

(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:

when τ is small $\frac{y'(t(k) + \tau) - y'(t(k))}{\tau}$ 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 τ , 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 τ , 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 τ , 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 τ :

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

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:²

$$\bullet \quad N \rightarrow \infty \text{ as } 1/\sqrt[p+1]{E} ;$$

$$\bullet \quad \text{For every } k: ET(k) \rightarrow 0 \text{ as } \sqrt[p+1]{E^p} = E^{\frac{p}{p+1}}$$

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

² 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*.