Notes on Runge-Kutta method

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I. EXPLICIT RUNGE-KUTTA SCHEME

For the fundamental therorem of calculus,

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(y(\tau), \tau) d\tau = y(t_n) + h \int_0^1 f(y(t_n + h\tau), t_n + h\tau) d\tau \tag{1}$$

replace the integral with a quadrature approximation

$$y_{n+1} = y_n + h\Sigma_{i=1}^{s} b_i f(y(t_n + c_i h), t_n + c_i h) \tag{2}$$

then we have to construct an approximation, denoted by $Y_i \simeq y(t_n + c_i h)$. With explicit Runge-Kutta methods you construct Y_i using

$$Y_1 = y_n, \quad f(Y_1, t_n), \quad f(Y_2, t_n + hc_2), \quad ..., \quad f(Y_{i-1}, t_n + hc_{i-1}). \tag{3}$$

Then

$$Y_1 = y_n, \tag{4}$$
$$Y_2 = y_n + ha_{21} f(Y_1, t_n), \tag{5}$$
$$Y_3 = y_n + ha_{31} f(Y_1, t_n) + ha_{32} f(Y_2, t_n + hc_2), \tag{6}$$
$$... \tag{7}$$
$$Y_s = y_n + h\Sigma_{i=1}^{s-1} a_{si} f(Y_i, t_n + hc_i). \tag{8}$$
$$y_{n+1} = y_n + h\Sigma_{i=1}^{s} b_i f(Y_i, t_n + hc_i) \tag{9}$$

More

$$y' = f(y, t) \tag{10}$$
$$y'' = \frac{d}{dt} y' = \left(\frac{\partial}{\partial t} + f \frac{\partial}{\partial y} \right) f = \frac{\partial f}{\partial t} + f \frac{\partial f}{\partial y} \tag{11}$$
$$y''' = \frac{d}{dt} y'' = \left(\frac{\partial}{\partial t} + f \frac{\partial}{\partial y} \right) \left(\frac{\partial f}{\partial t} + f \frac{\partial f}{\partial y} \right) \tag{12}$$
$$= \frac{\partial^2 f}{\partial t^2} + f \frac{\partial^2 f}{\partial t \partial y} + \frac{\partial f}{\partial t} \frac{\partial f}{\partial y} + f \frac{\partial^2 f}{\partial y \partial t} + f \frac{\partial f}{\partial y} \frac{\partial f}{\partial y} + f^2 \frac{\partial^2 f}{\partial y^2} \tag{13}$$
$$= \frac{\partial^2 f}{\partial t^2} + f^2 \frac{\partial^2 f}{\partial y^2} + 2f \frac{\partial^2 f}{\partial t \partial y} + \frac{\partial f}{\partial t} \frac{\partial f}{\partial y} + f \left(\frac{\partial f}{\partial y} \right)^2 \tag{14}$$

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A. Two-stage, second-order RK

$$Y_1 = y_n \tag{15}$$
$$Y_2 = y_n + ha_{21}f(Y_1, t_n) \tag{16}$$
$$y_{n+1} = y_n + hb_1 f(Y_1, t_n) + hb_2 f(Y_2, t_n + c_2 h) \tag{17}$$

Taylar expand about (y_n, t_n):

$$y_{n+1} = y_n + hb_1 f(y_n, t_n) + hb_2 \left[f + h\left(a_{21}\frac{\partial f}{\partial y} f + c_2 \frac{\partial f}{\partial t} \right) \right] + \mathcal{O}(h^3) \tag{18}$$
$$= y_n + h(b_1 + b_2) f + h^2 b_2 \left(a_{21}\frac{\partial f}{\partial y} f + c_2 \frac{\partial f}{\partial t} \right) + \mathcal{O}(h^3) \tag{19}$$

since

$$f(Y_2, t_n + c_2 h) = f(y_n + ha_{21}f(Y_1, t_n), t_n + c_2 h) \tag{20}$$
$$= f(y_n, t_n) + h\left[\frac{\partial f}{\partial y}(y_n, t_n) a_{21} f(y_n, t_n) + \frac{\partial f}{\partial t}(y_n, t_n) c_2 \right] + \mathcal{O}(h^2) \tag{21}$$

Compare to the Tayler expansion

$$y(t_n + h) = y(t_n) + hy'(t_n) + \frac{h^2}{2} y''(t_n) + \mathcal{O}(h^3) \tag{22}$$
$$= y_n + hf + \frac{h^2}{2}\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y} \right) + \mathcal{O}(h^3) \tag{23}$$

we have the order condition

$$b_1 + b_2 = 1 \tag{24}$$
$$b_2 a_{21} = \frac{1}{2} \tag{25}$$
$$b_2 c_2 = \frac{1}{2} \tag{26}$$

