PHYS 512 Problem Set 3

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The 4th order Runge-Kutta (RK4) method is a well defined algorithm for solving ODEs. For some first order ODE $\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y)$ and a step size h, RK4 is defined as

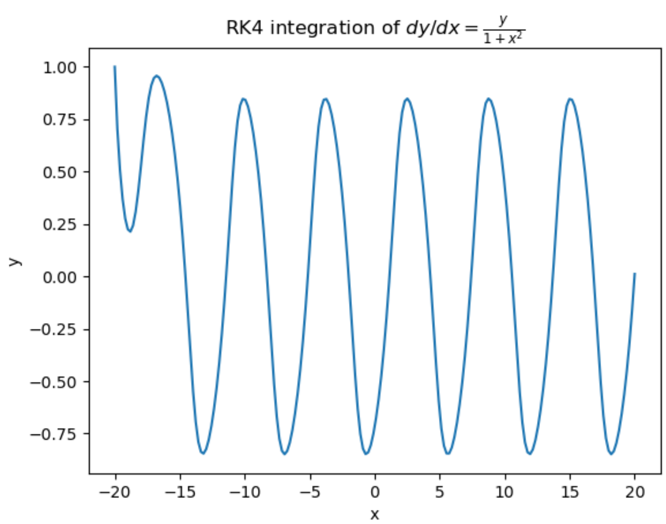
$$\begin{aligned}
k_1 &= h \cdot f(y, x) \\
k_2 &= h \cdot f(y + \frac{1}{2}k_1, x + \frac{1}{2}h) \\
k_3 &= h \cdot f(y + \frac{1}{2}k_2, x + \frac{1}{2}h) \\
k_4 &= h \cdot f(y + k_3, x + h) \\
y(x + h) &= y(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}$$

This algorithm is implemented directly in my "rk4_step" function which was used to evaluate

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{y}{1 + x^2}$$

as shown in figure 1.

Figure 1: basic RK4 integration of $\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{y}{1+x^2}$



Each of the RK4 terms after k_1 can be described as a second order Taylor expansion using the previous term.

$$
\begin{aligned}
k_1 &= h \cdot f(y, x) \\
k_2 &= h \cdot f(y + \frac{1}{2}k_1, x + \frac{1}{2}h) = h \cdot \left(f(y, x) + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}k_1 \right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) \right) \\
k_3 &= h \cdot f(y + \frac{1}{2}k_2, x + \frac{1}{2}h) = h \cdot \left(f(y, x) + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}k_2 \right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) \right) \right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) + \frac{h^2}{4}\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) \right) \\
k_4 &= h \cdot f(y + k_3, x + h) = h \cdot \left(f(y, x) + \frac{\mathrm{d}}{\mathrm{d}x}k_3 \right) \\
&= h \cdot \left(f(y, x) + h\frac{\mathrm{d}}{\mathrm{d}x}\left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(f(y, x) + \frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) \right) \right) \right) \\
&= h \cdot \left(f(y, x) + h\frac{\mathrm{d}}{\mathrm{d}x}f(y, x) + \frac{h^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(y, x) + \frac{h^3}{4}\frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) \right) \\
y_{rk4}(x + h) &= y(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

Given the proper coefficients, RK4 is equivalent to a 4th order polynomial so

$$y(x + h) = y_{rk4}(x + h) + \frac{h^5}{5!}\frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)$$

If the step size is reduced to $h/2$, repeating the second order expansion on k_1', k_2', k_3', and k_4' (' designates the $h/2$ step) produces

$$y_{rk4}(x + h/2) = y(x) + \frac{1}{6}(k_1' + 2k_2' + 2k_3' + k_4')$$

$$y(x + h/2) = y_{rk4}(x + h/2) + \left(\frac{h}{2}\right)^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)\ .$$

A second $h/2$ step (') gives

$$y_{rk4'}(x + h) = y(x + h/2) + \frac{1}{6}(k_1' + 2k_2' + 2k_3' + k_4')$$

$$y(x + h) = y(x + h/2) + \frac{1}{6}(k_1' + 2k_2' + 2k_3' + k_4') + \left(\frac{h}{2}\right)^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)$$

$$y(x + h) = y_{rk4}(x + h/2) + \left(\frac{h}{2}\right)^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6) + \frac{1}{6}(k_1' + 2k_2' + 2k_3' + k_4') + \left(\frac{h}{2}\right)^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)\ .$$

$$y(x + h) = y_{rk4}(x + h/2) + \frac{1}{6}(k_1' + 2k_2' + 2k_3' + k_4') + 2\left(\frac{h}{2}\right)^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)\ .$$

Thus, the leading error term for $y(x + h)$ after 2 RK4 steps of $h/2$ is $\frac{h^5}{16}\frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x)$ compared to $h^5\frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x)$ for a single step of length h. Using this result, I can make use of both step lengths to eliminate the 5^{th} order error term.

$$y_{h/2}(x + h) = y_{true}(x + h) - \frac{h^5}{16}\frac{\mathrm{d}^4}{\mathrm{d}x^4}f(y, x) + \mathcal{O}(h^6)$$

$$y_h(x+h) = y_{true}(x+h) - h^5 \frac{\mathrm{d}^4}{\mathrm{d}x^4} f(y,x) + \mathcal{O}(h^6)$$

$$\boxed{\frac{16 y_{h/2}(x+h) - y_h(x+h)}{15} = y(x+h) + \mathcal{O}(h^6)}\,.$$