

BSc Computing Mathematics
BSc Computing Maths with Business Studies

Year 2

MATHEMATICAL TECHNIQUES:

NUMERICAL METHODS

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NUMERICAL ANALYSIS

When handling problems using mathematical techniques it is usually necessary to establish a model, and to write down equations expressing the constraints and physical laws that apply. These equations must now be solved and a choice presents itself. One way is to proceed using conventional methods of mathematics, obtaining a solution in the form of a formula, or set of formulae. Another method is to express the equations in such a way that they may be solved computationally, ie by using methods of numerical analysis. This will lead directly to quantitative results, however if enough such results are obtained then qualitative results may emerge. Using these methods, large and complex physical systems may be modelled, and otherwise intractable problems can be solved with the help of modern computer systems.

Interpolation

We sometimes know the value of a function $f(x)$ at a set of points, without knowing the analytic expression for $f(x)$ that would allow us to calculate its value at some arbitrary point. Often the points at which we know the value of $f(x)$ are equally spaced, but not always. The task is to estimate $f(x)$ for a given value of x by, in some sense, drawing a smooth curve through (and perhaps beyond) the known values. If the desired value is in between the smallest and largest x -values already know, then the process is called *interpolation*. If x is outside that range, it is called *extrapolation*, which is considerably more hazardous. As a simple illustration, let us consider *linear interpolation*.

Before the advent of computers, if it was required, for example, to find the square root of a number x , a table of such numbers was consulted. If the number did not appear in the table, then the two numbers above and below x were used, and interpolation provided the solution. For example, suppose we wanted the square root of 2.155 and had a table such as shown below:

n	\sqrt{n}
2.140	1.46287
2.150	1.46629
2.160	1.46969
2.170	1.47309

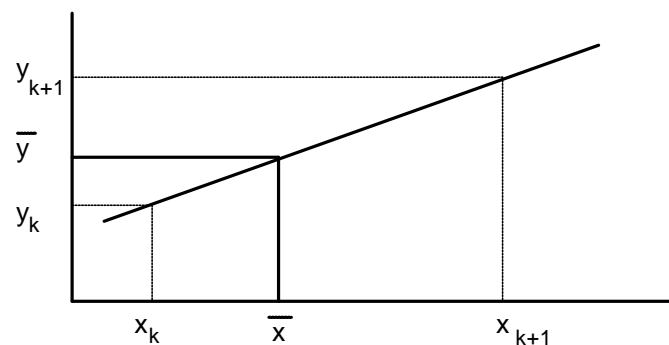
The difference between the square roots of 2.15 and 2.16 is 0.0034. Since 2.155 is half-way between 2.15 and 2.16 we could assume that its square root was half-way between the square roots of 2.15 and 2.16. This gives $\sqrt{2.155} = 1.46799$.

Had we wanted 2.153 we would have added 0.3 times 0.0034 to 2.15. This is the process of **LINEAR INTERPOLATION**, in which we assume a linear variation between the two known values to predict intermediate values.

Suppose we have a set of m numbers $x_1, x_2, x_3, \dots, x_m$ and that corresponding to each x_i there is a y_i , where y and x are related by some function f : $y = f(x)$. If we are given a value of x (not equal to one of the x_i) we want to find a value of y obtained by linear interpolation. Naturally we assume some functional relationship does indeed exist between x and y , and it is our responsibility to ensure that this is a valid assumption. Suppose that the required value of the variable x falls between the k^{th} and $k+1^{\text{th}}$ known values of x [we assume that the x 's are ordered in an ascending sequence so that $x_1 < x_2 < x_3 < \dots < x_m$]

$$\therefore x_k \leq \bar{x} \leq x_{k+1}$$

and we want to calculate the corresponding value of y . To do this, we draw a line segment joining the points (x_k, y_k) and (x_{k+1}, y_{k+1})



We then find the point on that line with an x -coordinate of \bar{x} .

The equation of the line through (x_k, y_k) and (x_{k+1}, y_{k+1}) is found by equating the slope of AB to that of BC:

$$i.e. \quad \frac{y - y_k}{x - x_k} = \frac{y_{k+1} - y_k}{x_{k+1} - x_k} \quad \therefore y = y_k + \frac{(x - x_k)(y_{k+1} - y_k)}{x_{k+1} - x_k}$$

Therefore, to find the required value of y we insert \bar{x} for x :

$$\therefore \bar{y} = y_k + \frac{(\bar{x} - x_k)(y_{k+1} - y_k)}{x_{k+1} - x_k} \quad (*)$$

Consider a simple example:

Suppose we have tabulated the values of $y = x^2$ for all integer x . Find 6.5^2 .

$$x_k = 6, \quad y_k = 36, \quad x_{k+1} = 7, \quad y_{k+1} = 49 \quad \text{and} \quad \bar{x} = 6.5$$

$$\text{Using } (*) \quad \bar{y} = 36 + \frac{(6.5 - 6)(49 - 36)}{7 - 6} = 36 + 0.5 \times 13 = 42.5$$

The correct value of 6.5^2 is 42.25 the error $E_T = -0.25$.

[Error = true value - calculated value].

A General Approach to Interpolation

We could investigate methods of interpolation using higher order polynomials, but although quadratic interpolation, for example, is likely to be more accurate than linear interpolation, it is by no means certain to provide sufficient accuracy all the time. We need to develop a general method which will also enable extra accuracy to be attained without having to resort to a new set of calculations. In order to do this we need to introduce the idea of a *difference table*.

Difference Table

As before, suppose that we have a set of values of an unknown function $y_1, y_2, y_3, \dots, y_n$ corresponding to a set of values of the (known) independent variable $x_1, x_2, x_3, \dots, x_n$ where $x_1 < x_2 < x_3 < \dots < x_n$.

A reliable formula for interpolation, to obtain the value of y corresponding to any x (where $x_1 < x_2 < x_3 < \dots < x_n$) will employ all the given information - ie it will be based on the values of the $n+1$ data entries. Instead of using these directly it is more convenient to use relationships dependent on these values. The relationship

$$y_{r+1} - y_r$$

is called the first difference of y_r , denoted by Δy_r : $\Delta y_r = y_{r+1} - y_r$

Similarly, the relationship $\Delta y_{r+1} - \Delta y_r$ is the *second difference*: $\Delta^2 y_r = \Delta y_{r+1} - \Delta y_r$

For example, $\Delta^2 y_0 = \Delta y_1 - \Delta y_0 = (y_2 - y_1) - (y_1 - y_0) = y_2 - 2y_1 + y_0$

Similarly $\Delta^2 y_1 = \Delta y_2 - \Delta y_1 = (y_3 - y_2) - (y_2 - y_1) = y_3 - 2y_2 + y_1$

In general terms: $\Delta^2 y_r = y_{r+2} - 2y_{r+1} + y_r \quad r = 0, 1, 2, \dots, n-2$

The *third differences* are $\Delta^3 y_r = y_{r+3} - 3y_{r+2} + 3y_{r+1} - y_r \quad r = 0, 1, 2, \dots, n-3$

Clearly, successive differences can be calculated and put into a table such as that shown below:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
x_0	y_0	Δy_0				
x_1	y_1	Δy_1	$\Delta^2 y_0$			
x_2	y_2	Δy_2	$\Delta^2 y_1$	$\Delta^3 y_0$	$\Delta^4 y_0$	
x_3	y_3	Δy_3	$\Delta^2 y_2$	$\Delta^3 y_1$	$\Delta^4 y_1$	$\Delta^5 y_0$
x_4	y_4	Δy_4	$\Delta^2 y_3$	$\Delta^3 y_2$		
x_5	y_5					

The polynomial interpolation formula, dependent on the $n+1$ entries, can be expressed in terms of these differences.

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
0	-2			
1	-1	1		
2	2	3	2	0
3	7	5	2	0
4	14	7	2	0
5	23	9	2	0
6	34	11		

In this example, all the differences after the second are zero. This is no coincidence - the n th differences of an n -degree polynomial are always constant, higher differences being zero.

Errors in a Difference Table

The first step in any interpolation procedure is the formation of a difference table from the given data. Since this often involves a large number of additions and subtractions it is an inevitable source of error. It is of interest to note how errors propagate in a difference table. Suppose y is subject to an error :

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
x_0	y_0			
		Δy_0		
x_1	y_1		$\Delta^2 y_0$	
		Δy_1		$\Delta^3 y_0 + e$
x_2	y_2		$\Delta^2 y_1 + e$	
		$\Delta y_2 + e$		$\Delta^3 y_1 - 3e$
x_3	$y_3 + e$		$\Delta^2 y_2 - 2e$	
		$\Delta y_3 - e$		$\Delta^3 y_2 + 3e$
x_4	y_4		$\Delta^2 y_3 + e$	
		Δy_4		$\Delta^3 y_3 - e$
x_5	y_5		$\Delta^2 y_4$	
		Δy_5		
x_6	y_6			

The error in the third difference column, for example, appears in four terms, with error coefficients given by the binomial coefficients of $(1 - e)^3$.

