RK4 Derivation

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November 25, 2020

Suppose $y(t_0) = y_0$ and we are estimating $y(t_0 + h)$. We assume a method of the form

$$y_n = y_0 + h \sum_{i=0}^{n-1} c_i f(t_0 + a_i h, y_i) \tag{1}$$

where

$$y_i = y_0 + h \sum_{j=0}^{i-1} b_{ij} f(t_0 + a_j h, y_j). \tag{2}$$

y_n will approximate $y(t_0 + h)$. We will assume that for $0 \le i \le n-1$,

$$a_i = \sum_{j=0}^{i-1} b_{ij} \tag{3}$$

and assume that f only depends on y. There is math that justifies this. We have

$$f(y_i) = f(y_0) + f_y(y_i - y_0) + \frac{1}{2} f_{yy}(y_i - y_0)^2 + \frac{1}{6} f_{yyy}(y_i - y_0)^3 + O(h^4). \tag{4}$$

Thus

$$\begin{aligned}
y_n &= y_0 + h \sum_{i=0}^{n-1} c_i f(y_i) && (5)\\
&= y_0 + h \sum_{i=0}^{n-1} c_i \left(f + f_y h \sum_{j=0}^{i-1} b_{ij} f(y_j) + \frac{1}{2} f_{yy} \left(h \sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^2 + \frac{1}{6} f_{yyy} \left(h \sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^3 \right) + O(h^5) && (6)\\
&= y_0 + hf \sum_{i=0}^{n-1} c_i + h^2 f_y \sum_{i=0}^{n-1} c_i \sum_{j=0}^{i-1} b_{ij} f(y_j) + \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^2 + \frac{1}{6} h^4 f_{yyy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^3 + O(h^5) && (7)\\
&= y_0 + T_1 + T_2 + T_3 + T_4 + O(h^5). && (8)
\end{aligned}$$

Expand h^2 term, T_2, to $O(h^5)$:

$$T_2 = h^2 f_y \sum_{i=0}^{n-1} c_i \sum_{j=0}^{i-1} b_{ij} f(y_j) \tag{9}$$

We need to expand $f(y_j)$ to $O(h^3)$. We have

$$
\begin{aligned}
f(y_j) &= f + f_y h \sum_{k=0}^{j-1} b_{jk} f(y_k) + \frac{1}{2} f_{yy} h^2 \left(\sum_{k=0}^{j-1} b_{jk} f(y_k) \right)^2 + O(h^3) && (10) \\
&= f + f_y h \sum_{k=0}^{j-1} b_{jk} \left(f + f_y h \sum_{l=0}^{k-1} b_{kl} f(y_l) + O(h^2) \right) + \frac{1}{2} f_{yy} h^2 \left(\sum_{k=0}^{j-1} b_{jk} f + O(h) \right)^2 + O(h^3) && (11) \\
&= f + f_y h \sum_{k=0}^{j-1} b_{jk} \left(f + f_y h \sum_{l=0}^{k-1} b_{kl} f \right) + \frac{1}{2} f_{yy} h^2 \left(\sum_{k=0}^{j-1} b_{jk} f \right)^2 + O(h^3) && (12) \\
&= f + h f_y f \sum_{k=0}^{j-1} b_{jk} + h^2 f_y^2 f \sum_{k=0}^{j-1} b_{jk} \sum_{l=0}^{k-1} b_{kl} + \frac{1}{2} h^2 f_{yy} f^2 \left(\sum_{k=0}^{j-1} b_{jk} \right)^2 + O(h^3) && (13)
\end{aligned}
$$

Thus

$$
\begin{aligned}
T_2 &= h^2 f_y \sum_{i=0}^{n-1} c_i \sum_{j=0}^{i-1} b_{ij} \left(f + h f_y f \sum_{k=0}^{j-1} b_{jk} + h^2 f_y^2 f \sum_{k=0}^{j-1} b_{jk} \sum_{l=0}^{k-1} b_{kl} + \frac{1}{2} h^2 f_{yy} f^2 \left(\sum_{k=0}^{j-1} b_{jk} \right)^2 \right) + O(h^5) && (14) \\
&= h^2 f_y \sum_{i=0}^{n-1} c_i \sum_{j=0}^{i-1} b_{ij} \left(f + h f_y f a_j + h^2 f_y^2 f \sum_{k=0}^{j-1} b_{jk} a_k + \frac{1}{2} h^2 f_{yy} f^2 a_j^2 \right) + O(h^5) && (15) \\
& && (16)
\end{aligned}
$$

Expand h^3 term, T_3, to $O(h^5)$:

$$
\begin{aligned}
T(h^3) &= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^2 && (17) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} \left(f + h f_y \sum_{k=0}^{j-1} b_{jk} f(y_k) + O(h^2) \right) \right)^2 && (18) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} \left(f + h f_y \sum_{k=0}^{j-1} b_{jk} f + O(h^2) \right) \right)^2 && (19) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(f \sum_{j=0}^{i-1} b_{ij} + h f_y f \sum_{j=0}^{i-1} b_{ij} \sum_{k=0}^{j-1} b_{jk} + O(h^2) \right)^2 && (20) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(f \sum_{j=0}^{i-1} b_{ij} + h f_y f \sum_{j=0}^{i-1} b_{ij} \sum_{k=0}^{j-1} b_{jk} \right)^2 + O(h^5) && (21) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(f^2 \left(\sum_{j=0}^{i-1} b_{ij} \right)^2 + 2 h f_y f^2 \sum_{j=0}^{i-1} b_{ij} \cdot \sum_{j=0}^{i-1} b_{ij} \sum_{k=0}^{j-1} b_{jk} \right) + O(h^5) && (22) \\
&= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(f^2 a_i^2 + 2 h f_y f^2 a_i \sum_{j=0}^{i-1} b_{ij} a_j \right) + O(h^5) && (23)
\end{aligned}
$$

