

Zero subscripts  
have been avoided  
as they are not  
acceptable in some  
programming  
languages.

FRAME 44 (continued)

degree 3 and so only the first, or any, four points need to be used when finding  $f(x)$ .

Find  $f(2)$  for the simplest curve satisfying the points

x	0	1	-2	3	-3	6	10
$f(x)$	3	0	21	6	36	45	153

\*\*\*\*\*

The divided difference table

44A

0	3	
1	0	-3
-2	21	2
3	6	-3
-3	36	2
6	45	1
10	153	27

indicates that  $f(x)$  is of degree 2. Consequently only three points need be used, say  $(0, 3)$ ,  $(1, 0)$  and  $(3, 6)$ . Then

$$\frac{f(2)}{2 \times 1 \times (-1)} = \frac{3}{2 \times (-1) \times (-3)} + \frac{0}{1 \times 1 \times (-2)} + \frac{6}{-1 \times 3 \times 2}$$

from which  $f(2) = 1$ .

FRAME 45

Certain modifications to the Lagrange method have been suggested, for example, that due to Aitken. This will not be considered here, but, if you are interested, you will find it dealt with in several of the books on numerical work. One such book is "Computers and Computing" by J.M. Rushforth and J.L. Morris (John Wiley & Sons).

FRAME 46A Word of Warning

In all our work on interpolation it has been assumed that, if  $y$  is a function of  $x$ , then a polynomial  $f(x)$  exists which is such that  $y = f(x)$  is an adequate representation of the curve on which the points lie. This may not be so. For example, there is no polynomial in  $x$  which adequately represents  $f(x)$  as given in the following table:

x	0	0.5	1	1.5	2	2.5	3.0
$f(x)$	0	0.8409	1	1.1066	1.1892	1.2574	1.3161

Form a difference table from these values and see what happens when you do so.

\*\*\*\*\*

0	0					
0.5	0.8409	8409				
1.0	1.0000	1591	-6818			
1.5	1.1066	1066	-525	6293	-6008	
2.0	1.1892	826	-240	285	-189	5819
2.5	1.2574	682	-144	96	-47	142
3.0	1.3161	587	-95	49		

You will notice that there is no column containing only small differences.

## FRAME 47

A difference table like this would give us the clue that it is not reasonable to try and proceed further. The values tabulated above were taken from the function  $f(x) = x^4$  and here we have a situation somewhat analogous to that in analytical work if an attempt is made to obtain a Maclaurin series for  $x^4$ . If Lagrange's method is used there is no built in early warning system, because, although this method is based on divided differences, these do not have to be found.

## FRAME 48

Inverse Interpolation

The process we have concentrated on so far is: Given a table of values of  $x$  and  $f(x)$ , what is the value of  $f(x)$  at some other value of  $x$ ? The inverse problem is: Given a table of values of  $x$  and  $f(x)$ , what value of  $x$  will correspond to some other value of  $f(x)$ ? The problem of finding such an  $x$  is known as INVERSE INTERPOLATION. As an example of this, one might be asked: From the table in FRAME 3, at what time would the temperature have been  $70^\circ \text{C}$ ? As you might suspect from previous work, there are certain methods of dealing with a problem of this sort when the original table is given at unequal intervals of the independent variable and others which can only be used if the original table is an equal interval one.

## FRAME 49

To take an example, suppose a curve passes through the points  $(0, -4)$ ,  $(0.6, -3.64)$ ,  $(1, -3)$  and it is necessary to find the value of  $x$  when  $y = -3.5$ .

You will notice that the intervals between successive values of  $x$  are unequal. One way in which we can proceed is to find  $y$  using the Lagrangian interpolation formula in FRAME 40, put the result equal to  $-3.5$  and solve the equation so formed for  $x$ .

What will you get if you do it this way?  
\*\*\*\*\*

$$\frac{y}{x(x - 0.6)(x - 1)} = \frac{-4}{x(-0.6)(-1)} + \frac{-3.64}{(x - 0.6)0.6(-0.4)} + \frac{-3}{(x - 1)0.4},$$

49A

i.e.,  $y = x^2 - 4$  (49A.1)

$x^2 - 4 = -3.5$  gives  $x \approx \pm 0.71$ . To keep  $x$  within the range 0 to 1,  
i.e., within the range of the given three points, take  $x = 0.71$ .

FRAME 50

If  $f(x)$  is of higher degree than two, then the Newton-Raphson process can be used to solve the equation obtained for  $x$ .

A second method is to interchange the roles of  $x$  and  $y$ . This means that an equation is found for  $x$  as a polynomial function of  $y$ . Once this has been done, the given value of  $y$  can be inserted into it to give the required value of  $x$ . These two steps can be combined into one as in FRAME 42, but in order that you can see fully what is involved, this will not be done in this example.

Use the three points  $(0, -4)$ ,  $(0.6, -3.64)$ ,  $(1, -3)$  to obtain a Lagrangian interpolation formula for  $x$  in terms of  $y$ .