The Newton-Gregory Interpolation Formula

The unique polynomial satisfying any $n+1$ values is of degree n :

$$p(x) = A_0 + A_1x + A_2x^2 + \dots + A_nx^n$$

The $n+1$ constants A_i being found from the $n+1$ linear equations obtained by substituting in the data.

The Forward Interpolation Formula

Suppose the $(n+1)$ values are (x_i, y_i) $i=0,1,2,\dots,n$. We can write the polynomial as:

$$p(x) = a_0 + (x - x_0)a_1 + (x - x_0)(x - x_1)a_2 + \dots$$

If the equal intervals between successive values is h , then $x_r - x_s = (r - s)h$.

We then have the $n+1$ equations for the a_i :

$$y_r = a_0 + rha_1 + r(r-1)h^2a_2 + \dots + r(r-1)(r-2)\dots(r-n+1)h^na_n$$

$$= a_0 + \sum_{t=1}^n r(r-1)(r-2)\dots(r-t+1)h^ta_t \quad \text{with } r = 0, \dots, n$$

Forming successive differences gives:

$$\Delta y_r = y_{r+1} - y_r = ha_1 + \sum_{t=2}^n t \{r(r-1)(r-2)\dots(r-t+2)\} h^t a_t$$

$$\Delta^2 y_r = \Delta y_{r+1} - \Delta y_r = 2h^2 a_2 + \sum_{t=3}^n t(t-1) \{r(r-1)(r-2)\dots(r-t+3)\} h^t a_t$$

$$\Delta^3 y_r = \Delta^2 y_{r+1} - \Delta^2 y_r = 3 \cdot 2h^3 a_3 + \sum_{t=4}^n t(t-1)(t-2) \{r(r-1)(r-2)\dots(r-t+4)\} h^t a_t$$

$$\Delta^{n-1} y_r = (n-1)! h^{n-1} a_{n-1} + \{n(n-1)(n-2)\dots 2\} rh^n a_n$$

$$\Delta^n y_r = n! h^n a_n$$

From the above set of equations we may show that:

$$\begin{aligned} a_0 &= y_0 \\ a_1 &= \Delta y_0 / h \\ a_2 &= \Delta^2 y_0 / (2! h^2) \\ a_3 &= \Delta^3 y_0 / (3! h^3) \\ &\vdots \\ a_n &= \Delta^n y_0 / (n! h^n) \end{aligned}$$

and hence the polynomial is $p(x) = y_0 + \frac{x-x_0}{h} \Delta y_0 + \frac{(x-x_0)(x-x_1)}{h^2} \frac{\Delta^2 y_0}{2!} + \dots$

if we write $x - x_0 = kh$ where $0 \leq k \leq n$ then

$$p(x) = y_0 + k \Delta y_0 + k(k-1) \frac{\Delta^2 y_0}{2!} + \dots + k(k-1)(k-2)\dots(k-n+1) \frac{\Delta^n y_0}{n!}$$

By looking at the difference table we can see that this formula uses the values along the diagonal of the differences of y - it is a FORWARD DIFFERENCE formula. It is therefore used for interpolation near the beginning of a table where k is small.

Since the coefficients are binomial the formula may be written

$$y \cong y_0 + \sum_{r=1}^n {}^k C_r \Delta^r y_0$$

Example (i)

(i) In the following table, use the Newton-Gregory Forward Interpolation formula to find
 (a) $f(2.4)$ (b) $f(8.7)$.

x	2	4	6	8	10
f(x)	9.68	10.96	12.32	13.76	15.28

Solution Form a difference table and note that all differences > 2 are zero.

x	y=f(x)	Δy	$\Delta^2 y$
2	9.68		
		1.28	
4	10.96		0.08
		1.36	
6	12.32		0.08
		1.44	
8	13.76		0.08
		1.52	
10	15.28		

(a) $x = 2.4$; $x = 2$; $h = 2$; $k = 0.2$

$$\text{we get } f(2.4) \cong 9.68 + \frac{2.4-2}{2} \times 1.28 + \frac{(2.4-2)(2.4-4)}{4} \times \frac{0.08}{2}$$

$$\text{so } f(2.4) \cong 9.68 + 0.2 \times 1.28 + 0.1 \times (-1.6) \times 0.04 = 9.9296$$

(b) $x = 8.7$; $x = 2$; $h = 2$; $k = 3.35$

$$\text{we get } f(8.7) \cong 9.68 + 3.35 \times 1.25 + 3.35 \times 2.35 \times 0.04 = 14.2829$$

Example (ii)

In the following table of e^x use the Newton-Gregory formula of forward interpolation to calculate

(a) $e^{0.12}$, (b) $e^{2.00}$.

x	0.1	0.6	1.1	1.6	2.1
e^x	1.1052	1.8221	3.0042	4.9530	8.1662

Solution: Form a difference table.

Note that in this case there is no difference column that is constant. This is to be expected since e^x cannot be represented by a polynomial function of finite degree.

x	y=e ^x	Δy	Δ ² y	Δ ³ y	Δ ⁴ y
0.1	1.1052				
		0.7169			
0.6	1.8221		0.4652		
		1.1821		0.3015	
1.1	3.0042		0.7667		0.1962
		1.9488		0.4977	
1.6	4.9530		1.2644		
		3.2132			
2.1	8.1662				

(a) With $x = 0.12$, $x_0 = 0.1$, $h = 0.5$, $k = 0.04$

$$\therefore e^{0.12} \cong 1.1052 + 0.04 \times 0.7169 + 0.04 \times (-0.96) \frac{0.4652}{2} + 0.04 \times (-0.96) \times (-1.96) \frac{0.3015}{6} + 0.04 \times (-0.96) \times (-1.96) \times (-2.96) \frac{0.1962}{24}$$

$\therefore e^{0.12} = 1.1269$ (correct value to 5 d.p. is 1.12750)

(b) $x = 2$, $x_0 = 0.1$, $h = 0.5$, $k = 3.8$

$$e^2 \cong 1.1052 + 2.72422 + 2.47486 + 0.96239 + 0.12525$$

$\therefore e^2 \cong 7.3919$ (to 4 dp). (correct value 7.3891 to 4 dp)

In Example (i) the interpolation formula is identical with $f(x)$, which is a quadratic function, and the results for $f(2.4)$ and $f(8.7)$ will therefore be correct to the number of decimal places retained.

In example (ii) the function e^x is replaced by a 4th degree polynomial which takes the value of e^x at the five given entries. Because the successive difference decrease, higher differences are relatively small and the value of the estimate converges. From direct calculation it turns out that the error in the estimate for $e^{0.12}$ is about 0.05 percent and for $e^{2.00}$ it is about 0.04 percent. It is important to note that interpolation may not always yield a valid result. Consider the following example:

Example (iii)

Use the Newton-Gregory forward interpolation formula to estimate $f(2.5)$ from the following data:

x	2	3	4	5	6
f(x)	1	2	6	24	120

Solution: Form the forward difference table:

x	y=f(x)	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
2	1				
		1			
3	2		3		
		4		11	
4	6		14		53
		18		64	
5	24		78		
		96			
6	120				

With $x = 2.5$, $x_0 = 2$, $h = 1$ then $k = 0.5$ and we obtain

$$f(2.5) \cong 1 + 0.5 - 0.375 + 0.6875 - 2.0703 = -0.2578.$$

The function $f(x)$ in this example happens to be the GAMMA FUNCTION written

$$\Gamma(x) = (x-1)!$$

providing x is a positive integer.

In fact the value of $f(2.5)$ is known to be 1.3293, and the value estimated by interpolation is obviously incorrect. The reason for this is that the successive differences are increasingly rapidly and the series obtained from the formula is divergent. The values of $f(x)$ are increasing so rapidly that it is not possible for a fourth-degree polynomial to represent the function accurately even though it is exact at the five given values. In other words, there is not enough information given - it is necessary to fix the value of the function at more closely spaced intervals of x since it is varying so rapidly.

