Brief notes for using the Runge-Kutta method

R. Shankar Subramanian Department of Chemical and Biomolecular Engineering Clarkson University

These notes are intended to help you in using a numerical technique, known as the Runge-Kutta method, which is employed for solving a set of ordinary differential equations. In a typical numerical scheme, we begin with the dependent variables at some point and march forward, taking small steps in the independent variable and calculating the values of the dependent variables at the end of the step. Runge-Kutta methods are based on approximating the Taylor series of the dependent variables in the independent variable about some point, to varying degrees of accuracy in the step size being taken (1,2). The term "fourth order" implies that we are exactly matching the Taylor series to $O(h^4)$ where h is the step size being taken. You can find a discussion as well as a detailed derivation of the scheme in many books on numerical methods. Here, I'll simply give you the recipe to be used.

First, consider a first order differential equation

y' = f(x, y), along with the starting condition $y(x_0) = y_0$.

The fourth order Runge-Kutta equations for this problem are given below.

$$x_{n+1} = x_n + h$$

$$y_{n+1} = y_n + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = hf (x_n, y_n)$$

$$k_2 = hf \left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2} \right)$$

$$k_3 = hf \left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2} \right)$$

$$k_4 = hf (x_n + h, y_n + k_3)$$

So, we would begin the calculations at $x = x_0$, with the corresponding value of y being y_0 and take a small step h. Once we calculate the value of y_1 by using the above recipe, we make n = 1, and proceed to calculate y_2 . The process is continued until we reach the other end of the interval in which the equation needs to be solved. If we have a higher order differential equation, we first break it down into a set of first order differential equations by defining intermediate variables. For example, a second order differential equation is written as a set of two first order differential equations by defining y' as some new variable. Once that is done for the given differential equation of order m, let us call our set of dependent variables Y^{j} , where j runs from 1 to m. Then, we can write

$$Y^{j'} = f^{j}(x, Y^{1}, Y^{2}, Y^{3}, \cdots Y^{m}), \quad j = 1, 2, 3, \cdots m$$

where f^{j} are known functions of their arguments.

Integration by the Runge-Kutta method is just as straightforward as it is for a single equation. Here is the recipe.

$$\begin{aligned} x_{n+1} &= x_n + h \\ Y_{n+1}^{j} &= Y_n^{j} + \frac{1}{6} \Big(k_1^{j} + 2k_2^{j} + 2k_3^{j} + k_4^{j} \Big) \\ k_1^{j} &= h f^{j} \Big(x_n, Y_n^{1}, Y_n^{2}, Y_n^{3}, \cdots Y_n^{m} \Big) \\ k_2^{j} &= h f^{j} \bigg(x_n + \frac{h}{2}, Y_n^{1} + \frac{k_1^{1}}{2}, Y_n^{2} + \frac{k_1^{2}}{2}, Y_n^{3} + \frac{k_1^{3}}{2}, \cdots Y_n^{m} + \frac{k_1^{m}}{2} \Big) \\ k_3^{j} &= h f^{j} \bigg(x_n + \frac{h}{2}, Y_n^{1} + \frac{k_2^{1}}{2}, Y_n^{2} + \frac{k_2^{2}}{2}, Y_n^{3} + \frac{k_2^{3}}{2}, \cdots Y_n^{m} + \frac{k_2^{m}}{2} \Big) \\ k_4^{j} &= h f^{j} \bigg(x_n + h, Y_n^{1} + k_3^{1}, Y_n^{2} + k_3^{2}, Y_n^{3} + k_3^{3}, \cdots Y_n^{m} + k_3^{m} \Big) \end{aligned}$$

When calculating k_i^j , you need to evaluate them for every value of j at a given level i before proceeding to the next level. That is, you would first calculate all the k_1^j , $j = 1, 2, 3 \cdots m$ before calculating k_2^j .

To assure that you have produced a working code that yields correct results, try your program on a third order linear ordinary differential equation with constant coefficients for which you can write an analytical solution. Compare the results from the numerical and analytical solutions. Determine the right value of h to use to get sufficient accuracy in your numerical solution by trial and error. This will give you some experience before trying the homework. Here is an example problem.

$$y''' + 2y'' - y' - 2y = 0$$
 with
 $y(0) = 4, \quad y'(0) = -3, \quad y''(0) = 7$

The analytical solution is

 $y = e^x + 2e^{-x} + e^{-2x}$

References

1. F.B. Hildebrand, Advanced Calculus for Applications, Prentice-Hall, New Jersey 1976.

2. W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery, Numerical Recipes in FORTRAN, Cambridge University Press, Cambridge, UK, 1992.