Derivation of 4th Order Runge-Kutta Method

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Consider the initial value problem given by

$$\begin{cases} y'(t) = f(t, y(t)) \\ y(t_0) = y_0 \end{cases}$$

for a function Lipschitz continuous function f. To approximate the solution $y(t)$, the Runge-Kutta method uses an intermediate y value to enhance the approximation of each successive approximation $y_k \approx y(t_k)$ as

$$\begin{aligned} \widetilde{y}_{k+\alpha} &= y_k + \alpha h f(t_k, y_k) \\ y_{k+1} &= y_k + \beta h f(t_k, y_k) + \gamma h f(t_k + \alpha h, \widetilde{y}_{k+\alpha}) \end{aligned}$$

for some α, β, and γ that must be consistent with the Taylor expandion of $y' = f$. Define f_y and f_t as the partial derivatives of f with respect to y and t respectively. Moreover, since f is continuously differentiable, the mixed partials of f are equivalent. Then the chain rule and Taylor's theorem gives us

$$\begin{aligned} f(t_k + \alpha h, \widetilde{y}_{k+\alpha}) &= f(t_k + \alpha h, y_k + \alpha h f(t_k, y_k)) \\ &= f(t_k, y_k) + \alpha h \left[f_t + f f_y\right] + \frac{(\alpha h)^2}{2}\left[f_{tt} + f f_{ty} + f^2 f_{yy}\right] + \frac{(\alpha h)^3}{6}\left[f_{ttt} + 3 f f_{tty} + 3 f^2 f_{tyy} + f^3 f_{yyy}\right] \\ &\quad + \frac{(\alpha h)^4}{24}\left[f_{tttt} + 4 f f_{ttty} + 6 f^2 f_{ttyy} + 4 f^3 f_{tyyy} + f^4 f_{yyyy}\right] + \mathcal{O}(h^5) \end{aligned}$$

Then the iterative step for y_{k+1} is given by

$$\begin{aligned} y_{k+1} &= y_k + \beta h f(t_k, y_k) + \gamma h f(t_k + \alpha, \widetilde{y}_{k+\alpha}) \\ &= y_k + (\beta + \gamma) h f(t_k, y_k) + \gamma \alpha h^2 \left[f_t + f f_y\right] + \gamma \frac{\alpha^2 h^3}{2}\left[f_{tt} + f f_{ty} + f^2 f_{yy}\right] + \gamma \frac{\alpha^3 h^4}{6}\left[f_{ttt} + 3 f f_{tty} + 3 f^2 f_{tyy} + f^3 f_{yyy}\right] \\ &\quad + \gamma \frac{\alpha^4 h^5}{24}\left[f_{tttt} + 4 f f_{ttty} + 6 f^2 f_{ttyy} + 4 f^3 f_{tyyy} + f^4 f_{yyyy}\right] + \mathcal{O}(h^5) \end{aligned}$$

Moreover, the Taylor expansion of the actual solution $y(t_{k+1})$ is given by

$$\begin{aligned} y(t_{k+1}) &= y(t_k) + h y'(t_k) + \frac{h^2}{2} y''(t_k) + \frac{h^3}{6} y'''(t_k) + \frac{h^4}{24} y^{(4)}(t_k) + \frac{h^5}{120} y^{(5)}(t_k) + \mathcal{O}(h^6) \\ &= y(t_k) + h f + \frac{h^2}{2}\left[f_t + f f_y\right] + \frac{h^3}{6}\left[f_{tt} + f f_{ty} + f^2 f_{yy}\right] + \frac{h^4}{24}\left[f_{ttt} + 3 f f_{tty} + 3 f^2 f_{tyy} + f^3 f_{yyy}\right] \\ &\quad + \frac{h^5}{120}\left[f_{tttt} + 4 f f_{ttty} + 6 f^2 f_{ttyy} + 4 f^3 f_{tyyy} + f^4 f_{yyyy}\right] + \mathcal{O}(h^6) \end{aligned}$$

Hence, we must choose α, β, and γ so that $y(t_{k+1}) = y_{k+1}$. Since, the corresponding coefficients of h must be equal we obtain a system of equations given by

$$
\begin{aligned}
\beta + \gamma &= 1 && h^0 \\
\gamma\alpha &= \frac{1}{2} && h^1 \\
\gamma\alpha^2 &= \frac{1}{3} && h^2 \\
\gamma\alpha^3 &= \frac{1}{4} && h^3 \\
\gamma\alpha^4 &= \frac{1}{5} && h^4
\end{aligned}
$$

Note that it is clear that for any order the additional equations will be of the form $\gamma\alpha^k = 1/(k+1)$.