The Newton-Gregory Backward Interpolation Formula

The formula derived in the previous section is appropriate when the required value (x_0, y_0) lies near the beginning of the tabulated data. When (x_0, y_0) is near the end of the table, it is necessary to find a polynomial satisfying the $(n+1)$ values (x_i, y_i) , $i=0,1,2,\dots,n$. This may be achieved in a parallel manner to the previous section. It follows that the backward formula is

$$y = f(x) \cong y_0 + k\nabla y_0 + k(k+1)\frac{\nabla^2 y_0}{2!} + k(k+1)(k+2)\frac{\nabla^3 y_0}{3!} + \dots + k(k+1)\dots(k+n-1)\frac{\nabla^n y_0}{n!}$$

which may alternatively be written as

$$y \cong y_0 + \sum_{r=1}^n {}^{k+r-1}C_r \nabla^r y_0 \quad \text{where} \quad {}^{k+r-1}C_r = \frac{k(k+1)(k+2)\dots(k-r+1)}{r!}$$

The following table shows the paths of the forward and backward interpolation formulae through the difference table for $n = 5$.

x_{-5}	y_{-5}								
x_{-4}	y_{-4}								
x_{-3}	y_{-3}								
x_{-2}	y_{-2}								
x_{-1}	y_{-1}								
x_0	y_0								
x_1	y_1								
x_2	y_2								
x_3	y_3								
x_4	y_4								
x_5	y_5								

∇y_0	$\nabla^2 y_0$	$\nabla^3 y_0$	$\nabla^4 y_0$	$\nabla^5 y_0$	Backward
Δy_0	$\Delta^2 y_0$	$\Delta^3 y_0$	$\Delta^4 y_0$	$\Delta^5 y_0$	Forward

Example

Apply the backward formula to find $e^{2.00}$ in Example (ii) of the previous section.

x	y=e ^{2.00}	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
0.1	1.1052				
		0.7169			
0.6	1.8221		0.4652		
		1.1821		0.3015	
1.1	3.0042		0.7667		0.1962
		1.9488		0.4977	
1.6	4.9530		1.2644		
		3.2132			
2.1	8.1662				

We have: $x = 2.0$, $x_0 = 2.10$, $h = 0.5$ and $k = -0.2$

$$\begin{aligned}e^{2.00} &\cong 8.1662 - 0.2 \times 3.2132 - 0.2 \times 0.8 \times \frac{1.2644}{2} - 0.2 \times 0.8 \times 1.8 \times \frac{0.4977}{6} + \dots \\ &= 7.3920.\end{aligned}$$

It has been observed that the two Newton-Gregory formulae use the information in the difference table obtained by proceeding through the table along different paths. Both formulae will give accurate results when the interval h in the given data is not too large (compared with the variability in the driving function) and providing always that higher differences decrease in value and eventually become negligible.

Test Exercises

1. Form a difference table from the following data and deduce that $f(x)$ is a quadratic function.

Use the table to find $f(0)$.

Use the Newton-Gregory forward interpolation formula based on $x = 0$ to find $f(x)$.

x	2	3	4	5	6
f(x)	3.00	4.28	5.88	7.8	10.04

2. Use an appropriate interpolation formula to estimate $f(16.4)$ and $f(23.5)$ from the following data table:

x	16	18	20	22	24
f(x)	261.3	293.7	330.0	372.2	422.3

Central differences

We have already defined the forward difference operator by

$$\Delta y_r = y(x_r + h) - y(x_r) = y_{r+1} - y_r$$

and the backwards difference operator by

$$\nabla y_r = y(x_r) - y(x_r - h) = y_r - y_{r-1}$$

We now define the central difference operator, \mathbf{d} , by

$$\mathbf{d}y_r = y\left(x_r + \frac{h}{2}\right) - y\left(x_r - \frac{h}{2}\right) = y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}}$$

The forwards and backwards difference operators may be written in terms of the central difference operator

$$\begin{aligned} \Delta y_r &= y(x_r + h) - y(x_r) = y\left\{\left(x_r + \frac{h}{2}\right) + \frac{h}{2}\right\} - y\left\{\left(x_r + \frac{h}{2}\right) - \frac{h}{2}\right\} \\ &= \mathbf{d}y\left(x_r + \frac{h}{2}\right) = \mathbf{d}y_{r+\frac{1}{2}} \end{aligned}$$

Similarly it may be shown that $\nabla y_r = \mathbf{d}y\left(x_r - \frac{h}{2}\right) = \mathbf{d}y_{r-\frac{1}{2}}$

The difference table, expressed in terms of central differences is as follows

\mathbf{x}	\mathbf{y}	$\mathbf{d}y$	$\mathbf{d}^2 y$	$\mathbf{d}^3 y$	$\mathbf{d}^4 y$
x_0	y_0	$\mathbf{d}y_{\frac{1}{2}}$		$\mathbf{d}^3 y_{\frac{1}{2}}$	
x_1	y_1	$\mathbf{d}y_{\frac{3}{2}}$	$\mathbf{d}^2 y_1$		
x_2	y_2	$\mathbf{d}y_{\frac{5}{2}}$	$\mathbf{d}^2 y_2$	$\mathbf{d}^3 y_{\frac{5}{2}}$	$\mathbf{d}^4 y_2$
x_3	y_3	$\mathbf{d}y_{\frac{7}{2}}$	$\mathbf{d}^2 y_3$		$\mathbf{d}^4 y_3$
x_4	y_4			$\mathbf{d}^3 y_{\frac{7}{2}}$	

We may develop an interpolation formula in terms of central differences. We first define the *shift operator* E by $Ey_r = y_{r+1}$

$$\begin{aligned} \text{Now, } \Delta y_r &= y_{r+1} - y_r & \therefore y_{r+1} &= y_r + \Delta y_r = (1 + \Delta)y_r \\ \text{so } Ey_r &= (1 + \Delta)y_r & \therefore E &\equiv 1 + \Delta \end{aligned}$$

$$\text{Also} \quad \Delta y_r = \mathbf{d}y_{r+\frac{1}{2}} = \mathbf{d}E^{\frac{1}{2}}y_r$$

$$\text{Note that} \quad E^{\frac{1}{2}}\mathbf{d}y_r = E^{\frac{1}{2}}(y_{r+\frac{1}{2}} - y_r) = E^{\frac{1}{2}}y_{r+\frac{1}{2}} - E^{\frac{1}{2}}y_r = y_{r+1} - y_r$$

$$\text{so} \quad E^{\frac{1}{2}}\mathbf{d}y_r = \Delta y_r = \mathbf{d}E^{\frac{1}{2}}y_r \quad \Rightarrow \text{the operators } E \text{ and } \delta \text{ commute}$$

$$\therefore \quad \Delta \equiv E^{\frac{1}{2}}\mathbf{d}$$

$$\text{and} \quad E \equiv 1 + \Delta \equiv 1 + E^{\frac{1}{2}}\mathbf{d} \quad \therefore \quad \Delta^2 \equiv (E^{\frac{1}{2}}\mathbf{d})(E^{\frac{1}{2}}\mathbf{d}) \equiv E\mathbf{d}^2 \equiv (1 + E^{\frac{1}{2}}\mathbf{d})\mathbf{d}^2$$

$$\therefore \quad \Delta^2 \equiv \mathbf{d}^2 + E^{\frac{1}{2}}\mathbf{d}^3$$

$$\text{and} \quad \Delta^3 \equiv \Delta\Delta^2 \equiv E^{\frac{1}{2}}\mathbf{d}(\mathbf{d}^2 + E^{\frac{1}{2}}\mathbf{d}^3) \equiv E^{\frac{1}{2}}\mathbf{d}^3 + E\mathbf{d}^4 \equiv E^{\frac{1}{2}}\mathbf{d}^3 + (1 + E^{\frac{1}{2}}\mathbf{d})\mathbf{d}^4$$

$$\therefore \quad \Delta^3 \equiv E^{\frac{1}{2}}\mathbf{d}^3 + \mathbf{d}^4 + E^{\frac{1}{2}}\mathbf{d}^5$$

We may substitute in the Newton-Gregory forward formula

$$y(x_r + kh) = (1 + \Delta)^k y_r$$

$$= \left[1 + k\Delta + k(k-1)\frac{\Delta^2}{2!} + k(k-1)(k-2)\frac{\Delta^3}{3!} + \dots \right] y_r$$

$$= \left[1 + kE^{\frac{1}{2}}\mathbf{d} + \frac{k(k-1)}{2!}(\mathbf{d}^2 + E^{\frac{1}{2}}\mathbf{d}^3) + \frac{k(k-1)(k-2)}{3!}(E^{\frac{1}{2}}\mathbf{d}^3 + \mathbf{d}^4 + E^{\frac{1}{2}}\mathbf{d}^5) + \dots \right] y_r$$

$$= \left[1 + kE^{\frac{1}{2}}\mathbf{d} + \frac{k(k-1)}{2!}\mathbf{d}^2 + \frac{k(k-1)(k-2)}{3!}E^{\frac{1}{2}}\mathbf{d}^3 + \dots \right] y_r$$

We now consider the relationship between backward differences and central differences.