Expand h^4 term, T_4, to $O(h^5)$:

$$
\begin{aligned}
T(h^4) &= \frac{1}{6} h^4 f_{yyy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} f(y_j) \right)^3 && (24) \\
&= \frac{1}{6} h^4 f_{yyy} \sum_{i=0}^{n-1} c_i \left(\sum_{j=0}^{i-1} b_{ij} f \right)^3 + O(h^5) && (25) \\
&= \frac{1}{6} h^4 f_{yyy} f^3 \sum_{i=0}^{n-1} c_i a_i^3 + O(h^5) && (26)
\end{aligned}
$$

Thus

$$
y_n = y_0 + T_1 + T_2 + T_3 + T_4 + O(h^5) \tag{27}
$$

where

$$
\begin{aligned}
T_1 &= hf \sum_{i=0}^{n-1} c_i && (28) \\
T_2 &= h^2 f_y \sum_{i=0}^{n-1} c_i \sum_{j=0}^{i-1} b_{ij} \left(f + h f_y f a_j + h^2 f_y^2 f \sum_{k=0}^{j-1} b_{jk} a_k + \frac{1}{2} h^2 f_{yy} f^2 a_j^2 \right) && (29) \\
T_3 &= \frac{1}{2} h^3 f_{yy} \sum_{i=0}^{n-1} c_i \left(f^2 a_i^2 + 2h f_y f^2 a_i \sum_{j=0}^{i-1} b_{ij} a_j \right) && (30) \\
T_4 &= \frac{1}{6} h^4 f_{yyy} f^3 \sum_{i=0}^{n-1} c_i a_i^3. && (31)
\end{aligned}
$$

Now we need the Taylor series for $y(t_0 + h)$. We have

$$
\begin{aligned}
y' &= f && (32) \\
y'' = f' &= f_y f, && (33) \\
y''' = f'' &= f_{yy} f^2 + f_y^2 f, && (34) \\
y'''' = f''' &= f_{yyy} f^3 + f_{yy} 2 f f_y f + 2 f_y f_{yy} f^2 + f_y^3 f && (35) \\
&= f_{yyy} f^3 + 4 f_{yy} f_y f^2 + f_y^3 f && (36)
\end{aligned}
$$

Thus the first order condition is

$$
\sum_{i=0}^{n-1} c_i = 1. \tag{37}
$$

The second order condition is

$$
\sum_{i=1}^{n-1} c_i a_i = \frac{1}{2}. \tag{38}
$$

The third order conditions are

$$
\begin{aligned}
\sum_{i=1}^{n-1} c_i a_i^2 &= \frac{1}{3}, && (39) \\
\sum_{i=2}^{n-1} c_i \sum_{j=1}^{i-1} b_{ij} a_j &= \frac{1}{6}. && (40)
\end{aligned}
$$

The fourth order conditions are

$$\sum_{i=1}^{n-1} c_i a_i^3 = \frac{1}{4} \tag{41}$$

$$\sum_{i=2}^{n-1} c_i \sum_{j=1}^{i-1} b_{ij} a_j^2 + 2 \sum_{i=2}^{n-1} c_i a_i \sum_{j=1}^{i-1} b_{ij} a_j = \frac{1}{3} \tag{42}$$

$$\sum_{i=3}^{n-1} c_i \sum_{j=2}^{i-1} b_{ij} \sum_{k=1}^{j-1} b_{jk} a_k = \frac{1}{24}. \tag{43}$$

More succinctly, and in Wikipedia's notation, which seems to be the standard notation:

The first order condition is

$$\sum_{i=0}^{n-1} b_i = 1. \tag{44}$$

The second order condition is

$$\sum_{i=1}^{n-1} b_i c_i = \frac{1}{2}. \tag{45}$$

The third order conditions are

$$\sum_{i=1}^{n-1} b_i c_i^2 = \frac{1}{3}, \tag{46}$$

$$\sum_{n>i>j>0} b_i a_{ij} c_j = \frac{1}{6}. \tag{47}$$

The fourth order conditions are

$$\sum_{i=1}^{n-1} b_i c_i^3 = \frac{1}{4} \tag{48}$$

$$\sum_{n>i>j>0} b_i a_{ij} c_j^2 + 2 \sum_{n>i>j>0} b_i c_i a_{ij} c_j = \frac{1}{3} \tag{49}$$

$$\sum_{n>i>j>k>0} b_i a_{ij} a_{jk} c_k = \frac{1}{24}. \tag{50}$$

For $n = 4$, this reads

$$b_0 + b_1 + b_2 + b_3 = 1 \tag{51}$$

$$b_1 c_1 + b_2 c_2 + b_3 c_3 = \frac{1}{2} \tag{52}$$

$$b_1 c_1^2 + b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3} \tag{53}$$

$$b_1 c_1^3 + b_2 c_2^3 + b_3 c_3^3 = \frac{1}{4} \tag{54}$$

$$b_2 a_{21} c_1 + b_3 a_{31} c_1 + b_3 a_{32} c_2 = \frac{1}{6} \tag{55}$$

$$b_2 a_{21} c_1^2 + b_3 a_{31} c_1^2 + b_3 a_{32} c_2^2 + 2(b_2 c_2 a_{21} c_1 + b_3 c_3 a_{31} c_1 + b_3 c_3 a_{32} c_2) = \frac{1}{3} \tag{56}$$

$$b_3 a_{32} a_{21} c_1 = \frac{1}{24}. \tag{57}$$