frac{1}{6}\{f_u(f_t + ff_u)\}_{t_j} + \cdots\right] \tag{6.101}$$

which shows that the method (6.95) is of second order. It may be noted that every Runge-Kutta method should reduce to a quadrature formula when $f(t, u)$ is independent of u, with W_i's as weights and c_i's as abscissas.

The free parameter c_2 is usually taken between 0 and 1. Sometimes, c_2 is chosen such that one of the W_i's in the method (6.95) is zero. For example, the choice $c_2 = 1/2$ makes $W_1 = 0$.

If $c_2 = 1/2$, we get

$$u_{j+1} = u_j + K_2$$

where $K_1 = hf(t_j, u_j)$,

$$K_2 = hf\left(t_j + \frac{h}{2},\ u_j + \frac{1}{2}K_1\right)$$

which is the Euler method with spacing $h/2$. It is also called the **modified Euler-Cauchy** method. It reduces to the mid-point quadrature rule when $f(t, u)$ is independent of u.

For $c_2 = 1$, we get

$$u_{j+1} = u_j + \frac{1}{2}(K_1 + K_2)$$

where $\quad K_1 = hf(t_j, u_j),$

$$K_2 = hf(t_j + h, u_j + K_1)$$

which reduces to the trapezoidal rule when $f(t, u)$ is independent of u. This method is also called as the **Euler-Cauchy** or **Heun** method.

Minimization of Local Truncation Error

An alternative way of choosing the arbitrary parameter is to **minimize the sum** of the absolute values of the coefficients in the term T_{j+1}. **Such a choice gives** an **optimal** method in the sense of minimum truncation error. **Here, we use the Lotkin's bounds** which are defined by

$$\left|\frac{\partial^{i+j} f}{\partial t^i \partial u^j}\right| < \frac{L^{i+j}}{M^{j-1}}, \; i, j = 0, 1, 2, \cdots$$

We find that

$$|f| < M, \; |f_u| < L, \; |f_t| < LM$$

$$|f_{tt}| < L^2 M, \; |f_{tu}| < L^2, \; |f_{uu}| < \frac{L^2}{M}.$$

Thus, $|T_{j+1}|$ becomes

$$|T_{j+1}| < ML^2h^3\left[4\left|\frac{1}{6} - \frac{c_2}{4}\right| + \frac{1}{3}\right].$$

The minimum value of T_{j+1} occurs for $c_2 = 2/3$ in which case $|T_{j+1}| < ML^2h^3/3$. We have the optimal method as

$$u_{j+1} = u_j + \frac{1}{4}(K_1 + 3K_2) \tag{6.102}$$

where $\quad K_1 = h\,f(t_j, u_j)$

$$K_2 = h\,f(t_j + \frac{2}{3}h, \; u_j + \frac{2}{3}K_1).$$

If the arbitrary parameters are determined by putting the leading coefficients in $|T_{j+1}|$ to zero, then such a formula is called **nearly optimal**. It may be noted that the explicit Runge-Kutta methods using two evaluations of f have one arbitrary parameter and have produced second order methods.