$$\text{By definition} \quad \nabla y_{r+1} = y_{r+1} - y_r \quad \therefore y_r = y_{r+1} - \nabla y_{r+1} = (1 - \nabla)y_{r+1}$$

$$\text{Also} \quad E y_r = y_{r+1} \quad \text{and} \quad y_r = E^{-1}y_{r+1} \quad \therefore E^{-1} \equiv (1 - \nabla)$$

$$\text{Also by definition} \quad \nabla y_{r+1} = y_{r+1} - y_r = \mathbf{d}y_{r+\frac{1}{2}} = \mathbf{d}E^{-\frac{1}{2}}y_{r+1} \quad \therefore \nabla \equiv \mathbf{d}E^{-\frac{1}{2}}$$

$$\text{or alternatively} \quad \nabla \equiv \mathbf{d}E^{-\frac{1}{2}}$$

$$\nabla^2 = (E^{-\frac{1}{2}}\mathbf{d})(E^{-\frac{1}{2}}\mathbf{d}) = E^{-1}\mathbf{d}^2 = (1 - \nabla)\mathbf{d}^2 = (1 - E^{-\frac{1}{2}}\mathbf{d})\mathbf{d}^2$$

$$\therefore \quad \nabla^2 = \mathbf{d}^2 - E^{-\frac{1}{2}}\mathbf{d}^3$$

$$\nabla^3 \equiv E^{-\frac{1}{2}}\mathbf{d}(\mathbf{d}^2 - E^{-\frac{1}{2}}\mathbf{d}^3) = E^{-\frac{1}{2}}\mathbf{d}^3 - E^{-1}\mathbf{d}^4 = E^{-\frac{1}{2}}\mathbf{d}^3 - (1 - E^{-\frac{1}{2}}\mathbf{d})\mathbf{d}^4$$

$$\therefore \quad \nabla^3 \equiv E^{-\frac{1}{2}}\mathbf{d}^3 - \mathbf{d}^4 + E^{-\frac{1}{2}}\mathbf{d}^5$$

We may substitute in the Newton-Gregory backward formula

$$\begin{aligned}
 y(x_r + kh) &= (1 - \nabla)^{-k} y_r \\
 &= \left[1 + k\nabla + k(k+1) \frac{\nabla^2}{2!} + k(k+1)(k+2) \frac{\nabla^3}{3!} + \dots \right] y_r \\
 &= \left[1 + kE^{-\frac{1}{2}}\mathbf{d} + \frac{k(k+1)}{2!}(\mathbf{d}^2 - E^{-\frac{1}{2}}\mathbf{d}^3) + \frac{k(k+1)(k+2)}{3!}(E^{-\frac{1}{2}}\mathbf{d}^3 - \mathbf{d}^4 + E^{-\frac{1}{2}}\mathbf{d}^5) + \dots \right] y_r \\
 &= \left[1 + kE^{-\frac{1}{2}}\mathbf{d} + \frac{k(k+1)}{2!}\mathbf{d}^2 + \frac{k(k+1)(k+2)}{3!}E^{-\frac{1}{2}}\mathbf{d}^3 + \dots \right] y_r
 \end{aligned}$$

We now take the average of the forward and backward formulae and obtain

$$y(x_r + kh) = \left[1 + k \left\{ \frac{E^{-\frac{1}{2}} + E^{\frac{1}{2}}}{2} \right\} \mathbf{d} + \frac{k^2}{2!} \mathbf{d}^2 + \frac{k(k-1)(k+1)}{3!} \left\{ \frac{E^{-\frac{1}{2}} + E^{\frac{1}{2}}}{2} \right\} \mathbf{d}^3 + \frac{k^2(k^2-1)}{4!} \mathbf{d}^4 + \dots \right] y_r$$

(The \mathbf{d}^4 term may be derived in the same way as the other terms were derived).

We introduce a final operator $\mathbf{m} = \frac{E^{-\frac{1}{2}} + E^{\frac{1}{2}}}{2}$, called the *averaging operator*.

The function of this averaging operator can be seen from the following:

$$\mathbf{m}y_r = \mathbf{m}(y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}}) = \left\{ \frac{E^{-\frac{1}{2}} + E^{\frac{1}{2}}}{2} \right\} (y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}}) = \frac{y_r + y_{r+1} - y_{r-1} - y_r}{2} = \frac{y_{r+1} - y_{r-1}}{2}$$

We have finally derived Stirling's formula for interpolating in terms of central differences.

Stirling's formula

$$y(x_r + kh) = \left[1 + k\mathbf{m}\mathbf{d} + \frac{k^2}{2!}\mathbf{d}^2 + \frac{k(k-1)(k+1)}{3!}\mathbf{m}\mathbf{d}^3 + \frac{k^2(k^2-1)}{4!}\mathbf{d}^4 + \dots \right] y_r$$

We may see how the terms relate to the difference table

x	y	dy	d²y	d³y	d⁴y
x_0	y_0				
x_1	y_1	$dy_{\frac{1}{2}}$			
x_{r-2}	y_{r-2}				
x_{r-1}	y_{r-1}	$dy_{r-\frac{3}{2}}$			
x_r	y_r	$dy_{r-\frac{1}{2}}$	$d^2 y_{r-1}$	$d^3 y_{r-\frac{1}{2}}$	
x_{r+1}	y_{r+1}	$dy_{r+\frac{1}{2}}$	$d^2 y_r$	$d^3 y_{r+\frac{1}{2}}$	$d^4 y_r$
x_{r+2}	y_{r+2}	$dy_{r+\frac{3}{2}}$	$d^2 y_{r+1}$		

Note that $mdy_r = \left\{ \frac{E^{-\frac{1}{2}} + E^{\frac{1}{2}}}{2} \right\} dy_r = \frac{1}{2} (E^{-\frac{1}{2}} dy_r + E^{\frac{1}{2}} dy_r) = \frac{1}{2} (dy_{r-\frac{1}{2}} + dy_{r+\frac{1}{2}})$

ie mdy_r is the average of the two differences highlighted in column 3 of the table.

Similarly $md^3 y_r = \frac{1}{2} (d^3 y_{r-\frac{1}{2}} + d^3 y_{r+\frac{1}{2}})$ and is the mean of the two differences in boxes in column 5 of the table.

Stirling's formula is useful for interpolating near the middle of a table, as the following example illustrates.

Example

Use Stirling's formula, with the difference table for e^x to obtain $e^{1.3}$.

x	$y=e^x$	dy	d^2y	d^3y	d^4y
0.1	1.1052				
		0.7169			
0.6	1.8221		0.4652		
		1.1821		0.3015	
1.1	3.0042		0.7667		0.1962
		1.9488		0.4977	
1.6	4.9530		1.2644		
		3.2132			
2.1	8.1662				

Solution

$$x = x_r + kh \qquad x = 1.3, \quad x_r = 1.1, \quad h = 0.5 \qquad k = \frac{x - x_r}{h} = 0.4$$

$$e^{1.3} \approx 3.0042 + 0.4 \left(\frac{1.1821 + 1.9488}{2} \right) + \frac{0.4^2}{2} 0.7667 \\ + \frac{0.4(0.4-1)(0.4+1)}{3!} \left(\frac{0.3015 + 0.4977}{2} \right) + \frac{0.4^2(0.4^2+1)}{4!} 0.1962 + \dots$$

$$\therefore e^{1.3} \approx 3.0042 + 0.62618 + 0.061336 - 0.0223776 - 0.0010987 = 3.6682$$

(Exact result $e^{1.3} = 3.6693$, to 4 dp)

NUMERICAL DIFFERENTIATION

Differentiation is a very important mathematical process and a great deal of effort has been devoted to the development of analytic techniques of finding the derivatives of various mathematical functions. It often occurs, however, that it is not possible to utilise these traditional methods. This happens when:

- (i) The function is too complex
- (ii) The function is unknown (when data are collected from some experiment).

In this section numerical techniques are described which provide an estimate of the derivative of a tabulated function.

Imagine that you have a procedure which computes a function $f(x)$ and you want to find its derivative $f'(x)$. Easy? The definition of the derivative is the limit, as $h \rightarrow 0$ of

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

practically suggests an algorithm: Pick a small value h , evaluate $f(x)$ and $f(x+h)$ and apply the above formula. The above procedure, however, contains two main sources of error: truncation error and roundoff error. The roundoff error depends upon the machine used to carry out the computation - it is necessary to ensure that the value used for h is exactly represented by the machine. Truncation error comes from the higher order terms in the Taylor series expansion:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(x) + \dots$$

which leads to $\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{1}{2}hf''(x) + \dots$

We will investigate methods of using difference tables to evaluate the derivatives of a function numerically. From page 6, the Newton-Gregory forward polynomial is:

$$f(x_k) \approx P_n(x_k) = f_0 + k\Delta f_0 + \frac{k^2}{2}C_2\Delta^2 f_0 + \dots + \frac{k^n}{n!}C_n\Delta^n f_0 \quad \text{where } k = (x - x_0)/h$$

Differentiating the above equation, remembering that $\frac{dP}{dx} = \frac{dP}{dk} \frac{dk}{dx}$

$$f'(x_k) \approx P'_n(x_k) = \frac{1}{h} \left\{ \Delta f_0 + \frac{1}{2}(2k-1)\Delta^2 f_0 + \frac{1}{2}(3k^2 - 6k + 2)\Delta^3 f_0 + \dots \right\}$$

We can simplify this considerably if we take $k = 0$, giving a derivative corresponding to $x = x_0$

$$f'(x_0) \approx \frac{1}{h} \left\{ \Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 + \dots - (-1)^n \frac{1}{n} \Delta^n f_0 \right\} \quad (1)$$

Example

Use the data in the table below to estimate $y'(1.7)$.

