Chapter 11

ORDINARY DIFFERENTIAL EQUATIONS

The general form of a first order differential equations is

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

with initial condition $y(a) = y_a$. We seek the solution $y = y(x)$ for $x > a$. This is shown in Figure 1, and is known as an "initial value problem". (Boundary value problems are more complicated, and will be discussed briefly later.)

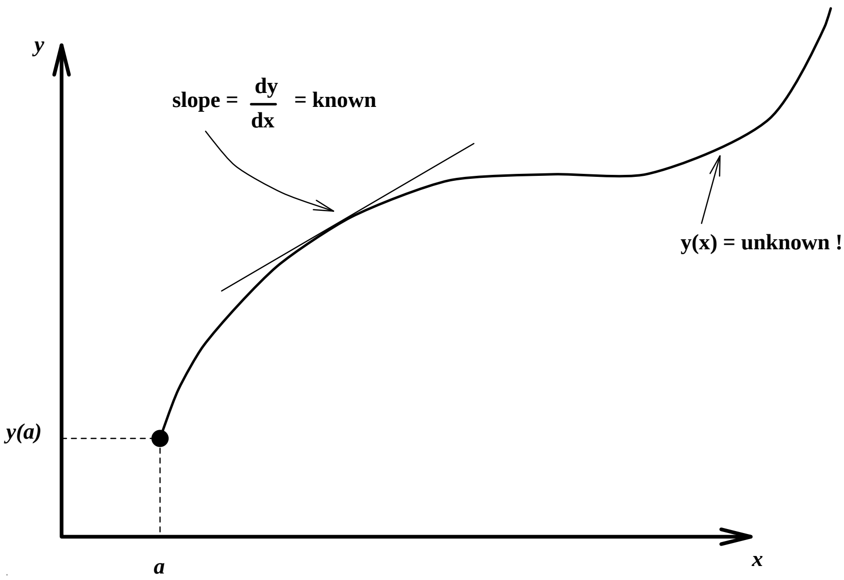

Figure 1: Geometrical interpretation of the problem.

Although some of these equations may be solved analytically (e.g. when f is linear in y, the equation is separable) most are not solvable by analytical techniques. Indeed, even when there is an analytical solution it is often of little practical use to us. For example, the d.e.:

$$\frac{dy}{dx} + 2xy = 1$$

with $y(0) = 0$ has solution

$$y(x) = e^{-x^2} \int_0^x e^{t^2} dt.$$

This integral must be evaluated numerically, and is no easier than doing the initial problem numerically from the start.

Note that numerical integration is simply a special case of solving a d.e. since

$$I = \int_a^b f(x) dx$$

is equivalent to solving for $I = y(b)$ with

$$\frac{dy}{dx} = f(x)$$

and $y(a) = 0$. Note that there is no y in the right-hand-side of the differential equation.

1. The Euler Method

This is the simplest (and least accurate) method, but it illustrates the general principles underlying the better schemes. We shall divide the area of integration, $[a, b]$, into n equal segments of width $h = (b - a)/n$, and define

$$x_i = a + ih \qquad i = 0, 1, \ldots, n.$$

This is shown in Figure 2.

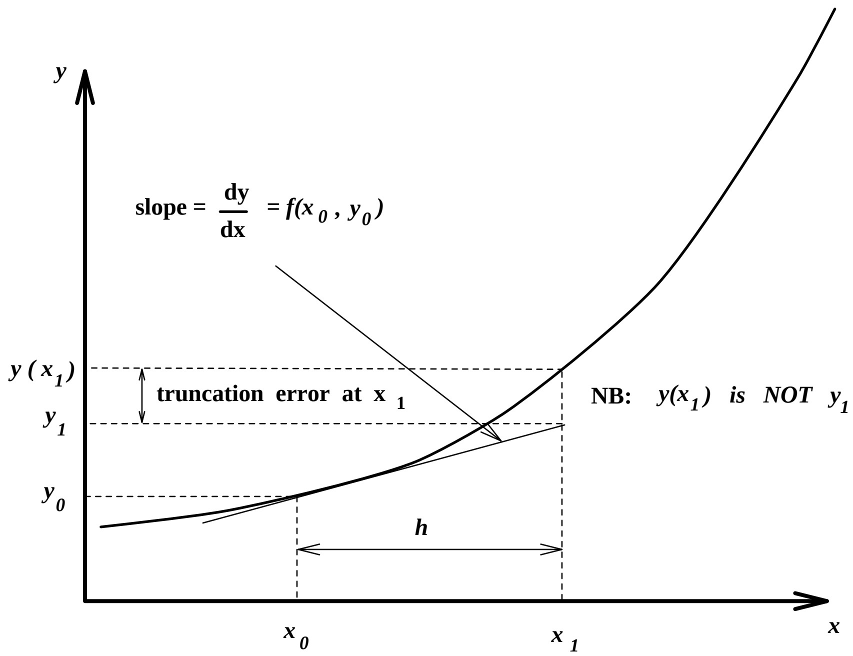

Figure 2: The Euler Method.

Clearly, from the diagram,

$$\begin{aligned} y_1 =& y_0 + \text{slope } \times h \\ =& y_0 + hf(x_0, y_0) \end{aligned}$$

and

$$y_2 = y_1 + hf(x_1, y_1)$$

which yields the general formula

$$y_{i+1} = y_i + hf(x_i, y_i).$$

An alternative derivation of this Euler formula is possible from the Taylor Series:

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \ldots$$

If we neglect terms of order h^2 (i.e. we "truncate"the series here, so that the "(local) truncation error" is $O(h^2)$):

$$\begin{aligned} y_{i+1} =& y_i + hy'(x_i) \\ =& y_i + hf(x_i, y_i). \end{aligned}$$

Note some salient features:

- — at *each step* we introduce an error due to truncation of the series, called the "local truncation error", which is $O(h^2)$ in this method.
- — the complete integration involves n steps, so that the "global" error is $\sim nh^2 \sim (nh)h$, and since $nh = (b-a) =$ constant, then the "global" error is $O(h)$.

e.g. Solve $\frac{dy}{dx} = y$ on $[0, 1]$ with $y(0) = 1$ using Euler's method with $n = 10$.

$$x_i = 0.1i \qquad\qquad i = 0, 1, \ldots, 10$$
$$y_i = y_i + hf(x_i, y_i)$$
$$= y_i + 0.1y_i = 1.1y_i$$

The exact solution is easily found to be $y = e^x$, so we can calculate the Euler Method value and compare with the exact solution: Thus the solution is:

x_i	y_i	% error
0.0	1.00	0.0
0.1	1.10	0.5
0.2	1.21	0.9
0.3	1.33	1.4
0.4	1.46	1.9
0.5	1.61	2.3
0.6	1.77	2.8
0.7	1.95	3.2
0.8	2.14	3.8
0.9	2.36	4.0
1.0	2.59	4.6

Note that the local error in this case is $\sim \frac{h^2}{2}y'' \sim h^2/2 \sim 0.04$. This is verified in the table: the error increases by $\frac{1}{2}$% per step to a total of $\sim n{\times}\frac{1}{2}\% \simeq 5\%$.

Obviously the global error here $\propto h$, so we can get more accurate results by decreasing h. Figure 3 shows the solution found by the Euler method with $h = 0.1$ together with the analytic solution. Figure 4 shows the improvement we obtain when we decrease h to 0.05. Cearly we cannot decrease h indefinitely, to obtain a given accuracy, because of the growth of round-off errors when the number of calculations increases. We can do better than this !

