

#### (4.C) RUNGE-KUTTA METHODS

##### (4.21) Example.

In the TS(2) method the user is required to determine and realize the functions:

$$G_2(t, x) \quad \text{to compute } x(k+1)$$

and:

$$G_3(t, x) \quad \text{in the choice of } h(k)$$

In general, the task is more difficult the higher the order of the method: in the TS(p) method the user must determine and realize the functions:

$$G_2(t, x), \dots, G_p(t, x) \quad \text{to compute } x(k+1)$$

and:

$$G_{p+1}(t, x) \quad \text{in the choice of } h(k)$$

The *Runge-Kutta methods* are designed to eliminate this burden.

To introduce the *structure* of the methods, let's see, in the TS(2) method, how the computation of  $x(k+1)$  is transformed when we use a numerical estimate of the value  $G_2(t, x)$ .

##### (4.22) Remark (numerical estimate of $G_2$ ).

The value  $G_2(t(k), x(k)) = y''(t(k))$  can be *estimated* with the following considerations:

(a) By definition:

$$\frac{y'(t(k) + \tau) - y'(t(k))}{\tau} \rightarrow y''(t(k)) \quad \text{as } \tau \rightarrow 0$$

hence:

$$\text{when } \tau \text{ is small } \frac{y'(t(k) + \tau) - y'(t(k))}{\tau} \text{ is a good approximation of } y''(t(k))$$

(b) Since  $y(t)$  is the solution of the differential equation whose value in  $t(k)$  is  $x(k)$  we have:

$$y'(t(k)) = F(t(k), y(t(k))) = F(t(k), x(k))$$

and:

$$y'(t(k) + \tau) = F(t(k) + \tau, y(t(k) + \tau))$$

This last value is *not computable* because, given  $\tau$ , the procedure does not know  $y(t(k) + \tau)$ . Then:

*we approximate  $y(t(k) + \tau)$  with  $y(t(k)) + y'(t(k)) \tau = x(k) + F(t(k), x(k)) \tau$*

Overall:

*using a small value of  $\tau$ , we estimate  $G_2(t(k), x(k)) = y''(t(k))$  with*

$$\frac{F(t(k) + \tau, x(k) + F(t(k), x(k)) \tau) - F(t(k), x(k))}{\tau}$$

This quantity, given  $\tau$ , *is computable without using  $G_2$* .

The estimate is *reasonable*. In fact, set  $F(k) = F(t(k), x(k))$  and consider the function of  $\tau$ :

$$H(\tau) = F(t(k) + \tau, x(k) + F(k) \tau)$$

Since we are assuming  $F(t, x)$  to have *continuous first partial derivatives*,  $H$  also has continuous first derivatives. Then:

$$H(\tau) = H(0) + H'(0) \tau + z(\tau) \tau \quad \text{where } z(\tau) \rightarrow 0 \text{ as } \tau \rightarrow 0$$

But:  $H(0) = F(k)$  and

$$H'(0) = \frac{\partial}{\partial t} F(t(k), x(k)) + \frac{\partial}{\partial x} F(t(k), x(k)) \cdot F(t(k), x(k)) = G_2(t(k), x(k)) = y''(t(k))$$

hence:

$$H(\tau) = F(k) + y''(t(k)) \tau + z(\tau) \tau$$

and:

$$\frac{H(\tau) - F(k)}{\tau} - y''(t(k)) = z(\tau) \rightarrow 0 \text{ as } \tau \rightarrow 0$$

(4.23) Remark (use of the numerical estimate).

In TS(2):

$$x(k+1) = x(k) + F(t(k), x(k)) h(k) + \frac{1}{2} G_2(t(k), x(k)) h(k)^2$$

Using  $\tau = h(k)$  in the estimate of Remark (4.22) we get:

$$G_2(t(k), x(k)) = \frac{F(t(k) + h(k), x(k) + F(t(k), x(k)) h(k)) - F(t(k), x(k))}{h(k)}$$

hence (remember that  $F(k) = F(t(k), x(k))$ ):

$$\begin{aligned} x(k+1) &= x(k) + F(k) h(k) + \frac{1}{2} [F(t(k) + h(k), x(k) + F(k) h(k)) - F(k)] h(k) \\ &= x(k) + \frac{1}{2} [F(k) + F(t(k) + h(k), x(k) + F(k) h(k))] h(k) \end{aligned}$$

This procedure for calculating  $x(k+1)$  can be rewritten, in a more compact way, as follows:  
*the value  $x(k+1)$  is obtained, after having chosen  $h(k)$ , by setting:*

- $ST_1 = F(t(k), x(k))$
- $ST_2 = F(t(k) + h(k), x(k) + ST_1 h(k))$

and then

$$x(k+1) = x(k) + \frac{1}{2} (ST_1 + ST_2) h(k)$$

(4.24) Definition (two and three stages Runge-Kutta methods).