Use $h = 0.2$ and find the result using 1, 2, 3 and 4 terms of the formula.

x	$y=e^x$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
1.3	3.669				
		0.813			
1.5	4.482		0.179		
		0.992		0.041	
1.7	5.474		0.220		0.007
		1.212		0.048	
1.9	6.686		0.268		0.012
		1.480		0.060	
2.1	8.166		0.328		0.012
		1.808		0.072	
2.3	9.974		0.400		
		2.208			
2.5	12.182				

With one term : $y'(1.7) = \frac{1}{0.2}(1.212) = 6.060$

With two terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268) = 5.390$

With three terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268 + \frac{1}{3}0.060) = 5.490$

With four terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268 + \frac{1}{3}0.060 - \frac{1}{4}0.012) = 5.475$

The data in the table are for $y = e^x$, rounded to 3 dp.

The error in the derivative is rather small for 4 terms, which can be anticipated since the fourth differences are approximately constant. This function is well-represented by a 4th degree polynomial.

The above formula (1) for derivatives is a forward-difference approximation, for which the fit provided by the interpolating polynomial is not symmetrical about x_0 - interpretation is more accurate near the centre of the range of fit.

For most purposes it is better to use central differences for the purpose of evaluating derivatives. We use Stirling's formula as the basis of derivatives in an analogous manner to the Newton-Gregory formula:

$$y(x_r) = \left\{ 1 + k \mathbf{m} \mathbf{d} y_r + \frac{k^2}{2!} \mathbf{d}^2 y_r + \frac{k(k-1)(k+1)}{3!} \mathbf{m} \mathbf{d}^3 y_r + \frac{k^2(k^2-1)}{4!} \mathbf{d}^4 y_r + \dots \right\}$$

$$k = (x - x_r) / h$$

and using the fact that $\frac{dy}{dx} = \frac{dy}{dk} \frac{dk}{dx}$

Differentiating gives $y'(x_r) = \frac{1}{h} \left\{ \mathbf{m}d + k\mathbf{d}^2 y_r + \frac{3k^2 - 1}{3!} \mathbf{m}d^3 y_r + \frac{4k^3 - 2k}{4!} \mathbf{m}d^4 y_r + \dots \right\}$

Using $\frac{d^2 y}{dx^2} = \frac{d}{dx} \frac{dy}{dx} = \frac{d}{dk} \frac{dy}{dx} \frac{dk}{dx} = \frac{d}{dk} \frac{dy}{dx} \frac{1}{h}$ we obtain

$$y''(x_r) = \frac{1}{h^2} \left\{ \mathbf{d}^2 y_r + \frac{6k}{3!} \mathbf{m}d^3 y_r + \frac{12k^2 - 2}{4!} \mathbf{d}^4 y_r + \dots \right\}$$

$$= \frac{1}{h^2} \left\{ \mathbf{d}^2 y_r + k\mathbf{m}d^3 y_r + \frac{12k^2 - 2}{4!} \mathbf{d}^4 y_r \right\}$$

Summary of results

At a tabular point $k = 0$ and so

$$y'(x_r) = \frac{1}{h} \left\{ \mathbf{m}d y_r - \frac{1}{6} \mathbf{m}d^3 y_r + \frac{1}{30} \mathbf{m}d^5 y_r + \dots \right\}$$

$$y''(x_r) = \frac{1}{h^2} \left\{ \mathbf{d}^2 y_r - \frac{1}{12} \mathbf{d}^4 y_r + \dots \right\}$$

$$y'''(x_r) \approx \frac{1}{h^3} \mathbf{m}d^3 y_r$$

$$y^{iv}(x_r) \approx \frac{1}{h^4} \mathbf{d}^4 y_r$$

Higher derivatives may be obtained in exactly the same way.

Writing the expressions out in full:

$$y'(x_r) \approx \frac{1}{h} \mathbf{m}d y_r = \frac{1}{h} \left[\frac{\mathbf{d}y_{r-\frac{1}{2}} + \mathbf{d}y_{r+\frac{1}{2}}}{2} \right] = \frac{1}{2h} (y_r - y_{r-1} + y_{r+1} - y_r) = \frac{y_{r+1} - y_{r-1}}{2h}$$

$$y''(x_r) \approx \frac{1}{h^2} \mathbf{d}^2 y_r = \frac{1}{h^2} \mathbf{d}(\mathbf{d}y_r) = \frac{1}{h^2} \mathbf{d}(y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}})$$

$$= \frac{1}{h^2} [y_{r+1} - y_r - y_r + y_{r-1}] = \frac{y_{r+1} - 2y_r + y_{r-1}}{h^2}$$

Example 1

Use the tabulated values of $y = e^x$ to approximate dy/dx and d^2y/dx^2 at $x = 1.1$.

x	y=e^x	dy	d²y	d³y	d⁴y
0.1	1.1052 (y_0)				
		0.7169			
0.6	1.8221 (y_1)		0.4652		
		1.1821		0.3015	
1.1	3.0042 (y_2)		0.7667		0.1962
		1.9488		0.4977	
1.6	4.9530 (y_3)		1.2644		
		3.2132			
2.1	8.1662 (y_4)				

$$\frac{dy_2}{dx} \approx \frac{y_3 - y_1}{2h} = \frac{4.9530 - 1.8221}{1} = 3.1309$$

(exact value 3.0042, to 4 d.p.)

$$\frac{d^2y_2}{dx^2} \approx \frac{1}{h^2}(y_3 - 2y_2 + y_1) = \frac{1}{0.5^2}(4.9530 - 2 \times 3.0042 + 1.8221) = 3.0668$$

(exact value 3.0042, to 4 d.p.)

Test Exercises

1. The following table is for $y = 1 + \log x$. Determine estimates of y' at $x = 0.15, 0.19$ and 0.23 using (a) one term, (b) two terms, (c) three terms of equation (1) at the beginning of this section. Determine the errors by comparison with the analytical values.

x	y=(1+logx)	Δy	$\Delta^2 y$	$\Delta^3 y$
0.15	0.1761			
0.17	0.2304			
0.19	0.2788			
0.21	0.3222			
0.23	0.3617			
0.25	0.3979			
0.27	0.4314			
0.29	0.4624			
0.31	0.4914			

2. A central-difference approximation for derivatives is more accurate than using a forward-difference approximation. Repeat Exercise 1(b) but use appropriate central difference formulae and compare the errors.

NUMERICAL SOLUTION OF DIFFERENTIAL EQUATIONS

Problems involving ordinary differential equations (ODEs) can always be reduced to the study of sets of first order differential equations. For example, the second order equation:

$$\frac{d^2 y}{dx^2} + q(x) \frac{dy}{dx} = r(x)$$

can be re-written as two first-order equations:

$$\frac{dy}{dx} = z(x) \qquad \frac{dz}{dx} = r(x) - q(x)z(x)$$

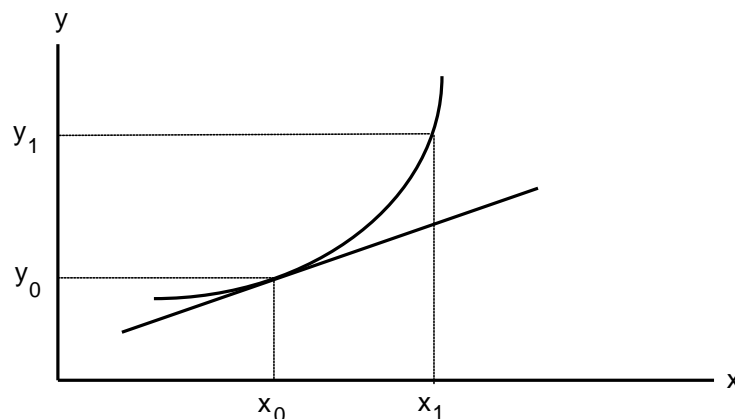
where z is a new variable. We shall therefore just consider *first-order ODEs*. Also, we shall consider **initial value problems** in which all the y values are known at some starting x value. The underlying idea of any method for solving the initial value problem is to rewrite the dy 's and dx 's in the formula above as finite steps Δy and Δx and multiply the equations by Δx . This gives algebraic formulas for the change in the functions when the independent variable x is "stepped" by one "stepsize" Δx . In the limit of small stepsize, a good approximation to the underlying differential equation is achieved. Literal implementation of this procedure results in *Euler's method*, below, which is NOT recommended for practical use because it is computationally inefficient. Euler's method is conceptually important, however, in that one way or another all practical methods come down to the same idea: add small increments to your functions corresponding to derivatives (right-hand sides of the equations), multiplied by stepsizes.