2. Improved Euler Method ("Huen's Method")

The principal contribution to the error in Euler's method is the neglect of curvature in the intervals $[x_i, x_{i+1}]$. Rather than take a constant slope across the interval equal to the initial value, we can use the average across the interval. This is shown in Figure 5 below.

Hence we can write

$$y_{i+1} = y_i + h\left[\frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1})}{2}\right].$$

The problem with this equation is that it is *implicit*, with y_{i+1} appearing on both sides of the equation. To avoid this problem we will **predict** a value of y_{i+1} to use on the right-hand-side, and then use this to provide a **corrected** value. We predict by using the Euler method:

$$\bar{y}_{i+1} = y_i + hf(x_i, y_i)$$

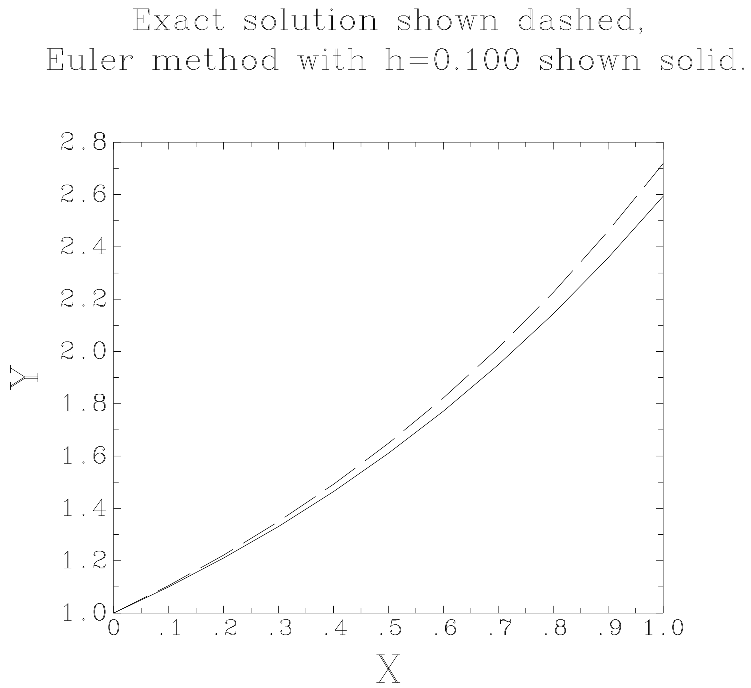

Figure 3: Results of Euler Method with $h = 0.1$.

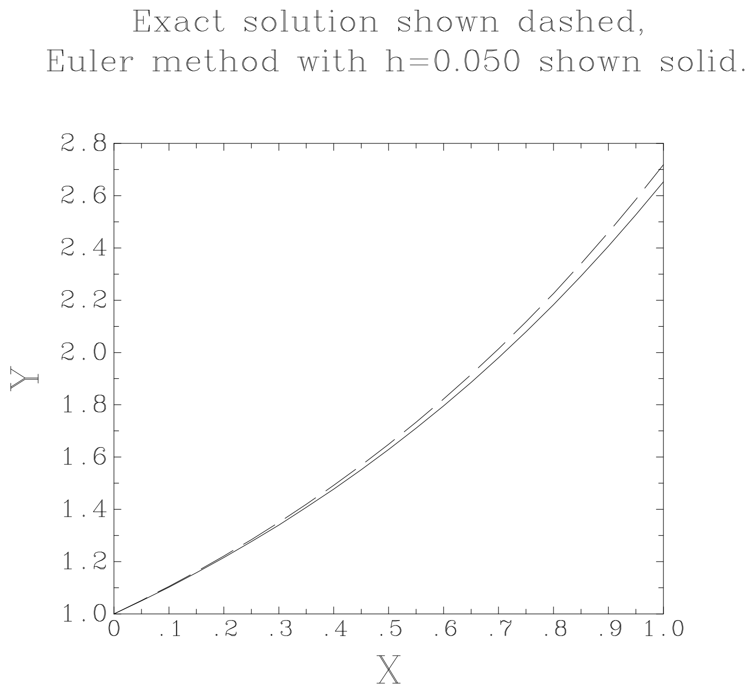

Figure 4: Results of Euler Method with $h = 0.05$.

and then use this in the above formula for y_{i+1}:

$$y_{i+1} = y_i + h \left[\frac{f(x_i, y_i) + f(x_{i+1}, \bar{y}_{i+1})}{2} \right].$$

e.g. Solve $\frac{dy}{dx} = y$ on $[0, 1]$ again, with $h = 0.1$.

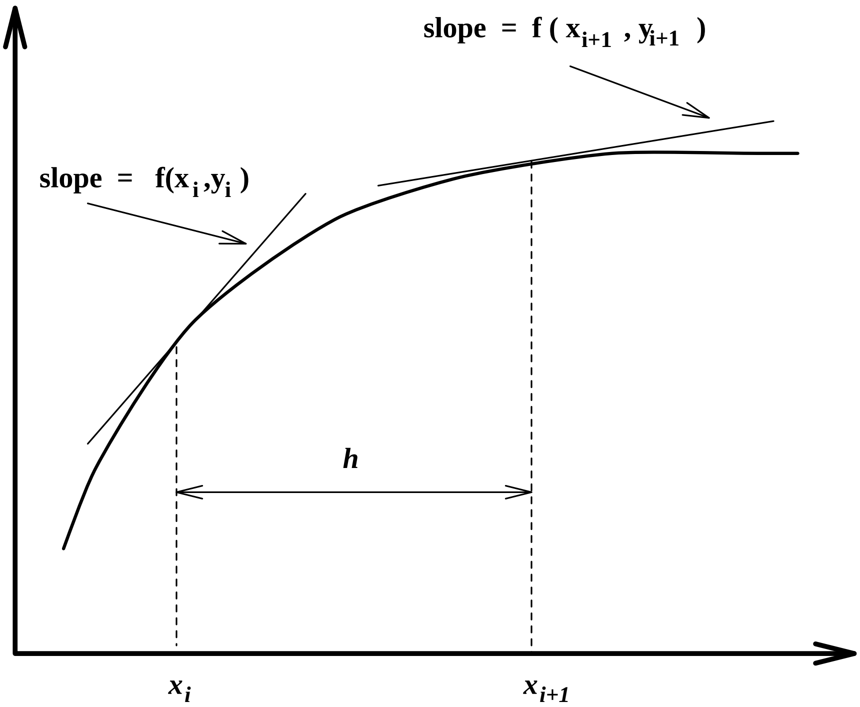

Figure 5: The Improved-Euler Method.

Here

$$\begin{aligned} \bar{y}_{i+1} =& y_i + hf(x_i, y_i) = y_i + 0.1y_i = 1.1y_i \quad \text{(the Euler method value)} \\ \Rightarrow \quad y_{i+1} =& y_i + \frac{h}{2}\left[f(x_i, y_i) + f(x_i + h, \bar{y}_{i+1})\right] \\ =& y_i + \frac{0.1}{2}\left[y_i + 1.1y_i\right] \\ =& 1.105y_i \end{aligned}$$

Using this we can construct the following table:

x_i	y_i	% error
0.0	1.000	0.00
0.1	1.105	0.02
0.2	1.221	0.03
0.3	1.349	0.05
0.4	1.491	0.06
0.5	1.647	0.08
0.6	1.820	0.09
0.7	2.012	0.11
0.8	2.223	0.12
0.9	2.456	0.14
1.0	2.714	0.15

Clearly this is much more accurate than the Euler method. Figure 6 shows this solution plotted against the exact solution, and Figure 7 shows the results obtained with $n = 20$.

