Module 6: Implicit Runge-Kutta Methods

Lecture 16: Derivation of Implicit Runge-Kutta methods

The Lecture Contains:

This lecture introduces the general R-stage implicit Runge-Kutta methods and derives such a method for the case with R=2.

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The general R-stage implicit Runge-Kutta method is defined by

$$y_{n+1} - y_n = h\,\emptyset(t_n, y_n, h) \quad (6.1)$$

where

$$\emptyset(t, y, h) = \sum_{r=1}^{R} c_r k_r$$

with

$$k_r = f(t + ha_r, y + h\sum_{s=1}^{R} b_{rs} k_s), \qquad r = 1, 2, \dots \dots \dots \dots, R \quad (6.2)$$

and

$$a_r = \sum_{s=1}^{R} b_{rs},\ r = 1, 2, \dots \dots \dots \dots \dots, R \quad (6.3)$$

The functions k_r are no longer defined explicitly but by a set of R implicit equations and thus making the derivation of such methods tedious. We shall consider here only the two-stage method obtained by setting $R = 2$ in (6.1)-(6.3). Let us also recall the expansion for $\phi_T(t, y, h)$ which is given by

$$\emptyset_T(t, y, h) = f + \frac{1}{2}hF + \frac{1}{6}h^2(Ff_y + G) + \frac{1}{24}h^3\left[\left(3f_{ty} + 3ff_{yy} + f_y^2\right)F + Gf_y + H\right] + 0(h^4) \quad (6.4)$$

where, extending the notation of (3.18)

$$F = f_t + ff_y$$

$$G = f_{tt} + 2ff_{ty} + f^2 f_{yy}$$

$$H = f_{ttt} + 3ff_{tty} + 3f^2 f_{tyy} + f^3 f_{yyy}$$

Now from (6.2) with $R = 2$, we have

$$K_r = f(t + ha_r, y + b_{r1}\, hk_1 + b_{r2}\, hk_2),\ r\ = 1, 2.$$

Expanding K_r by Taylor series about (f, y), we get

$$\begin{aligned} K_r = f + h\big[a_r f_t + (b_{r1}K_1 + b_{r2}K_2)f_y\big] \\ + \frac{1}{2}h^2\big[a_r^2 f_{tt} + 2a_r(b_{r1}K_1 + b_{r2}K_2)f_{ty} + (b_{r1}K_1 + b_{r2}K_2)^2 f_{yy}\big] \\ + \frac{1}{6}h^3\big[a_r^3 f_{ttt} + 3a_r^2(b_{r1}K_1 + b_{r2}K_2)f_{tty} + 3a_r(b_{r1}K_1 + b_{r2}K_2)^2 f_{tyy} \\ + (b_{r1}K_1 + b_{r2}K_2)^3 f_{yyy}\big] + 0(h^4) \end{aligned} \quad (6.5)$$

Since these two equations are implicit, we can no longer proceed by successive substitution as done in the case of explicit Runge-Kutta methods earlier. Let us assume instead, that the solutions for K_1 and K_2 may be expressed in the form

$$K_r\ = A_r + hB_r + h^2 C_r + h^3 D_r + 0(h^4) \qquad r\ =\ 1, 2 \quad (6.6)$$

Substituting for k_r by (6.6) in (6.5) we get

$$A_r + hB_r + h^2C_r + h^3D_r = f + h\big[a_r f_t + \{b_{r1}(A_1 + hB_1 + h^2C_1) + b_{r2}(A_2 + hB_2 + h^2C_2)\}f_y\big] + \frac{h^2}{2}\big[a_r^2 f_{tt} + 2a_r\{b_{r1}(A_1 + hB_1) + b_{r2}(A_2 + hB_2)\}f_{ty} + \{b_{r1}(A_1 + hB_1) + b_{r2}(A_2 + hB_2)\}^2 f_{yy}\big] + \frac{h^3}{6}\big[a_r^3 f_{ttt} + 3a_r^2(b_{r1}A_1 + b_{r2}A_2)f_{tty} + 3a_r(b_{r1}A_1 + b_{r2}A_2)^2 f_{tyy} + (b_{r1}A_1 + b_{r2}A_2)^3 f_{yyy}\big] + 0(h^4), \qquad r = 1, 2$$