EULER'S METHOD

Suppose we must solve the equation $\frac{dy}{dx} = f(x, y)$, given that $y = y_0$ when $x = x_0$.

Divide the range of values of x into n equal steps $x_0, x_1, x_2, \dots, x_n$.

The step width is then given by: $h = \frac{x_n - x_0}{n}$



$$y_1 = y_0 + h \left. \frac{dy}{dx} \right|_{x_0} = y_0 + hf(x_0, y_0)$$

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

$$\vdots \quad \quad \quad \vdots$$

$$y_n = y_{n-1} + hf(x_{n-1}, y_{n-1})$$

Example 1 $\frac{dy}{dx} = y^2 - x$ Find $y(2.3)$ given $y(2)=3$.

Take $h=0.1$: $y_1 = y_0 + 0.1(y_0^2 - x_0)$ $x_0 = 2, y_0 = 3$
 $y_{i+1} = y_i + 0.1(y_i^2 - x_i)$

i	x_i	y_i	y_i^2	$y_i^2 - x_i$	$0.1(y_i^2 - x_i)$	y_{i+1}
0	2.0	3.000				
1	2.1					
2	2.2					
3	2.3					

0	2.0	3.000	9.000	7.000	0.700	3.700
1	2.1	3.700	13.690	11.590	1.159	4.859
2	2.2	4.859	23.610	21.410	2.141	7.000
3	2.3	7.000				

Example 2

$$\frac{dy}{dx} = x + y \quad \text{Find } y(0.05) \text{ correct to 5 d.p. given that } y(0)=2$$

Take $h=0.01$: $y_{i+1} = y_i + 0.01(x_0 + y_0)$, $y_0 = 2$, $x_0 = 0$
 $\therefore y_{i+1} = y_i + 0.01y_i'$

i	x_i	y_i	y_i'	0.01y_i'	y_{i+1}
0	0.00	2	2	0.02	2.02
1	0.01	2.02	2.03	0.0203	2.0403
2	0.02	2.0403	2.0603	0.020603	2.060903
3	0.03	2.060903	2.090903	0.02090903	2.08181203
4	0.04	2.08181203	2.12181203	0.0212181203	2.1030301503
5	0.05	2.1030301503			

Example 3

$$\frac{dy}{dx} = 2(1 + x) - y \quad \text{Find } y \text{ for } x=2.0(0.2)3.0, \text{ given } y(2)=5$$

Take $h=0.2$ $y_{i+1} = y_i + 0.2y_i'$

i	x_i	y_i	y_i'
0	2	5	1
1	2.2	5.2	1.2
2	2.4	5.44	1.36
3	2.6	5.712	1.488
4	2.8	6.0096	1.5904
5	3.0	6.32768	

Example 4

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

Find y for x=1.0(0.2)2.0, given y(1)=2

Take h=0.2

$$y_{i+1} = y_i + 0.2 y_i'$$

i	x _i	y _i	y _i '
0	1.0	2	0
1	1.2	2	0.2
2	1.4	2.04	0.36
3	1.6	2.112	0.488
4	1.8	2.2096	0.5904
5	2.0	2.32768	0.67232

EXERCISES

Solve the following ODEs to obtain the required values of y, under the given initial conditions:

1. If $\frac{dy}{dx} = x + y$ find y for x=0,(0.1),0.5, given that y(0)=1.

(Solution: 1.0, 1.1, 1.22, 1.362, 1.5282, 1.72102)

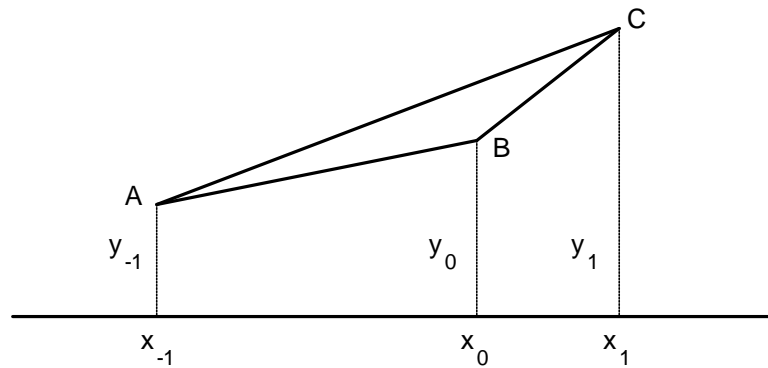
2. If $\frac{dy}{dx} = 1 + xy$ find y for x=0,(0.1),0.5, given that y(0)=1.

(Solution: 1.0, 1.1, 1.211, 1.3352, 1.4753, 1.6343)

3. Solve the above two equations by analytic methods and check your numerical results from questions 1 and 2.

SECOND-ORDER ODEs

To solve first order ODEs, one boundary/initial condition was required; for second order ODEs it becomes necessary to have two. We approximate the second derivative by the first term of the central difference formula presented earlier in this booklet. We can see from the following diagram how this can be derived geometrically:



Approximate slope at B may be given by:

$$(1) \quad \text{BC:} \quad \frac{dy}{dx} \approx \frac{y_1 - y_0}{h} \quad (\text{Forward difference})$$

$$(2) \quad \text{AB:} \quad \frac{dy}{dx} \approx \frac{y_0 - y_{-1}}{h} \quad (\text{Backward difference})$$

$$(3) \quad \text{AC:} \quad \frac{dy}{dx} \approx \frac{y_1 - y_{-1}}{2h} \quad (\text{Central difference})$$

For the second derivative:

$$\frac{d^2 y}{dx^2} \approx \frac{\frac{y_1 - y_0}{h} - \frac{y_0 - y_{-1}}{h}}{h} = \frac{y_1 - 2y_0 + y_{-1}}{h^2}$$

Example 1 $\frac{d^2y}{dx^2} = y$ Find $y(0.6)$, given $y(0)=1, y(0.1)=1.1$

$$h=0.1 \quad \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = y_i \Rightarrow y_{i+1} = 2.01y_i - y_{i-1}$$

i	x_i	y_i	2.01y_i-y_{i-1}
0	0	1	
1	0.1	1.1	1.211
2	0.2	1.211	1.33411
3	0.3	1.33411	1.4705611
4	0.4	1.4705611	1.6217178
5	0.5	1.6217178	1.7890917
6	0.6	1.7890917	

Example 2 $\frac{d^2y}{dx^2} = 4y$ Find $y(0.6)$, given $y(0)=0.5, y(0.1)=6.0$

$$h=0.1 \quad \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = y_i \Rightarrow y_{i+1} = 2.01y_i - y_{i-1}$$

i	x_i	y_i	2.01y_i-y_{i-1}
0	0	0.5	
1	0.1	6.0	11.56
2	0.2	11.56	17.2356
3	0.3	17.2356	23.083556
4	0.4	23.083556	29.162348
5	0.5	29.162348	35.532762
6	0.6	35.532762	

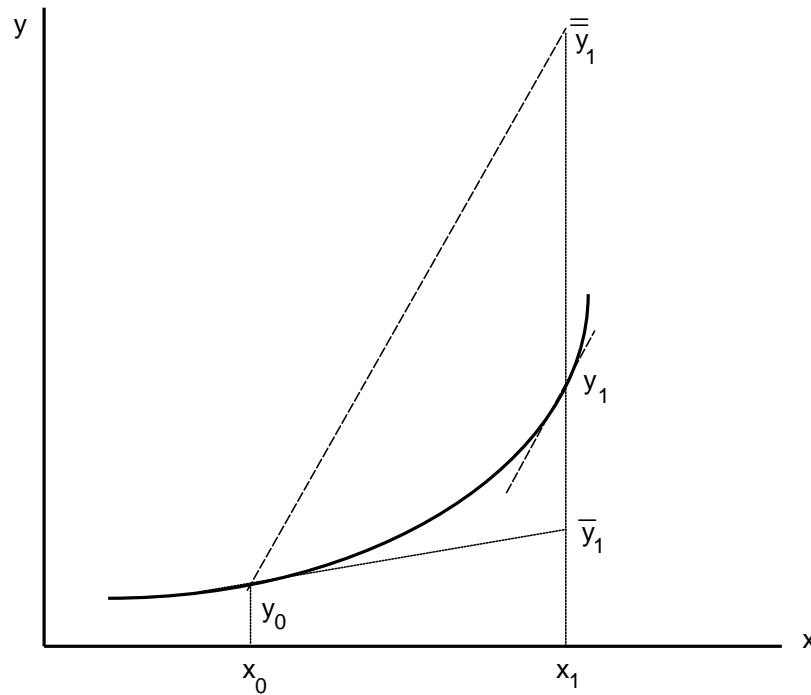
Example 3 $\frac{d^2y}{dx^2} - \frac{dy}{dx} - 2y = 0$ Find $y(0.05)$, given $y(0)=3$, $y(0.01)=3.1$