Let's look at the error in the Improved Euler Method. Using the Taylor's Series for 2 variables:

$$f(x_{i+1}, \bar{y}_{i+1}) = f(x_i + h, y_i + k)$$

where $k = hf(x_i, y_i)$ has been substituted to make the expansion clear. Proceeding with the expansion:

$$f(x_{i+1}, \bar{y}_{i+1}) = f(x_i, y_i) + h\frac{\partial f}{\partial x}(x_i, y_i) + k\frac{\partial f}{\partial y}(x_i, y_i) + O(h^2).$$

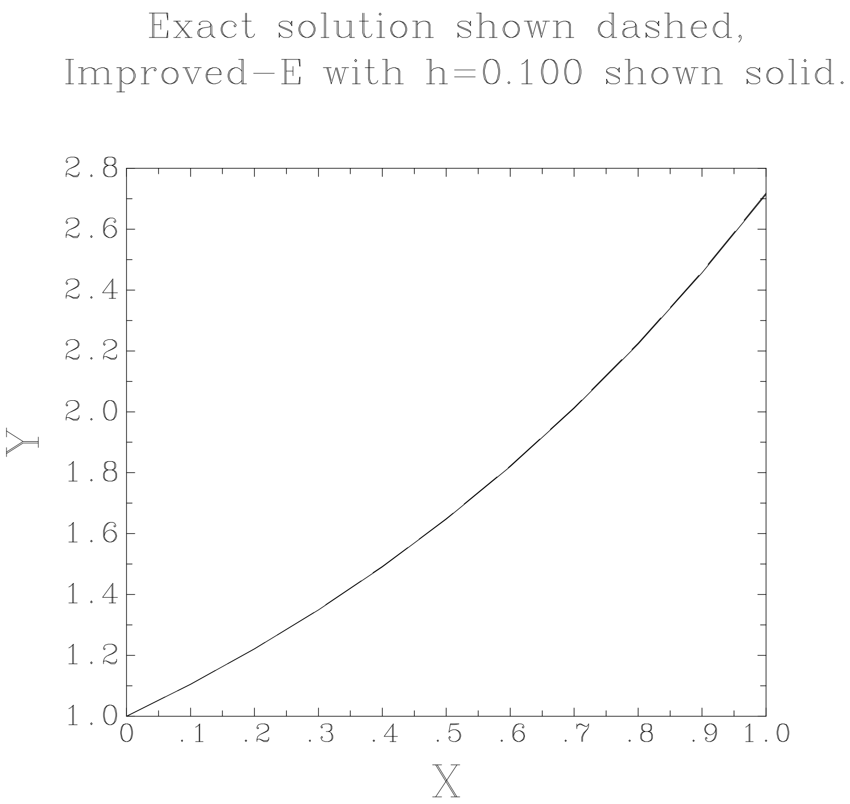

Figure 6: Results with Improved-Euler method and $h = 0.1$.

If we now substitute in the expression for k we find

$$\begin{aligned} f(x_{i+1}, \bar{y}_{i+1}) =& f(x_i, y_i) + h\frac{\partial f}{\partial x}(x_i, y_i) + (hf(x_i, y_i))\frac{\partial f}{\partial y}(x_i, y_i) + O(h^2) \\ =& \frac{dy}{dx} + h\left[\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx}\right] + O(h^2) \\ =& \frac{dy}{dx} + h\frac{df}{dx} + O(h^2). \end{aligned}$$

But $f = \frac{dy}{dx}$ so:

$$f(x_{i+1}, \bar{y}_{i+1}) = \frac{dy}{dx} + h\frac{d^2y}{dx^2} + O(h^2).$$

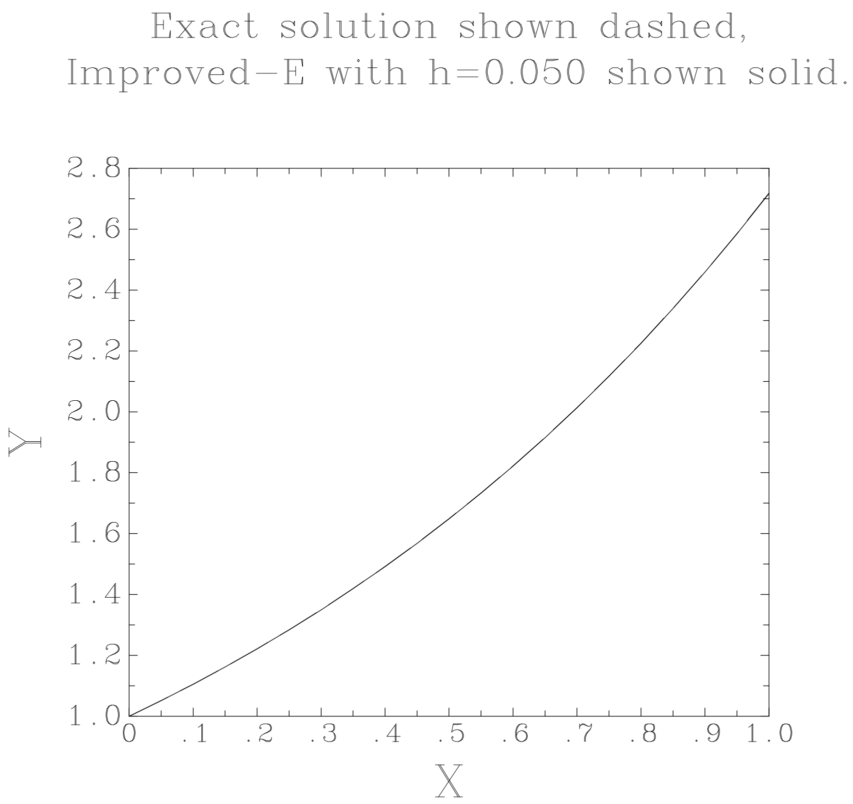

Figure 7: Results with Improved-Euler method and $h = 0.05$.

Hence, substituting this into the Improved Euler formula:

$$\begin{aligned} y_{i+1} =& y_i + \frac{h}{2}\left[f(x_i, y_i) + f(x_i + h, y_i + hf(x_i, y_i))\right] \\ =& y_i + \frac{h}{2}\left[\frac{dy}{dx} + \frac{dy}{dx} + h\frac{d^2y}{dx^2} + O(h^2)\right] \\ =& y_i + h\frac{dy}{dx} + \frac{h^2}{2}\frac{d^2y}{dx^2} + O(h^3). \end{aligned}$$

This is a Taylor Series to second order in h, and hence the local truncation error is $O(h^3)$. Thus the global error is $O(nh^3) \sim O(h^2)$ since $nh = b - a$.

In our previous example

$$\begin{aligned} y(1) =& 2.7172 \text{ with } n = 10: \text{ so the global error } = 0.15\% \\ y(1) =& 2.7140 \text{ with } n = 20: \text{ so the global error } = 0.04\% \end{aligned}$$

So with h decreasing by a factor of 2 the error decreased by a factor of 4, as expected. Note that to achieve an error of 0.1% at $x = 1$ would require

— $h = \frac{1}{12}$ with the Improved Euler Method,

— $h = \frac{1}{480}$ with the Euler Method.

