Notes on Implementing MC's Method

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I. EXPLICIT RUNGE-KUTTA SCHEME

To integrate the ODE

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

we start from the fundamental theorem of calculus

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

We can replace the integral with a quadrature approximation

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

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

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

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

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

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

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Further more for the chain rule.

$$y' = f(y, t) \tag{8}$$

$$y'' = \frac{d}{dt}y' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right)f = \frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}$$

$$y''' = \frac{d}{dt}y'' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right)\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)$$

$$= \frac{\partial^2 f}{\partial t^2} + f\frac{\partial^2 f}{\partial t\partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f\frac{\partial^2 f}{\partial y\partial t} + f\frac{\partial f}{\partial y}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2}$$

$$= \frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2} + f\left(\frac{\partial f}{\partial y}\right)^2$$

$$(10)$$

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.

$$Y_i = y_n + h\sum_{i=1}^{i-1} a_{ij} \simeq y(t_n + c_i h) = y_n + hc_i, \tag{11}$$

$$y_{n+1} = y_n + h\sum_{i=1}^s b_i = y_n + h. (12)$$

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

$$(13)$$

 $a_{21} = c_2$ for example.

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

$$y' = f, (14)$$

$$y'' = (f\frac{\partial}{\partial y})f = ff_y, \tag{15}$$

$$y''' = \left(f\frac{\partial}{\partial y}\right)(ff_y) = ff_y^2 + f^2 f_{yy} \tag{16}$$

Dense Output

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

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

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 $b_i(\theta)$ as

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

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

$$b_1(\theta) = \theta - \frac{3}{2}\theta^2 + \frac{2}{3}\theta^3, \tag{19}$$

$$b_2(\theta) = b_3(\theta) = \theta^2 - \frac{2}{3}\theta^3, \tag{20}$$

$$b_4(\theta) = -\frac{1}{2}\theta^2 + \frac{2}{3}\theta^3. \tag{21}$$

The dense output formula can be summarized as [2]

$$y(t_n + \theta h) = y_n + h \sum_{i=1}^4 b_i(\theta) k_i + \mathcal{O}(h^4), \tag{22}$$

$$y(t_n + \theta h) = y_n + h \sum_{i=1}^4 b_i(\theta) k_i + \mathcal{O}(h^4),$$

$$\frac{d^{(m)}}{dt^{(m)}} y(t_n + \theta h) = \frac{1}{h^{(m-1)}} \sum_{i=1}^s k_i \frac{d^{(m)}}{d\theta^{(m)}} b_i(\theta) + \mathcal{O}(h^{4-m}).$$
(22)

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]

$$k_1 = y', (24)$$

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

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

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).

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]

$$Y_1 = y_n, (27)$$

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

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

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