B. Three-stage, third-order RK

$$Y_i = y_n + h\Sigma_{j=1}^{i-1} a_{ij} f(Y_j, t_c + c_j h) \tag{27}$$
$$y_{n+1} = y_n + h\Sigma_{i=1}^{s} b_i f(Y_i, t_n + c_i h) \tag{28}$$

Consider $t_n = 0, y(t) = t \Rightarrow y(0) = 0, y' = 1$. For first order accuracy, need to obtain the exact solution of $y(t) = t$.

$$Y_i = y_n + h\Sigma_{j=1}^{i-1} a_{ij} \simeq y(t_n + c_i h) = y_n + hc_i, \tag{29}$$
$$y_{n+1} = y_n + h\Sigma_{i=1}^{s} b_i = y_n + h. \tag{30}$$

$$\Rightarrow \left\{ \begin{array}{c} \Sigma_{j=1}^{i-1} a_{ij} = c_i, \\ \Sigma_{i=1}^{s} b_i = 1. \end{array} \right. \Rightarrow \left\{ \begin{array}{c} a_{21} = c_2 \end{array} \right. \tag{31}$$

where is necessary for first-order accuracy.

For up to the 3-order conditions, it sufices to study the case of autonomous differential equations, $y' = f(y)$.

$$
\begin{aligned}
Y_1 &= y_n, && (32)\\
Y_2 &= y_n + hc_2 f, && (33)\\
Y_3 &= y_n + h(c_3 - a_{32})f(Y_1) + ha_{32}f(Y_2) && (34)\\
&= y_n + h(c_3 - a_{32})f + ha_{32}\left(f + hc_2 f f_y + \frac{(hc_2 f)^2}{2} f_{yy} + \mathcal{O}(h^3)\right) && (35)\\
&= y_n + hc_3 f + h^2 a_{32} c_2 f_y f + \frac{h^3 a_{32} c_2^2}{2} f_{yy} f^2 + \mathcal{O}(h^4) && (36)
\end{aligned}
$$

where we have used

$$
\begin{aligned}
f(Y_2) &= f(y_n + hc_2 f) = f + hc_2 f f_y + \frac{(hc_2 f)^2}{2} f_{yy} + \mathcal{O}(h^3) && (37)\\
f(Y_3) &= f(y_n + hc_3 f + h^2 a_{32} c_2 f_y f + \mathcal{O}(h^3)) && (38)\\
&= f + f_y\left(hc_3 f + h^2 a_{32} c_2 f_y f + \mathcal{O}(h^3)\right) + \frac{1}{2} f_{yy}\left(hc_3 f + h^2 a_{32} c_2 f_y f + \mathcal{O}(h^3)\right)^2 + \mathcal{O}(h^3) && (39)\\
&= f + hc_3 f f_y + h^2 a_{32} c_2 f_y^2 f + \frac{1}{2} f_{yy}(h^2 c_3^2 f^2) + \mathcal{O}(h^3) && (40)\\
&= f + hc_3 f f_y + h^2(a_{32} c_2 f_y^2 f + \frac{1}{2} c_3^2 f^2 f_{yy}) + \mathcal{O}(h^3) && (41)
\end{aligned}
$$

then

$$
\begin{aligned}
y_{n+1} = y_n &+ hb_1 f + hb_2\left(f + hc_2 f f_y + \frac{(hc_2 f)^2}{2} f_{yy}\right) && (42)\\
&+ hb_3\left(f + hc_3 f f_y + h^2(a_{32} c_2 f_y^2 f + \frac{1}{2} c_3^2 f^2 f_{yy})\right) + \mathcal{O}(h^4) && (43)\\
= y_n &+ h(b_1 + b_2 + b_3)f + h^2(c_2 b_2 + c_3 b_3) f_y f + h^3(\frac{1}{2}(b_2 c_3^2 + b_3 c_3^2) f_{yy} f^2 + b_3 a_{32} c_2 f_y^2 f) + \mathcal{O}(h^4) && (44)
\end{aligned}
$$

Tayler expansion

$$
y(t_n + h) = y_n + hf + \frac{h^2}{2}(f f_y) + \frac{h^3}{6}\left(f f_y^2 + f^2 f_{yy}\right) + \mathcal{O}(h^4) \qquad (45)
$$

where we have used

$$
y' = f, \quad y'' = (f\frac{\partial}{\partial y})f = f f_y, \quad y''' = (f\frac{\partial}{\partial y})(f f_y) = f f_y f_y + f^2 f_{yy} \qquad (46)
$$

Compare the above two equations, we got the order condition

$$
\begin{aligned}
& b_1 + b_2 + b_3 = 1, && (47)\\
& b_2 c_2 + b_3 c_3 = \frac{1}{2}, && (48)\\
& \frac{1}{2}(b_2 c_2^2 + b_3 c_3^3) = \frac{1}{6}, && (49)\\
& b_c a_{32} c_2 = \frac{1}{6}. && (50)
\end{aligned}
$$