Thus there are two important advantages of the Improved Euler over the Euler:

— the error is smaller for a given h

— decreasing h increases the accuracy more quickly in the Improved Euler than in the Euler.

Finally, consider the case where

$$\frac{dy}{dx} = f(x) \tag{1}$$

i.e. the right-hand-side does not include y. Then the predictor step is not required and the corrector equation is

$$y_{i+1} = y_i + \frac{h}{2}\left[f(x_i) + f(x_{i+1})\right].$$

We now demonstrate that this is equivalent to the Trapezoidal Rule. From (1):

$$\begin{aligned} \int_{y_i}^{y_{i+1}} dy &= \int_{x_i}^{x_{i+1}} f(x)dx \\ y_{i+1} - y_i &= \int_{x_i}^{x_{i+1}} f(x)dx \\ \text{or } y_{i+1} &= y_i + \int_{x_i}^{x_{i+1}} f(x)dx. \end{aligned}$$

Now, using the Trapezoidal Rule to evaluate the integral:

$$\int_{x_i}^{x_{i+1}} f(x)dx = \left(\frac{x_{i+1} - x_i}{2}\right)\left(f(x_{i+1}) + f(x_i)\right).$$

Substituting:

$$y_{i+1} = y_i + \frac{h}{2}\left[f(x_{i+1}) + f(x_i)\right],$$

as required. Thus the Improved Euler method is equivalent to the Trapezoidal Rule.

A goodway to estimate the relative amount of computer time required to solve a differential equation is to count the number of calls to the function routine. The overheads are essentially proportional to this figure, so twice as many calls will mean twice as long to run, in general. Note that the Improved Euler method uses two function calls per step, which is twice as many as the Euler method. So for the same amount of computer time (or actual dollar cost, if one is paying for time on a major computer) one can use steps which are half as small in the Euler Method than in the Improved Euler method. The advantage lies in the fact that the Improved Euler method with step $2h$ is usually more accurate than the Euler with step h, as we saw above.

3. Modified Euler Method

Another simple modification to the Euler Method is to use the slope of the mid-point of $[x_i, x_{i+1}]$:

$$y_{i+1} = y_i + hf(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}),$$

where $x_{i+\frac{1}{2}} = x_i + h/2$ and for $y_{i+\frac{1}{2}}$ we use the Euler method:

$$y_{i+\frac{1}{2}} = y_i + \frac{h}{2} f(x_i, y_i).$$

Like the Improved Euler method, the Modified Euler Method has a global error $O(h^2)$, and uses two function calls per step.

4. Fourth-Order Runge-Kutta Method

The Euler, Improved Euler and Modified Euler are particular examples of a class of techniques known as "Runge-Kutta" methods, which have the general form

$$y_{i+1} = y_i + h\phi$$

where ϕ is some approximation to the slope. For example:

a) $\phi = k_1$ where $k_1 = f(x_i, y_i)$ is the Euler Method.

b) $\phi = k_2$ where $k_2 = f(x_i + \frac{1}{2}h, y_i + h\frac{k_1}{2})$ is the Modified Euler Method.

c) $\phi = \frac{1}{2}(k_1 + k_2^\star)$ where $k_2^\star = f(x_i + h, y_i + hk_1)$ is the Improved Euler Method.

The most popular method of this class is the 4^{th} Order Runge-Kutta Method, which has a global error of order h^4 which means that the local truncation error is $O(h^5)$. In this method we take:

$$\begin{aligned} k_1 &= f(x_i, y_i) \\ k_2 &= f(x_i + \frac{h}{2}, y_i + \frac{hk_1}{2}) \\ k_3 &= f(x_i + \frac{h}{2}, y_i + \frac{hk_2}{2}) \\ k_4 &= f(x_i + h, y_i + hk_3) \end{aligned}$$

and

$$y_{i+1} = y_i + h\phi$$

where

$$\phi = \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right).$$

e.g. Solve $\frac{dy}{dx} = y$ (again !) with $y(0) = 1$ but with only TWO subdivisions of $h = \frac{1}{2}$.

The first step is

$$\begin{aligned} k_1 &= y_0 = 1 \\ k_2 &= y_0 + \frac{hk_1}{2} = 1.25 \\ k_3 &= y_0 + \frac{hk_2}{2} = 1.3125 \\ k_4 &= y_0 + hk_3 = 1.65625 \end{aligned}$$

And hence

$$y_1 = y_0 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 1.64844.$$

And the second step is

$$\begin{aligned}
k_1 =& y_1 = 1.64844 \\
k_2 =& y_1 + \frac{hk_1}{2} = 1.25y_1 \\
k_3 =& y_1 + \frac{hk_2}{2} = 1.3125y_1 \\
k_4 =& y_1 + hk_3 = 1.65625y_1
\end{aligned}$$

And hence

$$y_2 = y_1 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 2.71735.$$

Thus we have a global error of only 0.03% with $n = 2$! This is more accurate than the Improved Euler method with $n = 20$!

Concerning computational efficiency, we note that each step of the 4^{th} order Runge-Kutta method take 4 function evaluations (one per k value). So $n = 2$ uses 8 evaluations, whereas the Improved Euler with $n = 20$ uses 40 function evaluations ! So the RK4 method gave a better answer with less work. Figure 8 shows the log of the errors for this problem with $n = 10$ and each of the Euler, Improved Euler, and RK4 methods.

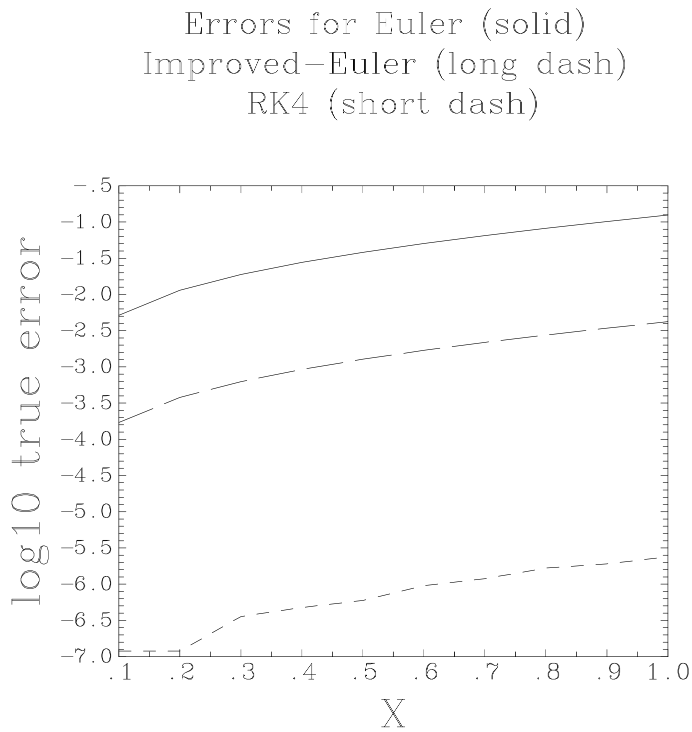

Figure 8: Comparison of errors with the different methods.