$$\begin{aligned}
 h=0.01 \quad \therefore \quad & \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} - \frac{y_{i+1} - y_{i-1}}{2h} - 2y_i = 0 \\
 \therefore \quad & (y_{i+1} - 2y_i + y_{i-1}) - \frac{h}{2}(y_{i+1} - y_{i-1}) - 2h^2y_i = 0 \\
 \therefore \quad & y_{i+1}\left(1 - \frac{h}{2}\right) = 2y_i - y_{i-1} + \frac{h}{2}y_{i-1} - 2h^2y_i \\
 \therefore \quad & y_{i+1} = \left[(2 - 2h^2)y_i + \left(\frac{h}{2} - 1\right)y_{i-1} \right] / \left[1 - \frac{h}{2} \right] \\
 \therefore \quad & y_{i+1} = 1.0050251(1.9998y_i - 0.995y_{i-1})
 \end{aligned}$$

i	x_i	y_i	1.9998y_i-0.995y_{i-1}
0	0.00	3	
1	0.01	3.1	3.21438
2	0.01	3.2305326	3.3759191
3	0.03	3.3928834	3.5707083
4	0.04	3.5886515	3.8006662
5	0.05	3.8197649	

IMPROVED EULER METHOD (IEM)

The ordinary Euler method may be improved by estimating the slope over the interval between points by the average of the slopes at the beginning and the end. We know the slope at the start point, so we can use this to estimate the y-value of the end point. From this we can estimate the slope at the end point. Taking the mean of the two slopes, we can then predict the true y-value with greater accuracy.



Estimate of y_1 based on slope at x_0 : $\bar{y}_1 = y_0 + hf(x_0, y_0)$

Estimate of y_1 based on slope at x_1 : $\bar{\bar{y}}_1 = y_0 + hf(x_1, \bar{y}_1)$

$$\text{Take } y_1 = \frac{1}{2}(\bar{y}_1 + \bar{\bar{y}}_1) = y_0 + \frac{1}{2}h\{f(x_0, y_0) + f(x_1, \bar{y}_1)\}$$

This will set up an *iterative* scheme as follows:

$$\begin{aligned} y_{1(1)} &= y_0 + hf(x_0, y_0) \\ y_{1(2)} &= y_0 + \frac{1}{2}h\{f(x_0, y_0) + f(x_1, y_{1(1)})\} \\ y_{1(3)} &= y_0 + \frac{1}{2}h\{f(x_0, y_0) + f(x_1, y_{1(2)})\} \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \end{aligned}$$

Summary of the method

The steps in the method are as follows:

1. We start with the given equation $y' = f(x, y)$, and with the initial condition that $y = y_0$ at $x = x_0$. We have to determine values of y for $x = x_0$ to x_n step h .
 2. From the equation and the initial values we can determine $y'_0 = f(x_0, y_0)$. This is the ordinary Euler method.
 3. We now know x_0, y_0, y'_0 and h , and can therefore calculate
 - (a) $x_1 = x_0 + h$
 - (b) $\bar{y}_1 = y_0 + hy'_0$ (again, this is the same step as the ordinary Euler method)
 - (c) We now calculate $f(x_1, \bar{y}_1)$, and then we can estimate
 - (d) $y_1 = y_0 + \frac{1}{2}h\{y'_0 + f(x_1, \bar{y}_1)\}$
 4. This is the first estimate of y_1 . We can, if we wish, repeat steps (c) and (d) in 3 above, replacing \bar{y}_1 with the calculated value y_1 and thereby finding an *improved* estimate of y_1 . This is known as the **recursive** method. We can continue to employ this recursion until we obtain enough accuracy (i.e. until the n^{th} decimal place remains unchanged).
 5. Finally, we can calculate $y'_1 = f(x_1, y_1)$ and repeat steps 3 and 4 to find x_2 and y_2 . This is then repeated for all the values of y that we are required to find.
-

Example 1

Apply the Improved Euler Method, without recursion, to solve:

$$\frac{dy}{dx} = x + y \quad \text{for } x=0.0 \text{ to } 0.5 \text{ step } 0.1, \quad \text{given that } y(0)=1.$$

We proceed in a step-by-step routine: we have the equation $y' = x + y$.

$$\begin{array}{lll} \text{Initial conditions} \Rightarrow & x_0 = 0, \quad y_0 = 1 & \therefore y'_0 = x_0 + y_0 = 1. \\ \text{Also} & h = 0.1 & \therefore x_1 = x_0 + h = 0.1 \end{array}$$

- (a) First calculate the value $\bar{y}_1 = y_0 + hy'_0 = 1 + 0.1 \times 1 = 1.1$
 - (b) $y_1 = y_0 + \frac{1}{2}h\{y'_0 + f(x_1, \bar{y}_1)\} = 1 + 0.05 \times \{1 + (0.1 + 1.1)\} = 1.11$
 - (c) So we have $x_1 = 0.1, y_1 = 1.1 \quad \therefore y'_1 = 0.1 + 1.11 = 1.21$
 - (d) We now take these last results in place of x_0, y_0 and y'_0 in the above calculations, and find the corresponding values for the next interval : x_2, y_2 and y'_2 . These values are shown in the following table:
-

n	x_n	y_n	y'_n
0	0.0	1.0	1.0
1	0.1	1.11	1.21
2	0.2	1.24205	1.44205
3	0.3	1.398465	1.698465
4	0.4	1.581804	1.981804
5	0.5	1.794893	2.294893

We now use recursion to obtain improved estimates of y .

As before, we have $x_0 = 0$, $x_1 = 0.1$, $y_0 = 1$ and $y'_0 = 1$.

We next calculate, as before, $\bar{y}_1 = y_0 + hy'_0 = 1.1$

$$\text{and estimate } y_1 = y_0 + \frac{1}{2}h\{y'_0 + f(x_1, \bar{y}_1)\} = 1 + 0.05 \times (1 + 1.2) = 1.11$$

So far, this is all identical to the previous calculation, however, instead of stopping now and using this value as the final estimate for y_1 we substitute this value back into the last formula above in place of \bar{y}_1 . For the value found so far we use the notation $y_{1(1)}$.

$$\text{We therefore proceed to find: } y_{1(2)} = y_0 + \frac{1}{2}h\{y'_0 + f(x_1, y_{1(1)})\} = 1 + 0.05 \times (1 + 0.1 + y_{1(1)})$$

We now have a **recursion relation** which can be simplified by multiplying out the constants to give:

$$y_{1(n)} = 1.055 + 0.05y_{1(n-1)}$$

and we can then tabulate the values of $y_{1(n)}$ for increasing values of n :

n	$y_{1(n)}$
1	1.1
2	1.11
3	1.1105
4	1.110525
5	1.1105263
6	1.1105263

Note that after 5 iterations we have achieved 7 decimal place accuracy in the solution and that the estimate without recursion is in error by 0.0005263, or 0.0474144%.