*Two-stage Runge-Kutta (RK) methods* are those in which, after choosing appropriate real numbers  $c_2$ ,  $a_{21}$ ,  $b_1$  and  $b_2$ , the value  $x(k+1)$  is obtained, after having chosen  $h(k)$ , by setting:

- $ST_1 = F(t(k), x(k))$
- $ST_2 = F(t(k) + c_2 h(k), x(k) + a_{21} ST_1 h(k))$

and then

- $x(k+1) = x(k) + (b_1 ST_1 + b_2 ST_2) h(k)$

*Three-stage Runge-Kutta (RK) methods* are those in which, after having chosen appropriate real numbers  $c_2$ ,  $c_3$ ,  $a_{21}$ ,  $a_{31}$ ,  $a_{32}$ ,  $b_1$ ,  $b_2$  and  $b_3$ , the value  $x(k+1)$  is obtained, after having chosen  $h(k)$ , by setting:

- $ST_1 = F(t(k), x(k))$
- $ST_2 = F(t(k) + c_2 h(k), x(k) + a_{21} ST_1 h(k))$
- $ST_3 = F(t(k) + c_3 h(k), x(k) + [a_{31} ST_1 + a_{32} ST_2] h(k))$

and then

- $x(k+1) = x(k) + (b_1 ST_1 + b_2 ST_2 + b_3 ST_3) h(k)$

(4.25) Definition (order of a method as  $h \rightarrow 0$ )

Let  $s(h)$  be the deviation function for the method under consideration. The integer  $p$  is called the *order of the method as  $h \rightarrow 0$*  if:

$$s^{(m)}(0) = 0 \quad \text{for } m = 0, \dots, p \quad \text{and} \quad s^{(p+1)}(0) \neq 0$$

that is, if the first term of the Taylor expansion of  $s(h)$  for  $h = 0$  is that of order  $p+1$ :

$$s(h) = \frac{1}{(p+1)!} s^{(p+1)}(0) h^{p+1} + \dots$$

(4.26) Remark (how to find the parameters in a Runge-Kutta method).

In a multi-stage Runge-Kutta method the values of the parameters  $c_i$ ,  $a_{ij}$ ,  $b_i$  are determined

(*not uniquely*) by the condition that: for *each* function  $F$  defining the Cauchy Problem, the order of the method for  $h \rightarrow 0$ , is *as high as possible*.

(4.27) Example.

Consider the two-stage Runge-Kutta method. For each  $k$ , let  $y(t) = y(t; x(k), t(k))$ . Then we have:

$$s(h) = x(k) + [b_1 ST_1 + b_2 ST_2(h)] h - y(t(k) + h)$$

Hence:

$$s^{(1)}(h) = b_1 ST_1 + b_2 ST_2'(h) h + b_2 ST_2(h) - F[t(k) + h, y(t(k) + h)]$$

$$s^{(2)}(h) = b_2 ST_2''(h) h + 2 b_2 ST_2'(h) - \partial_t F[t(k) + h, y(t(k) + h)] - F[t(k) + h, y(t(k) + h)] \cdot \partial_t F[t(k) + h, y(t(k) + h)]$$

and, since  $ST_2(0) = ST_1 = F[t(k), x(k)]$ :

$$s^{(0)}(0) = s(0) = x(k) - y(t(k)) = 0$$

$$s^{(1)}(0) = (b_1 + b_2 - 1) F[t(k), x(k)]$$

$$s^{(2)}(0) = 2 b_2 ST_2'(0) - \partial_t F[t(k), x(k)] - F[t(k), x(k)] \cdot \partial_t F[t(k), x(k)]$$

Then, set  $F_k(h) = F[t(k) + c_2 h, x(k) + a_{21} ST_1 h]$  and hence  $ST_1 = F[t(k), x(k)] = F_k(0)$ , it is:

$$ST_2'(h) = c_2 \partial_t F_k(h) + a_{21} F_k(0) \partial_x F_k(h)$$

and:

$$s^{(2)}(0) = (2 b_2 c_2 - 1) \partial_t F_k(0) + (2 b_2 a_{21} - 1) F_k(0) \partial_x F_k(0)$$

Finally:

$$s^{(1)}(0) = 0 \text{ for every } F \Leftrightarrow b_1 + b_2 - 1 = 0$$

$$s^{(2)}(0) = 0 \text{ for every } F \Leftrightarrow 2 b_2 c_2 - 1 = 0 \text{ and } 2 b_2 a_{21} - 1 = 0$$

and the method is of order *at least* two for  $h \rightarrow 0$  if and only if:

$$b_1 + b_2 = 1, \quad 2 b_2 c_2 = 1, \quad 2 b_2 a_{21} = 1$$

For example:

$$b_1 = b_2 = 1/2, \quad c_2 = a_{21} = 1 \quad (\text{Heun method})^1$$

$$b_1 = 0, \quad b_2 = 1, \quad c_2 = a_{21} = 1/2 \quad (\text{modified Euler method or midpoint method})$$

(4.28) Remark.

For a method of order  $p$  we have:<sup>2</sup>

- $N \rightarrow \infty$  as  $1/\sqrt[p+1]{E}$  ;
- For every  $k$ :  $ET(k) \rightarrow 0$  as  $\sqrt[p+1]{E^p} = E^{\frac{p}{p+1}}$

<sup>1</sup> It is the method of Example (4.23), also called 'improved Euler method'.

<sup>2</sup> Proof omitted.

(4.29) Remark.

Definition (4.24) extends to methods with any number of stages. Furthermore: the maximum order of a one-stage method is *one* (there is only one one-stage method of order one: the TS(1) method), of a two-stage method it is *two*, and of a three-stage method it is *three*. In general, *the maximum order of a method is less than or equal to the number of stages*.