5. Errors

We'll now look at an example, but keep the number of function evaluations constant, so that each method takes the same amount of computer time. Consider now the d.e.

$$\frac{dy}{dx} = -y + 1$$

over the interval $[0, 0.5]$ with $y(0) = 0$. Suppose we solve this with RK4 using $h = 0.1$, so that $n = 5$. This is 20 function evaluations. If the Improved Euler method is to step across this interval with 20 function evaluations, then we need 10 steps of $h = 0.05$ because each step takes two function evaluations. And for the Euler Method, as each step needs one function evaluation, then we take 20 steps across the interval, or $h = 0.025$. The table below shows the results:

x	E ($h = 0.025$)	IE ($h = 0.05$)	RK4 ($h = 0.1$)	Exact
0.1	0.096312	0.095120	0.09516250	0.09516258
0.2	0.183348	0.181198	0.18126910	0.18126925
0.3	0.262001	0.259085	0.25918158	0.25918178
0.4	0.333079	0.329085	0.32967971	0.32967995
0.5	0.397312	0.393337	0.39346906	0.39346934

This shows quite clearly that even for the same amount of work. the RK4 method is significantly better, and hence the method of choice.

In figure 9 we apply the three methods we have developed to the solution of the d.e.

$$\frac{dy}{dx} = 5x^4$$

with $y(-1) = -1$, and $n = 10$. In figure 10 we repeat this, but with $n = 20$. For the Euler Method the log of the error decreases from about -0.3 to -0.6, which is a factor of 2 smaller when h was halved. For the Improved Euler method the log of the error decreases from -1.3 to -1.8, which is about a factor of 4 smaller. And, for RK4 the log of the error goes from about -4 or -5 to -5.2 or -6.5, which is about a factor of 16 smaller. Thus the errors decrease as

— h for the Euler method,

— h^2 for the Improved Euler method,

— h^4 for the RK4 method.

Finally, Figure 11 shows the solution to

$$\frac{dy}{dx} = y + x$$

with $y(0) = 0$ and the three methods discussed so far. Again, we have adjusted n in each case so that the amount of work done in each case is identical. The solid line is the analytical solution, and we see that even though we used only $n = 5$ for the RK4 method, the solution is very good, and well ahead of both the Improved Euler (with $n = 10$) and the Euler (with $n = 20$).

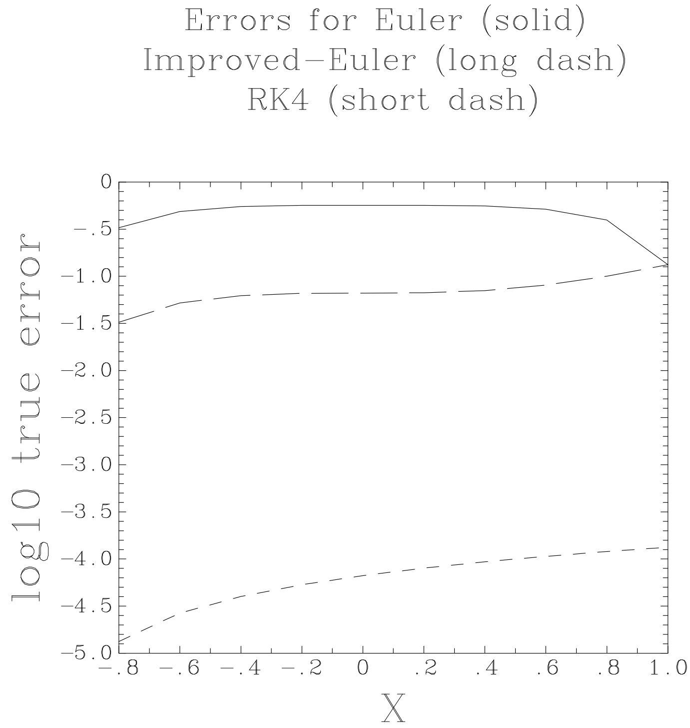

Figure 9: Comparison of errors in solving $\frac{dy}{dx} = 5x^4$ with $n = 10$.

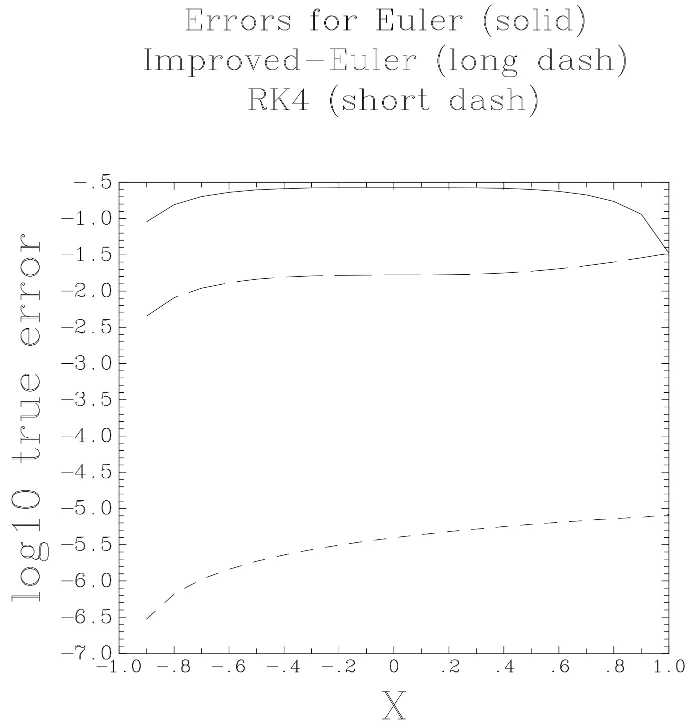

Figure 10: Comparison of errors in solving $\frac{dy}{dx} = 5x^4$ with $n = 20$.

6. Error Control: The Runge-Kutta-Fehlberg Method

Ideally, we wish to specify the maximum error we will accept in our numerical solution, and then expend the minimum effort necessary to achieve this. In general this is not consistent with a constant step-length. So we now look at a method which uses an adaptive step-length h.

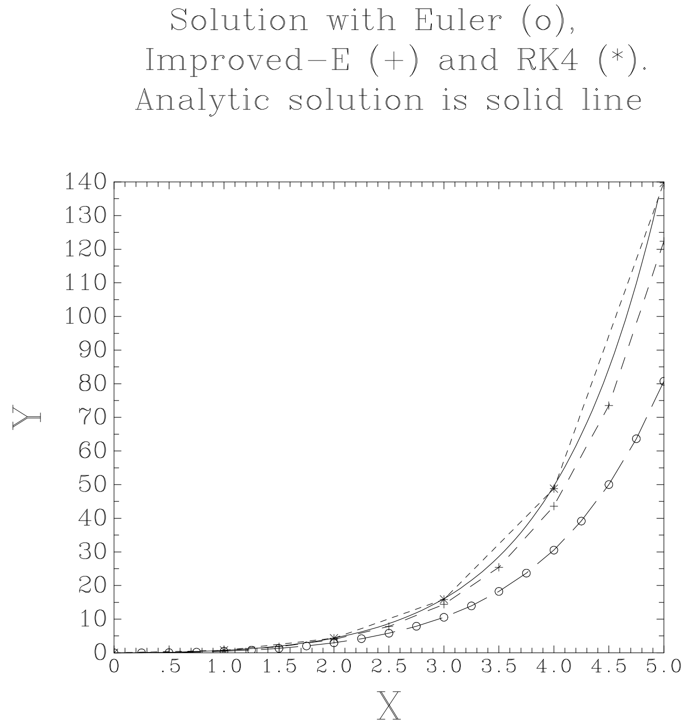

Figure 11: Comparison with different n but same amount of CPU time.

