Mathematics 20: Ordinary Differential Equations

In this section we will review the solving of ordinary differential equations. The generic problem is:

$$\frac{dy}{dx} = f(x, y) \qquad (*)$$

At first sight this appears to restrict attention to first-order equations, but if we permit the quantity y to become a *vector* then we can handle any order. Let us use the equation:

$$\frac{d^2y}{dx^2} + y = 0$$

as an example. We use a two-dimensional vector to describe the problem:

$$y_1 = y \qquad\qquad y_2 = \frac{dy}{dx}$$

in terms of which:

$$\begin{aligned}\frac{dy_1}{dx} =& y_2\\ \frac{dy_2}{dx} =& -y_1\end{aligned}$$

which is of the required form ($*$). Obviously, we can handle any order of differential equation by using all the derivatives up to the largest as the components of a 'vector'.

The simplest way of solving ordinary differential equations is by Euler's method. We use Taylor's Theorem:

$$y(x+h) = y(x) + hy^{(1)}(x) + \frac{h^2}{2!}y^{(2)}(x) + \frac{h^3}{3!}y^{(3)}(x) + \ldots + \frac{h^n}{n!}y^{(n)}(x)\ldots$$

in terms of the derivatives:

$$y^{(n)}(x) \equiv \frac{d^n y}{dx^n}(x)$$

at it's simplest to yield:

$$y(x+h) = y(x) + hy^{(1)}(x) + O(h^2) = y(x) + hf(x, y(x)) + O(h^2)$$

which enables us to integrate our equation to $x+h$. Provided that the step length, h, is small then an integration from a to b with N steps gives an error of order $O(Nh^2) = O(h)$ which can be made arbitrarily small.

Probably the most widely used algorithms are the so-called Runge-Kutta algorithms. These techniques involve 'multiple-steps', ie several function evaluations at each step, in order to increase the order of agreement with Taylor's Theorem. We will derive some second-order techniques as examples:

We define the quantities:

$$\begin{aligned}k_1 =& hf(x + a_1 h, y(x))\\ k_2 =& hf(x + a_2 h, y(x) + b_{21}k_1)\\ k_3 =& hf(x + a_3 h, y(x) + b_{31}k_1 + b_{32}k_2)\\ k_4 =& hf(x + a_4 h, y(x) + b_{41}k_1 + b_{42}k_2 + b_{43}k_3)\end{aligned}$$

and so on.. We then construct the next step as:

$$y(x+h) = y(x) + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots \qquad (**)$$

where the parameters; $w_1, w_2, w_3, \dots$ and $a_1, a_2, a_3, \dots$ and $b_{21}, b_{31}, b_{32}, \dots$ are parameters which are chosen so that $(**)$ agrees with Taylor's Theorem to as many orders of h as is desired.

Second-order Runge-Kutta: At this order we need only two terms:

$$y(x+h) = y(x) + hw_1 f(x + a_1 h, y(x)) + hw_2 f(x + a_2 h, y(x) + b_{21} h f(x + a_1 h, y(x)))$$

and so:

$$y(x+h) = y(x) + hw_1 f(x,y) + hw_2 f(x,y) + h^2 w_1 a_1 f_x(x,y) + h^2 w_2 a_2 f_x(x,y)$$
$$+ h^2 w_2 b_{21} f(x,y) f_y(x,y) + O(h^3)$$

from simply expanding to leading order, where we are using the notation:

$$\begin{aligned} f_x(x,y) &= \frac{\partial f}{\partial x}(x,y) \\ f_y(x,y) &= \frac{\partial f}{\partial y}(x,y) \end{aligned}$$

etc.. Now:

$$y^{(2)}(x) = \frac{d}{dx} f(x,y) = f_x(x,y) + f_y(x,y) y^{(1)}(x) = f_x(x,y) + f(x,y) f_y(x,y)$$

and so we get agreement with Taylor's Theorem at second order provided that:

$$\begin{aligned} w_1 + w_2 &= 1 \\ w_1 a_1 + w_2 a_2 &= \frac{1}{2} \\ w_2 b_{21} &= \frac{1}{2} \end{aligned}$$

There are many possible solutions to these equations: eg; $w_1 = 0$, $w_2 = 1$, $a_1 = 1$, $a_2 = 1/2$, $b_{21} = 1/2$, leading to:

$$\begin{aligned} k_1 &= hf(x+h, y) \\ k_2 &= hf(x + \frac{h}{2}, y + \frac{k_1}{2}) \\ y(x+h) &= y(x) + k_2 \end{aligned}$$

or: $w_1 = 1/2$, $w_2 = 1/2$, $a_1 = 0$, $a_2 = 1$, $b_{21} = 1$, leading to:

$$\begin{aligned} k_1 &= hf(x,y) \\ k_2 &= hf(x+h, y+k_1) \\ y(x+h) &= y(x) + \frac{1}{2}(k_1 + k_2) \end{aligned}$$

