Notes on Implementing MC's Method

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Contents

I. EXPLICIT RUNGE-KUTTA SCHEME

To integrate the ODE

$$\frac{dy}{dt} = f(y,t), \tag{1}$$

we start from the fundamental therorem of calculus

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(y(\tau),\tau)d\tau = y(t_n) + h\int_0^1 f(y(t_n + h\tau), t_n + h\tau)d\tau. \tag{2}$$

We can replace the integral with a quadrature approximation

$$y_{n+1} = y_n + h\Sigma_{i=1}^s b_i f(y(t_n + c_i h), t_n + c_i h), \tag{3}$$

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

$$y_n, \quad f(Y_1, t_n + hc_1), \quad f(Y_2, t_n + hc_2), \quad ..., \quad f(Y_{i-1}, t_n + hc_{i-1}). \tag{4}$$

Then the explicit Runge-Kutta method can be sum up as the following,

$$\boxed{\begin{aligned} Y_s &= y_n + h\Sigma_{i=1}^{s-1} a_{si} f(Y_i, t_n + hc_i), & (5)\\ y_{n+1} &= y_n + h\Sigma_{i=1}^s b_i f(Y_i, t_n + hc_i). & (6)\end{aligned}}$$

We can also introduce the intermediate slopes as $k_i := f(Y_i, t_n + hc_i)$, then

$$y_{n+1} = y_n + h\Sigma_{i=1}^s b_i k_i. \tag{7}$$

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Further more for the chain rule,

$$
\begin{aligned}
y' &= f(y,t) && (8)\\
y'' &= \frac{d}{dt}y' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right) f = \frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y} && (9)\\
y''' &= \frac{d}{dt}y'' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right)\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\\
&= \frac{\partial^2 f}{\partial t^2} + f\frac{\partial^2 f}{\partial t \partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f\frac{\partial^2 f}{\partial y \partial t} + f\frac{\partial f}{\partial y}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2}\\
&= \frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t \partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2} + f\left(\frac{\partial f}{\partial y}\right)^2 && (10)
\end{aligned}
$$

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

$$
\begin{aligned}
Y_i &= y_n + h\Sigma_{j=1}^{i-1} a_{ij} \simeq y(t_n + c_i h) = y_n + hc_i, && (11)\\
y_{n+1} &= y_n + h\Sigma_{i=1}^{s} b_i = y_n + h. && (12)
\end{aligned}
$$

$$
\Rightarrow \begin{cases} \Sigma_{j=1}^{i-1} a_{ij} = c_i, \\ \Sigma_{i=1}^{s} b_i = 1, \end{cases} \tag{13}
$$

$a_{21} = c_2$ for example.

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

$$
\begin{aligned}
y' &= f, && (14)\\
y'' &= (f\frac{\partial}{\partial y})f = ff_y, && (15)\\
y''' &= (f\frac{\partial}{\partial y})(ff_y) = ff_y^2 + f^2 f_{yy} && (16)
\end{aligned}
$$

A. Dense Output

Consider formulas of the form for a 4-stage Runge-Kutta method [1]

$$
u(\theta) = y_n + h\Sigma_{i=1}^{4} b_i(\theta) k_i. \tag{17}
$$

where k_i is defined below eq. (6), and $b_i(\theta)$ are polynomicals to be determined such that $u(\theta) - y(x_0 + \theta h) = \mathcal{O}(h^{p^*+1})$. We write the polynomials $b_j(\theta)$ as

$$
b_j(\theta) = \Sigma_{q=1}^{p^*} b_{jq}\theta^q. \tag{18}
$$

For the 4-stage RK4 with $p^* = 3$ the order condition produce a unique solution

$$
\begin{aligned}
b_1(\theta) &= \theta - \frac{3}{2}\theta^2 + \frac{2}{3}\theta^3, && (19)\\
b_2(\theta) &= b_3(\theta) = \theta^2 - \frac{2}{3}\theta^3, && (20)\\
b_4(\theta) &= -\frac{1}{2}\theta^2 + \frac{2}{3}\theta^3. && (21)
\end{aligned}
$$

The dense output formula can be summarized as [2]

$$
\boxed{
\begin{aligned}
y(t_n + \theta h) &= y_n + h\Sigma_{i=1}^{4} b_i(\theta) k_i + \mathcal{O}(h^4), && (22)\\
\frac{d^{(m)}}{dt^{(m)}} y(t_n + \theta h) &= \frac{1}{h^{(m-1)}}\Sigma_{i=1}^{s} k_i \frac{d^{(m)}}{d\theta^{(m)}} b_i(\theta) + \mathcal{O}(h^{4-m}). && (23)
\end{aligned}
}
$$

B. Taylor expansion of k_i for RK4 up to $\mathcal{O}(h^2)$

The taylor expansion of k_i around t_n are [2]

$$k_1 = y', \tag{24}$$

$$k_2 = y' + \frac{h}{2}y'' + \frac{h^2}{8}(y''' - f_y y''), \tag{25}$$

$$k_3 = y' + \frac{h}{2}y'' + \frac{h^2}{8}(y''' + f_y y''). \tag{26}$$

where $f_y y'' \equiv (y'')^2/y' = \frac{4(k_3^{(c)} - k_2^{(c)})}{h_{(c)}^2}$, and y', y'', y''' can be represented with $k_i^{(c)}$ of coarse grid using the dense output formula (22)-(23). Obviously, h appears here are $h^{(f)}$, while h appears in (22)-(23) are $h^{(c)}$.

C. Taylor expansion of Y_i for RK4 up to $\mathcal{O}(h^3)$

Similarly, we can also expand Y_i instead of k_i [3]

$$Y_1 = y_n, \tag{27}$$

$$Y_2 = y_n + \frac{h}{2}y', \tag{28}$$

$$Y_3 = y_n + \frac{h}{2}y' + \frac{h^2}{4}y'' + \frac{h^3}{16}(y''' - f_y y'') \tag{29}$$

$$Y_4 = y_n + hy' + \frac{h^2}{2}y'' + \frac{h^3}{8}(y''' + f_y y'') \tag{30}$$

where $f_y y'' \equiv (y'')^2/y' = \frac{4(k_3^{(c)} - k_2^{(c)})}{h_{(c)}^2}$, and y', y'', y''' can be represented with $k_i^{(c)}$ of coarse grid using the dense output formula (22)-(23).

1. Pseudocode of MC's method

1. Integrate coarse grid from t_n to $t_n + h^{(c)}$ and store $k_i^{(c)}$ somewhere.
2. Interpolate in time for y, y', y'', y''' using (22)-(23) with stored $k_i^{(c)}$
   (a) at $\theta = 0.0$ for the first fine step,
   (b) at $\theta = 0.5$ for the second fine step.
3. Calculate Y_i for the first and second fine steps using (27)-(30).
4. Interpolate in space to fill Y_i in the fine ghost points.
5. Repeat.

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[1] Roger Alexander. Solving ordinary differential equations i: Nonstiff problems (e. hairer, sp norsett, and g. wanner). Siam Review, 32(3):485, 1990.
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[3] Peter McCorquodale and Phillip Colella. A high-order finite-volume method for conservation laws on locally refined grids. Communications in Applied Mathematics and Computational Science, 6(1):1–25, 2011.