One technique, as we saw in Richardson Extrapolation, is to do the calculation once with h and then again with $h/2$, enabling us to estimate the errors. We shall use a related, but more advanced technique here.

Suppse $Y(x)$ is an exact solution of

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

Let y be a solution from a method with global error $O(h^4)$, such as the RK4 method. Let z be a solution from a method with global error $O(h^5)$ (e.g. a different RK scheme, say RK5). Then the local truncation error is

$$\begin{aligned} y_i &= Y_i + \alpha h^5, \\ z_i &= Y_i + \beta h^6. \end{aligned}$$

Thus

$$\begin{aligned} |y_i - z_i| &= Y_i + \alpha h^5 - (Y_i + \beta h^6) \\ &= \alpha h^5 + O(h^6). \end{aligned} \tag{1}$$

Suppose we now want to make the same step but with $h' = sh$. Then the solution $\bar{y}_i$ has truncation error:

$$\bar{y}_i - Y_i = \alpha(sh)^5 = \alpha s^5 h^5.$$

If we limit this error to the value T then

$$\begin{aligned} \alpha s^5 h^5 &= T, \\ \Rightarrow \alpha h^5 &= \frac{T}{s^5}. \end{aligned}$$

Substituting this into (1):

$$\begin{aligned} |y_i - z_i| =& \frac{T}{s^5} \\ \Rightarrow s =& \left(\frac{T}{|y_i - z_i|} \right)^{1/5}. \end{aligned}$$

This determines s, given y_i and z_i, and hence tells us the new step to use so that our error is below the specified tolerance. To be sure, one usually replaces T by $T/2$ so that

$$s = \left(\frac{T}{2|y_i - z_i|} \right)^{1/5}.$$

Alternatively, one can look at the global error:

$$y_i = Y_i + \alpha(sh)^4$$

and hence

$$|y_i - Y_i| = \alpha s^4 h^4 = T \quad \Rightarrow \alpha h^4 = \frac{T}{s^4}.$$

Substituting this into equation (1):

$$\frac{hT}{s^4} = |y_i - z_i|$$

and

$$\Rightarrow s = \left(\frac{hT}{|y_i - z_i|} \right)^{1/4}.$$

Note that this is a factor of $h^{1/4}$ stricter than our previous criterion. Again, it is common to let $T \to T/2$:

$$s = \left(\frac{hT}{2|y_i - z_i|} \right)^{1/4}. \tag{2}$$

The problem that remains is to find y and z !

Well, we already have a method which has global error $O(h^4)$—this is the RK4 method. If we can devise a 5^{th} order method it will, in general, have it's own 5 k's, giving a total of 9 k's to be evaluated at each step. This is very expensive in computer time. But these k's are not unique, and Fehlberg (in 1966) found a set of 6 k's which would allow a 4^{th} order **and** a 5^{th} order solution ! This is only one function evaluation more than any 5^{th} order method. This is the so-called "Runge-Kutta-Fehlberg" method (RKF). It uses

$$\begin{aligned} y_{i+1} =& y_i + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5. \\ z_{i+1} =& z_i + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 + \frac{9}{50}k_5 + \frac{2}{55}k_6. \end{aligned}$$

where

$$\begin{aligned}
k_1 =& hf(x_i, y_i) \\
k_2 =& hf(x_i + \frac{h}{4}, y_i + \frac{1}{4}k_1) \\
k_3 =& hf(x_i + \frac{3h}{8}, y_i + \frac{3}{32}k_1 + \frac{9}{32}k_2) \\
k_4 =& hf(x_i + \frac{12h}{13}, y_i + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3) \\
k_5 =& hf(x_i + h, y_i + \frac{439}{210}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4) \\
k_6 =& hf(x_i + \frac{1}{2}h, y_i - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2566}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5)
\end{aligned}$$

Then we adjust $h \rightarrow sh$ according to

$$s = \left(\frac{hT}{2|y_i - z_i|} \right)^{1/4}.$$

Typically we restrict the rate of change of h with something like:

```
if (s > 2) then
        Set h = 2h
else if (s < 0.5) then
        Set h = 0.5h
else
        Set h = sh
endif
if (h < h_min) set h = h_min
if (h > h_max) set h = h_max
```

It is important to note neither of our formulae for s will actually work in practice. The reason is because we are using the *current* values of y and z, and these include all accumulated differences from the first step. In reality, we need the difference in the addition to y and z at the current step. So the denominator in the equations for s should not really be $|y_i - z_i|$ but $|y(_i - y_{i-1}) - z(_i - z_{i-1})|$. This is purely because we derived the formula assuming that we started with the exact valuye Y, and looked at the change. If we accumulate the change, however, then the errors begin to accumulate also. Hence we must look only at the difference in the increments. Think about this, and it should all become clear (eventually).

7. Higher-Order Differential Equations

The earlier methods can be easily extended to 2^{nd} or higher order differential equations. Here we seek a solution of

$$\frac{d^2y}{dx^2} = F(x, y, \frac{dy}{dx}),$$

where F is given and $y(x_0) = y_0$ and $\frac{dy}{dx}(x_0) = z_0$, say. Note that we have two (because it is a second order equation) **initial** conditions, and hence this is an **initial** value problem. If we have $y(x_0) = y_0$ and $y(x_n) = y_n$ then we have **boundary** conditions and we say the problem is a **boundary** value problem. These are more subtle, and we will discuss them briefly later.

The basis of our approach is to split the 2^{nd} order d.e. into two first order d.e.s by defining a new dependent variable:

$$z = \frac{dy}{dx}.$$

Then we must solve

$$\begin{aligned}\frac{dy}{dx} =& z\\ \frac{dz}{dx} =& F(x,y,z).\end{aligned}$$

This is a special case of the coupled pair of equations

$$\begin{aligned}\frac{dy}{dx} =& G(x,y,z)\\ \frac{dz}{dx} =& F(x,y,z)\end{aligned}$$

where $G = z$. But the principle is the same for both: we simply apply our chosen method to the two first order d.e.s (noting that the z_i and y_i resulting from $\frac{dz}{dx}$ and $\frac{dy}{dx}$ are then used in each d.e. Note that this principle can be generalised to any number of coupled d.e.s, and hence to any d.e. of any order.

So, for a second order d.e. solved by the Euler Method we have:

$$\begin{aligned}y_{i+1} &= y_i + hz_i\\ z_{i+1} &= z_i + hF(x_i, y_i, z_i)\end{aligned}$$

for $i = 0, 1, \ldots, n$. Note that these equations are coupled: we need both y_i and z_i before we can get y_{i+1} or z_{i+1}, We cannot solve for all the y_i and then the z_i (or vice versa).