Example 1

$$\frac{dy}{dx} = x^2 y \quad x_0 = 1, \quad x_1 = 1.1, \quad y_0 = 3, \quad f(x, y) = x^2 y$$

$$y_{1(i)} = y_0 + hf(x_0, y_0)$$

$$y_{1(i+1)} = y_0 + \frac{1}{2}h[f(x_0, y_0) + f(x_1, y_{1(i)})]$$

here

$$y_{1(i)} = 3 + 0.1(3)$$

$$y_{1(i+1)} = 3 + 0.05(3 + 1.1^2 y_{1(i)}) = 3.15 + 0.0605 y_{1(i)}$$

i	y1(i)	y1(i+1)=3.15+0.0605y1(i)
0	3	
1	3.3	3.34965
2	3.34965	3.35265
3	3.35265	3.35283
4	3.35283	3.35285
5	3.35285	

Example 2 $\frac{dy}{dx} = \frac{1}{y^2}$ $x_0 = 1, x_1 = 1.1, y_0 = 1, f(x, y) = \frac{1}{y^2}$

Euler's Method: $y_1 = y_0 + hf(x_0, y_0) = 1 + 0.1\left(\frac{1}{1}\right) = 1.1$

Improved Euler Method: $y_{1(i)} = y_0 + hf(x_0, y_0)$

$$y_{1(i+1)} = y_0 + \frac{1}{2}h\left[f(x_0, y_0) + f(x_1, y_{1(i)})\right]$$

here

$$y_{1(1)} = 1.1$$

$$y_{1(i+1)} = 1 + \frac{1}{2}0.1\left(1 + \frac{1}{y_{1(i)}^2}\right) = 1.05 + \frac{0.05}{y_{1(i)}^2}$$

i	y1(i)	y1(i+1)=1.05+0.05/y1(i)²
0	1	
1	1.1	1.09132
2	1.09132	1.09198
3	1.09198	1.09193
4	1.09193	

Exact Solution: $\frac{dy}{dx} = \frac{1}{y^2} \quad \therefore y^2 dy = dx \quad \frac{y^3}{3} = x + c \quad \therefore y = \sqrt[3]{3x - 2}$

$$\therefore y(1.1) \cong 1.091392$$

Example 3

$$\frac{dy}{dx} = x + y \quad x_0 = 0, \quad x_1 = 0.1, \quad y_0 = 1, \quad f(x, y) = x + y$$

$$y_{1(i)} = y_0 + hf(x_0, y_0)$$

$$y_{1(i+1)} = y_0 + \frac{1}{2}h[f(x_0, y_0) + f(x_1, y_{1(i)})]$$

for y_1

here

$$y_{1(0)} = 1 + 0.1(1) = 1.1$$

$$y_{1(i+1)} = 1 + 0.05(1 + 0.1 + y_{1(i)}) = 1.055 + 0.05y_{1(i)}$$

i	y1(i)	y1(i+1)=1.055+0.05y1(i)
0	1.1	1.11
1	1.11	1.1105
2	1.1105	1.110525
3	1.110525	1.1105263
4	1.1105263	1.1105263
5	1.1105263	

$$\therefore y_1 \cong 1.1105263$$

for y_2 :

$$x_1 = 0.1, \quad x_2 = 0.2, \quad y_1 = 1.1105263, \quad f(x, y) = x + y$$

$$y_{2(i)} = y_0 + hf(x_0, y_0)$$

$$y_{2(i+1)} = y_0 + \frac{1}{2}h[f(x_0, y_0) + f(x_1, y_{2(i)})]$$

here

$$f(x_1, y_1) = x_1 + y_1 = 1.2105263$$

$$y_{2(0)} = 1.1105263 + 0.1(1.2105263) = 1.2315789$$

$$y_{2(i+1)} = 1.1105263 + 0.05(1.2105263 + 0.2 + y_{2(i)}) = 1.1810526 + 0.05y_{2(i)}$$

i	y2(i)	y2(i+1)=1.1810526+0.05y2(i)
0	1.2315789	1.2426315
1	1.2426315	1.2431842
2	1.2431842	1.2432118
3	1.2432118	1.2432132
4	1.2432132	1.2432133
5	1.2432133	

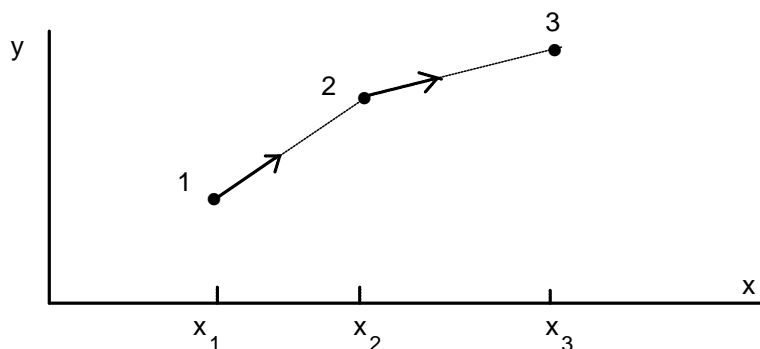
$$\therefore y_2 \cong 1.2432133$$

THE RUNGE-KUTTA METHOD

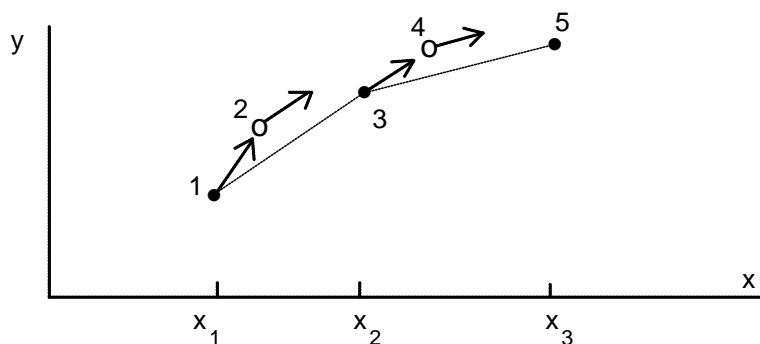
The Euler method, which has the formula

$$y_{n+1} = y_n + hf(x_n, y_n)$$

advances a solution from x_n to $x_{n+1} \equiv x_n + h$. The formula is non-symmetric - it advances a solution through an interval h using derivative information only at the beginning of the interval, as illustrated in the figure below:



There are several reasons why Euler's method is not recommended for practical use, among them (i) it is not very accurate when compared with other methods run at the equivalent stepsize and (ii) it is not very stable. Consider, however, the use of a step like in the above illustration to take a "trial" step to the midpoint of the interval. Then use the value of both x and y at that midpoint to compute the "real" step across the whole interval. The following diagram illustrates the method:



Mathematically, this can be written as

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

$$k_2 = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1)$$

$$y_{n+1} = y_n + k_2 + O(h^3)$$

This procedure is called the **second-order Runge-Kutta method** (a method is conventionally called n^{th} order if its error term is $O(h^{n+1})$).

We need not stop there. There are a number of ways of evaluating the right-hand-side $f(x,y)$ that all agree to first order, but that have different coefficients of higher-order error terms. Adding up the right combination of these, we can eliminate the error terms order by order. This is the basic idea of the Runge-Kutta method. By far the most commonly used of these methods is the classical **fourth-order Runge-Kutta formula**:

Fourth-Order Runge-Kutta Formula

$$\begin{aligned}
 k_1 &= hf(x_n, y_n) \\
 k_2 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1) \\
 k_3 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2) \\
 k_4 &= hf(x_n + h, y_n + k_3) \\
 y_{n+1} &= y_n + \frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4 + O(h^5)
 \end{aligned}$$

The fourth-order Runge-Kutta method required four evaluations of the right hand side per step h . This will be superior to the second-order method if at least twice as large a step is possible for the same accuracy. Is this so? The answer is: often, perhaps even usually, but not always. This emphasises the fact that *high order* does not always mean *high accuracy*. A good system should exert some adaptive control over its own progress, making frequent changes to its stepsize to maintain the error within predetermined limits. This, however, is beyond the scope of this unit.

Example 1

Solve $\frac{dy}{dx} = x + y$, given that $y(0) = 1$

$$x_0 = 0, y_0 = 1, y'_0 = 1, h = 0.1 \qquad x_1 = x_0 + h = 0.1$$

$$k_1 = hy'_0 = 0.1$$

$$k_2 = hf(0 + 0.05, 1 + 0.05) = hf(0.05, 1.05) \qquad \therefore k_2 = 0.11$$

$$k_3 = hf(0 + 0.05, 1 + 0.055) = hf(0.05, 1.055) \qquad \therefore k_3 = 0.1105$$

$$k_4 = 0.12105$$

$$\therefore y_1 = 1.110342$$

Exercises

1. Using the 4th order Runge Kutta method,

(a) compute an estimate of $x(0.75)$ for the initial value problem:

$$\frac{dx}{dt} = x + t + xt, \quad x(0) = 1$$

using a step size of $h = 0.15$.

(Solution: 3.2345)

(b) compute an estimate of $x(2)$ for the initial value problem

$$\frac{dx}{dt} = \frac{1}{x+t}, \quad x(1) = 2$$

using a step size of $h = 0.1$.

(Solution: 2.2771)

2. Solve $y' = x + y$ with $y = 1$ at $x = 0$.

Determine the function values for y for $x=0(0.1)0.5$.

(Solution: 1.0, 1.110342, 1.242806, 1.399718, 1.583649, 1.797442)

3. Solve $y' = y^2 - xy$ with $y = 0.4$ at $x = 0$.

Determine the function values for y for $x=0(0.2)1.0$.

(Solution: 0.4, 0.4259, 0.4374, 0.4319, 0.4085, 0.3689)

4. Solve $y' = \frac{y-x}{y+x}$ with $y = 1$ at $x = 0$.

Determine the function values for y for $x=0(0.2)1.0$.

(Solution: 1.0, 1.1679, 1.2902, 1.3817, 1.4497, 1.4983)