Fourth-order Runge-Kutta: At this order we need four terms. The algebra is much worse, but a nice example is:

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

The final problem that might be met is so-called 'mixed' boundary conditions. These 'stepping' techniques provide a method for following a solution over a range of x. Often, we are presented with boundary conditions which involve both $x = a$ and $x = b$. In this case our methods will enable us to start at a and then solve across to b. The boundary condition at a can be put in at the start, but there is freedom at a which corresponds to the choices of behaviour at b. One requires to vary the freedom at a until the solution has the required boundary condition at b. This type of problem is seen in Quantum-mechanical bound-state problems, where one of the boundary conditions is the $\psi(\infty) = 0$, while the other is $\psi(0)$. If the equations are *linear* then linear superposition of any two solutions will provide the required boundary conditions. Unfortunately, neither the Schrodinger problem nor the screening problem is of this type. For non-linear problems one is dealing with finding the solution to an algebraic equation: The freedom at a may be deemed the variable, and the difference between the actual and desired boundary condition at b being required to vanish. Due to the *dramatic* behaviour of the solution to most non-linear differential equations, it is best to use the simplest 'root finding' technique: Bisection. The root is bracketed by trial and error, and then the interval is sequentially bisected with the half-interval containing the root being retained at each step.

A sequence of Runge-Kutta techniques of increasing order:

$$
\begin{aligned}
k_1 &= hf(x, y) \\
y(x + h) &= y(x) + k_1
\end{aligned}
\tag{1}
$$

$$
\begin{aligned}
k_1 &= hf(x, y) \\
k_2 &= hf(x + h, y + k_1) \\
y(x + h) &= y(x) + \frac{1}{2}(k_1 + k_2)
\end{aligned}
\tag{2}
$$

$$
\begin{aligned}
k_1 &= hf(x, y) \\
k_2 &= hf(x + \frac{h}{2}, y + \frac{k_1}{2}) \\
k_3 &= hf(x + h, y + 2k_2 - k_1) \\
y(x + h) &= y(x) + \frac{1}{6}(k_1 + 4k_2 + k_3)
\end{aligned}
\tag{3}
$$

$$
\begin{aligned}
k_1 &= hf(x,y)\\
k_2 &= hf(x+\frac{h}{2}, y+\frac{k_1}{2})\\
k_3 &= hf(x+\frac{h}{2}, y+\frac{k_2}{2})\\
k_4 &= hf(x+h, y+k_3)\\
y(x+h) &= y(x)+\frac{1}{6}(k_1+2k_2+2k_3+k_4)
\end{aligned}
\tag{4}
$$

$$
\begin{aligned}
k_1 &= hf(x,y)\\
k_2 &= hf(x+\frac{h}{4}, y+\frac{k_1}{4})\\
k_3 &= hf(x+\frac{h}{2}, y+\frac{k_1}{2})\\
k_4 &= hf(x+\frac{h}{2}, y+\frac{k_1}{7}+\frac{2k_2}{7}+\frac{k_3}{14})\\
k_5 &= hf(x+\frac{3h}{4}, y+\frac{3k_1}{8}-\frac{k_3}{2}+\frac{7k_4}{8})\\
k_6 &= hf(x+h, y-\frac{4k_1}{7}+\frac{12k_2}{7}-\frac{2k_3}{7}-k_4+\frac{8k_5}{7})\\
y(x+h) &= y(x)+\frac{7}{90}(k_1+k_6)+\frac{16}{45}(k_2+k_5)-\frac{k_3}{3}+\frac{7k_4}{15}
\end{aligned}
\tag{5}
$$

$$
\begin{aligned}
k_1 &= hf(x,y)\\
k_2 &= hf(x+\frac{h}{4}, y+\frac{k_1}{4})\\
k_3 &= hf(x+\frac{h}{4}, y+\frac{k_1}{8}+\frac{k_2}{8})\\
k_4 &= hf(x+\frac{h}{2}, y+\frac{k_3}{2})\\
k_5 &= hf(x+\frac{h}{2}, y-\frac{k_1}{12}-k_2+\frac{5k_3}{3}-\frac{k_4}{12})\\
k_6 &= hf(x+\frac{3h}{4}, y+\frac{7k_1}{24}+\frac{7k_2}{8}-\frac{13k_3}{12}+\frac{2k_5}{3})\\
k_7 &= hf(x+\frac{3h}{4}, y-\frac{k_1}{24}-\frac{k_2}{8}+\frac{5k_3}{6}-\frac{k_5}{6}+\frac{k_6}{4})\\
k_8 &= hf(x+h, y-\frac{4k_2}{7}+\frac{8k_3}{7}+\frac{k_4}{7}-\frac{2k_5}{7}+\frac{4k_7}{7})\\
y(x+h) &= y(x)+\frac{7}{90}(k_1+k_8)+\frac{8}{45}(2k_3+k_6+k_7)+\frac{2k_5}{15}
\end{aligned}
\tag{6}
$$