For the improved Euler method we have a predictor and a corrector step for each variable:

$$\begin{aligned}\text{Predict:}\qquad \bar{y}_{i+1} =& y_i + hz_i\\ \bar{z}_{i+1} =& z_i + hF(x_i, y_i, z_i)\\ \text{Correct:}\qquad y_{i+1} =& y_i + \frac{1}{2}h(z_i + \bar{z}_{i+1})\\ z_{i+1} =& z_i + \frac{1}{2}h\Big(F(x_i, y_i, z_i) + F(x_{i+1}, \bar{y}_{i+1}, \bar{z}_{i+1})\Big)\end{aligned}$$

e.g. Consider the d.e.

$$\frac{d^2y}{dx^2} + 2\frac{dy}{dx} + y = 1,$$

with $y(0) = 0$ and $\frac{dy}{dx}(0) = 0$. Here we set $\frac{dy}{dx} = z$ and thus

$$\frac{d^2y}{dx^2} = \frac{dz}{dx} = 1 - 2\frac{dy}{dx} - y.$$

We have $y_0 = 0$ and $z_0 = 0$. Using 2 steps of the Improved Euler Method yields:

$$\begin{aligned}\bar{y}_1 &= y_0 + hz_0 = 0 & \bar{z}_1 &= z_0 + h(1 - y_0 - 2z_0) = \frac{1}{2}\\ y_1 &= y_0 + \frac{1}{2}h(z_0 + \bar{z}_1) & z_1 &= z_0 + \frac{1}{2}h\left[(1 - y_0 - 2z_0) + (1 - \bar{y}_1 - 2\bar{z}_1)\right]\\ &= \frac{1}{8} & &= \frac{1}{4}\\ \bar{y}_2 &= y_1 + hz_1 = \frac{1}{4} & \bar{z}_2 &= z_1 + h(1 - y_1 - 2z_1) = \frac{7}{16}\\ y_2 &= y_1 + \frac{1}{2}h(z_1 + \bar{z}_2) & z_2 &= z_1 + \frac{1}{2}h\left[(1 - y_1 - 2z_1) + (1 - \bar{y}_2 - 2\bar{z}_2)\right]\end{aligned}$$

$$= \frac{19}{64} \qquad\qquad = \frac{5}{16}$$

Thus we estimate $y(1) = 19/64 \simeq 0.297$. Using $h = \frac{1}{4}$ yields $y(1) \simeq 0.270$. The exact solution is

$$y(x) = 1 - (x+1)e^{-x}$$

and hence $y(1) = 0.2642$. Of course, one can now use Richardson Extrapolation on our two 2^{nd} order approximations to obtain:

$$y(1) \simeq \frac{4}{3}\times 0.270 - \frac{1}{3}0.297 \simeq 0.261.$$

Alternatively, of course, we could use the RK4 scheme. In this case we would have

$$\begin{aligned} y_{i+1} =& y_i + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \\ z_{i+1} =& z_i + \frac{h}{6}\left(\ell_1 + 2\ell_2 + 2\ell_3 + \ell_4\right) \end{aligned}$$

where

$$\begin{aligned} k_1 =& f(x_i, y_i, z_i) = z_i \\ k_2 =& f(x_i + \frac{h}{2}, y_i + \frac{hk_1}{2}, z_i + \frac{h\ell_1}{2}) = (z_i + \frac{h\ell_1}{2}) \\ k_3 =& f(x_i + \frac{h}{2}, y_i + \frac{hk_2}{2}, z_i + \frac{h\ell_2}{2}) = (z_i + \frac{h\ell_2}{2}) \\ k_4 =& f(x_i + h, y_i + hk_3, z_i + h\ell_3) = (z_i + h\ell_3) \end{aligned}$$

$$\begin{aligned} \ell_1 =& g(x_i, y_i, z_i) \\ \ell_2 =& g(x_i + \frac{h}{2}, y_i + \frac{hk_1}{2}, z_i + \frac{h\ell_1}{2}) \\ \ell_3 =& g(x_i + \frac{h}{2}, y_i + \frac{hk_2}{2}, z_i + \frac{h\ell_2}{2}) \\ \ell_4 =& g(x_i + h, y_i + hk_3, z_i + h\ell_3) \end{aligned}$$

One could also use the RKF method, etc etc. And, as said earlier, this technique can be used to solve any system of o.d.e.s of any order.

8. Boundary Value Problems

We limit our discussion in this section to 2^{nd} order differential equations. In this case we do not know $\frac{dy}{dx}$ initially, but rather we know $y(a) = A$ and $y(b) = B$. There are two main techniques for solving these problems:

i) the shooting method

ii) finite-difference methods.

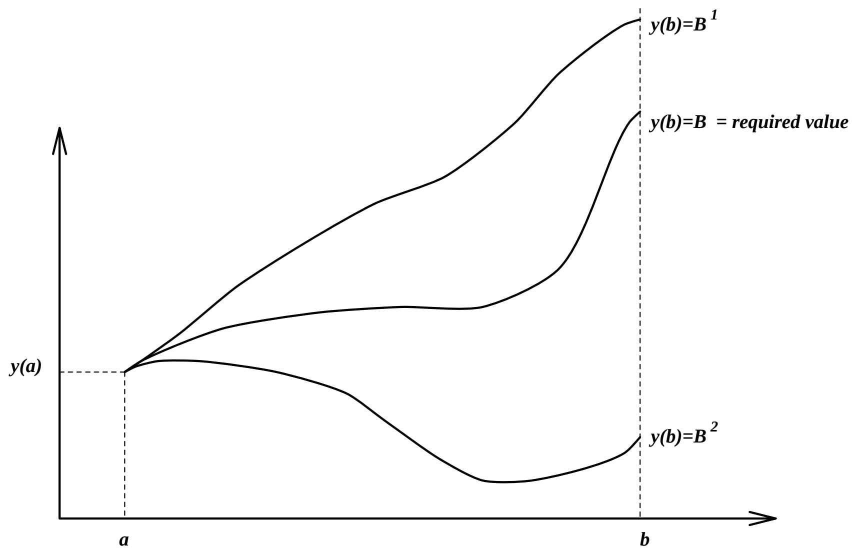

Figure 12: The Shooting Method.

8.1 The Shooting Method

The basis of this method is to guess an initial value for $\frac{dy}{dx}$ and use an initial-value method (*e.g.* RK4). Of course, we won't have $y = y(b) =$ the desired value $= B$. So we now choose a different initial value of $\frac{dy}{dx}$ and repeat. This is shown schematically in figure 12.

Let our first guess for $\frac{dy}{dx}$ at $x = a$ be $A'^{(1)}$ and suppose this resulted in $y(b) = B^{(1)}$. Suppose now that our second guess for $\frac{dy}{dx}$ at $x = a$ was $A'^{(2)}$ and suppose this resulted in $y(b) = B^{(2)}$. Clearly we wish to find A' so that $y(b) = B$. Effectively, we can think of $y(b)$ as a non-linear function g of A'. Then we want the root of

$$g(A') - B = 0.$$

We can solve this using

i) Secant method

ii) Bisection method

iii) False-Position method

We cannot use the Newton-Raphson method, of course, because we do not know how to differentiate g. Nevertheless, we can now solve this equation for A'. But note that each iteration involves an RK4 integration ! Hence the Shooting Method is not very efficient.