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On equating powers of h we obtain

$$A_r = f$$

$$B_r = a_r f_t + (b_{r1}A_1 + b_{r2}A_2)f_y$$

$$C_r = (b_{r1}B_1 + b_{r2}B_2)f_y + \frac{1}{2}a^2{}_r f_{tt} + a_r(b_{r1}A_1 + b_{r2}A_2)\ f_{ty} + \frac{1}{2}(b_{r1}A_1 + b_{r2}A_2)^2 f_{yy}$$

$$\begin{aligned} D_r = \big(b_{r1,}C_1 + b_{r2}C_2\big)f_y + a_r(b_{r1}\,B_1 + b_{r2}\,B_2)f_{ty} + (b_{r1}A_1 + b_{r2}A_2)(b_{r1}B_1 + b_{r2}B_2)f_{yy} \\ + \frac{1}{6}a_r^3 f_{ttt} + \frac{1}{2}a_r^2(b_{r1}A_1 + b_{r2}A_2)f_{tty} + \frac{1}{2}a_r(b_{r1}A_1 + b_{r2}A_2)^2 f_{tyy} \\ + \frac{1}{6}(b_{r1}A_1 + b_{r2}A_2)^3 f_{yyy};\ r = 1, 2 \end{aligned}$$

This set of equations is seen to be explicit and can be solved by successive substitution. Making use of (6.3), we obtain

$$A_r = f$$

$$B_r = a_r F$$

$$C_r = (b_{r1}a_1 + b_{r2}a_2)F\,f_y + \tfrac{1}{2}a_r^2 G$$

$$\begin{aligned} D_r = [b_{r1}(b_{11}a_1 + b_{12}a_2) + b_{r2}(b_{21}a_1 + b_{22}a_2)].Ff_y^2 + a_r(b_{r1}a_1 + b_{r2}a_2)F\big(f_{ty} + ff_{yy}\big) + \\ \tfrac{1}{2}(b_{r1}a_1^2 + b_{r2}a_2^2)Gf_y + \tfrac{1}{6}a_r^3 H \quad\ r = 1, 2 \end{aligned} \qquad (6.7)$$

Using (6.6), the expansion for $\phi(t, y, h)$ defined by (6.2) may be written as

$$\phi(t, y, h) = c_1 A_1 + c_2 A_2 + h(c_1 B_1 + c_2 B_2) + h^2(c_1 C_1 + c_2 C_2) + h^3(c_1 D_1 + c_2 D_2) + 0(h^4)$$

where the coefficients $A_r, B_r, C_r, D_r, r = 1{,}2$ are given by (6.7). Comparing this with the expansion (6.4) for $\phi_T(t, y, h)$, we see that the two stage implicit Runge-Kutta method will have order one if

$$C_1 + C_2 = 1 \qquad (6.8)$$

order two, if

$$C_1 + C_2 = 1$$

&

$$C_1 a_1 + C_2 a_2 = \frac{1}{2} \qquad (6.9)$$

and order three, if

$$C_1 + C_2 = 1$$

$$C_1 a_1 + C_2 a_2 = \frac{1}{2}$$

$$C_1(b_{11} a_1 + b_{12} a_2) + C_2(b_{21} a_1 + b_{22} a_2) = \frac{1}{6} \qquad (6.10)$$

$$C_1 a_1^2 + C_2 a_2^2 = \frac{1}{3}$$

and order four, if

$$C_1 + C_2 = 1$$

$$C_1 a_1 + C_2 a_2 = \frac{1}{2}$$

$$C_1(b_{11}a_1 + b_{12}a_2) + C_2(b_{21}a_1 + b_{22}a_2) = \frac{1}{6}$$

$$C_1 a_1^2 + C_2 a_2^2 = \frac{1}{3}$$

$$(C_1 b_{11} + C_2 b_{21})(b_{11}a_1 + b_{12}a_2) + (C_1 b_{12} + C_2 b_{22})(b_{21}a_1 + b_{22}a_2) = \frac{1}{24}$$

$$C_1 a_1(b_{11}a_1 + b_{12}a_2) + C_2 a_2(b_{21}a_1 + b_{22}a_2) = \frac{1}{8}$$

$$C_1(b_{11}a_1^2 + b_{12}a_2) + C_2(b_{21}a_1^2 + b_{22}a_2^2) = \frac{1}{12}$$

$$C_1 a_1^3 + C_2 a_2^3 = \frac{1}{4} \qquad (6.11)$$

Moreover, from (6.3) we must have

$$a_1 = b_{11} + b_{12}$$

$$a_2 = b_{21} + b_{22}$$

In view of this last requirement, there are only six undetermined coefficients, namely $C_1, C_2, a_1, a_2, b_{12}, b_{21}$.