8.2 Finite-Difference Methods

An alternative method is to approximate the derivatives with approximate formulae known as "difference" formulae. To see this, consider the Taylor Series expansions:

$$\begin{aligned} y(x_{i+1}) =& y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i)\ldots \\ y(x_{i-1}) =& y(x_i) - hy'(x_i) + \frac{h^2}{2}y''(x_i)\ldots \end{aligned}$$

If we now add these two equations (and write y_i for $y(x_i)$):

$$y_{i+1} + y_{i-1} = 2y_i + h^2 y_i'' + O(h^4),$$

which yields

$$y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + O(h^4).$$

Alternatively, if we subtract the two Taylor Series:

$$y_i' = \frac{y_{i+1} - y_{i-1}}{2h} + O(h^2).$$

Using this technique we can determine approximate formulae for various derivatives. These can then be substituted into the d.e. and hence we obtain a set of simultaneous algebraic equations to solve for the y_i !

e.g. Consider the differential equation

$$\alpha\frac{d^2y}{dx^2} + \beta\frac{dy}{dx} + \gamma y = \delta$$

where α, β, γ and δ are constants. Then let $y(a) = y_0$ and $y(b) = y_e$ at the end-point. Divide the interval $b - a$ into n equal intervals of width $h = (b - a)/n$. Then substitute the difference equations:

$$\begin{aligned} y_i'' &= \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \\ y_i' &= \frac{y_{i+1} - y_{i-1}}{2h} \end{aligned}$$

into the differential equation to obtain:

$$\frac{\alpha}{h^2}\left(y_{i+1} - 2y_i + y_{i-1}\right) + \frac{\beta}{2h}\left(y_{i+1} - y_{i-1}\right) + \gamma y_i = \delta$$

for $i = 0, 1, \ldots, n$. The resulting y_i will be approximate solutions for $y(x_i)$. Now, we can re-write these equations as

$$\begin{aligned} \alpha(y_2 - 2y_1 + y_0) + \frac{\beta h}{2}(y_2 - y_0) + \gamma y_1 h^2 &= \delta h^2 \\ \alpha(y_3 - 2y_2 + y_1) + \frac{\beta h}{2}(y_3 - y_1) + \gamma y_2 h^2 &= \delta h^2 \\ \vdots \qquad\qquad \vdots \qquad\qquad & \quad \vdots \\ \alpha(y_n - 2y_{n-1} + y_{n-2}) + \frac{\beta h}{2}(y_n - y_{n-1}) + \gamma y_n h^2 &= \delta h^2. \end{aligned}$$

We can write this in matrix form as:

$$\begin{pmatrix} \gamma h^2 - 2\alpha & \alpha + \frac{\beta h}{2} & 0 & 0 & \cdots & 0 \\ \alpha - \frac{\beta h}{2} & \gamma h^2 - 2\alpha & \alpha + \frac{\beta h}{2} & 0 & \cdots & 0 \\ 0 & \alpha - \frac{\beta h}{2} & \gamma h^2 - 2\alpha & \alpha + \frac{\beta h}{2} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \alpha - \frac{\beta h}{2} & \gamma h^2 - 2\alpha & \alpha + \frac{\beta h}{2} \\ 0 & \cdots & \cdots & 0 & \alpha - \frac{\beta h}{2} & \gamma h^2 - 2\alpha \end{pmatrix} \underset{\sim}{y} = \begin{pmatrix} \delta h^2 - (\alpha - \frac{\beta h}{2})y_0 \\ \delta h^2 \\ \delta h^2 \\ \vdots \\ \delta h^2 \\ \delta h^2 + (\alpha - \frac{\beta h}{2})y_n \end{pmatrix},$$

where

$$\underset{\sim}{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

Note that this is a tri-diagonal system ! This is another example of why the Thomas Algorithm is so important. An advantage of this finite-difference technique is that the constants α, β, γ and δ can very easily be made functions of x.

e.g. Solve the differential equation

$$y'' + 2y' + y = 0$$

with $y(0) = 1$ and $y(1) = 0$. Using finite-differences with n segments we get

$$\left(\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}\right) + 2\left(\frac{y_{i+1} - y_{i-1}}{2h}\right) + y_i = 0$$

which becomes

$$(1-h)y_{i-1} + (h^2 - 2)y_i + (1+h)y_{i+1} = 0.$$

With $h = 0.2$ (i.e. $n = 5$ intervals) and $y_0 = 1$ and $y_5 = 0$:

$$\begin{pmatrix} -1.96 & 1.2 & 0 & 0 \\ 0.8 & -1.96 & 0 & 0 \\ 0 & 0.8 & -1.96 & 1.2 \\ 0 & 0 & 0.8 & -1.96 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} -0.8 \\ 0 \\ 0 \\ -1.2 \end{pmatrix}.$$

Using the Thomas algorithm yields:

$$\underset{\sim}{y} = \begin{pmatrix} 0.65 \\ 0.40 \\ 0.22 \\ 0.09 \end{pmatrix} \simeq \begin{pmatrix} y(0.2) \\ y(0.4) \\ y(0.6) \\ y(0.8) \end{pmatrix}.$$

The exact solution is

$$y(x) = (1-x)e^{-x}$$

so that this finite-difference solution is accurate to 2 decimal places. One can control the error by using higher accuracy difference formulae, which are beyond the scope of this introductory course.

Exercises:

1. Use Euler's method with $h = 0.2$ to determine approximate values of the solutions of each of the following differential equations in [0,1]:

$$\text{(a)}\quad \frac{dy}{dx} = -y \qquad\qquad \text{(b)}\quad \frac{dy}{dx} = 2x$$

where $y(0) = 1$ in each case. Determine the exact solution and plot both your results and the exact solution. Calculate the errors at each point.

2. Repeat Question 1 but with $h = 0.1$ and show that the errors at each point $x = 0.2$, 0.4, 0.6, 0.8 and 1.0 are halved from the case where $h = 0.2$.

3. Repeat Question 1(a) using the Improved Euler (Huen's) Method and $h = 0.2$. Recalculate the solution with $h = 0.1$ and identify the factor by which the error is reduced when h is halved.

4. Calculate the approximate solution of the differential equation

$$\frac{dy}{dx} = -y^2, \qquad\qquad y(0) = 1$$

using both the Improved Euler method and the Modified Euler method for two steps with $h = 0.5$. Repeat using four steps of $h = 0.25$ and compare the errors in each case.

5. Use the fourth order Runge-Kutta method to determine an approximate value of $y(1)$ for the differential equation

$$\frac{dy}{dx} = 2xy,$$

given $y(0) = 2$. Use $n = 2$, 5 and 10.

6. Use Euler's method, the Improved Euler method and the fourth-order Runge-Kutta method to determine the approximate solution of the equation

$$\frac{dy}{dx} = x + y, \qquad\qquad y(0) = 0.$$

Integrate from $x = 0$ to $x = 1$ and in each case use $n = 10$. Plot all 3 graphs on the same axes together with the exact solution. Repeat, again with $n = 10$, but this time over the interval $x = 0$ to $x = 5$.

7. Again consider the differential equation in Question 6. Plot the solutions obtained with

i) the Euler method with $n = 20$,

ii) the Improved Euler method with $n = 10$,

iii) the fourth-order Runge-Kutta method with $n = 5$, on the same axes.

Note that these all involve the same number of function evaluations, yet the RK4 solution is clearly superior.

8. Show that each step of the fourth-order Runge-Kutta method for the aproximate solution of the differential equation

$$\frac{dy}{dx} = y$$

using a step-length in x of h yields approximate values y_i for $y(x_i)$ which can be written as

$$y_i = Ay_{i-1}$$

where

$$A = 1 + h + \frac{h^2}{2} + \frac{h^3}{6} + \frac{h^4}{24}.$$

Identify the value of A for the exact solution and hence show that the error in A is $O(h^5)$.