\*\*\*\*\*

50A

$$\frac{x}{(y + 4)(y + 3.64)(y + 3)} = \frac{0}{(y + 4)(-0.36)(-1)} + \frac{0.6}{(y + 3.64)0.36(-0.64)} + \frac{1}{(y + 3)0.64}$$

$$x = -1.04167y^2 - 6.29167y - 8.5 \quad (50A.1)$$

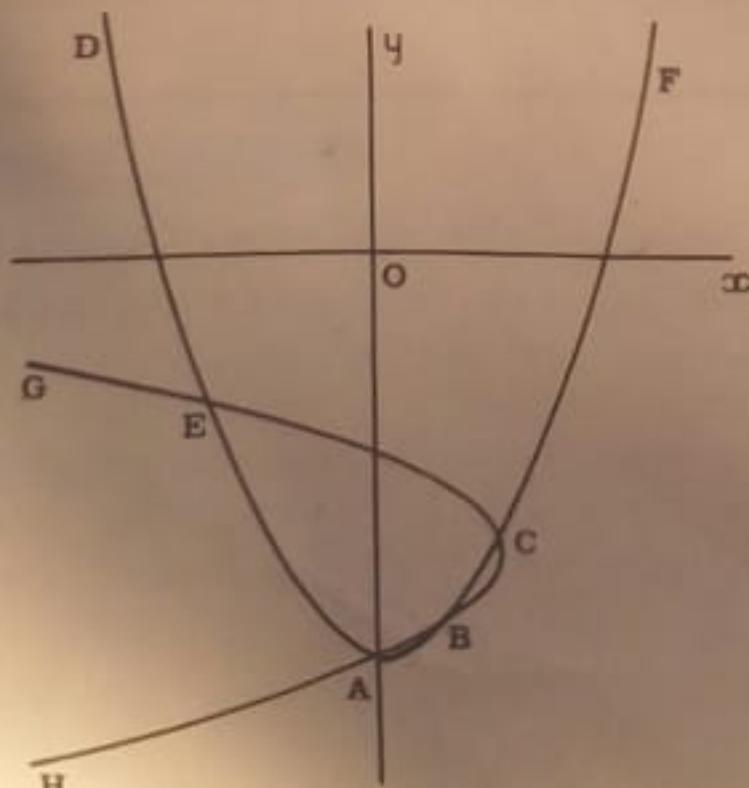
FRAME 51

When  $y = -3.5$ , this gives  $x \approx 0.76$ , which is not the same as that obtained before. So the question now is: Why the difference?

Can you spot the reason? [Don't worry if you can't, it is a bit tricky. As a hint, it is suggested that you consider sketches of the two curves represented by (49A.1) and (50A.1).]

\*\*\*\*\*

51A



In both 49A and 50A you found a parabola passing through the three given points, A, B and C. However the one found in 49A had its axis parallel to  $Oy$  (the parabola DEABC) while that found in 50A had its axis parallel to  $Ox$  (GECBAH), and these two parabolas are not the same. For an intermediate value of  $y$ , they give different values for  $x$ .

As only three points are known, and there is actually no information about what happens in between these points, one cannot be definite and say, with no shadow of doubt, which, if indeed either, should be taken. As we have based our direct interpolation on a polynomial of the form  $y = f(x)$ , it would seem logical to continue to use one of this form for inverse interpolation and so quote the answer as approximately 0.71. Sometimes an answer can be immediately discarded. For example, in 41A you found a polynomial to fit the points  $(-1, -3), (0, -1), (1, 1)$  and (3, 29). Suppose you were required to find the value of  $x$  when  $y = 20$ , knowing in addition that, over the range given,  $y$  is increasing as  $x$  increases. The value you would find by the second method is approximately 6.4 and so you would immediately reject it under the conditions given.

When the original table is given at equal intervals of  $x$ , both of the methods just given can be used, care being taken to reject any ridiculous answers. Alternatively, finite differences can now be used, the method, however, being basically similar to that in FRAME 49 and 49A. To see how it works, let us return to the difference table in 20A and seek the value of  $x$  for which  $f(x) = 0.08$ . Obviously the value required will lie between 2.0 and 2.2. For this calculation,  $x_0$  is now put equal to 2.0 and  $x_1$ , 2.2. Any convenient interpolation formula is now used, putting in it  $f_p = 0.08$ ,  $f_0 = 0.0739$ , etc., but leaving  $p$  as  $p$ .

Suppose we use Bessel's formula. What equation will you get when you make these substitutions?

\*\*\*\*\*

$$\begin{aligned} 0.08 &= 0.0821 + (p - \frac{1}{2}) \times 0.0164 + \frac{p(p - 1)}{2} \times 0.00325 \\ &\quad + \frac{p(p - 1)(p - \frac{1}{2})}{6} \times 0.0005 + \frac{(p + 1)p(p - 1)(p - 2)}{24} \times 0.0002, \end{aligned}$$

stopping at the fourth differences as no more are reliable.

This is now a quartic equation in  $p$ , but instead of solving it, as is possible, by Newton-Raphson, an alternative iterative technique is often used at this stage. By solving for the  $p$  in the term  $(p - \frac{1}{2}) \times 0.0164$ , the quartic can be rewritten as

$$\begin{aligned} p &= 0.37195 - 0.09909(p - 1) - 0.00508(p - 1)(p - \frac{1}{2}) \\ &\quad - 0.00051(p + 1)p(p - 1)(p - 2) \end{aligned} \tag{54.1}$$

A first estimate of  $p$  can be taken as  $p_0 = 0.372$ , say (i.e. the constant term on the R.H.S.). A second estimate,  $p_1$ , is obtained by substituting this value of  $p$  into the R.H.S. Thus

$$\begin{aligned} p_1 &= 0.37195 - 0.09909 \times 0.372 \times (-0.628) \\ &\quad - 0.00508 \times 0.372 \times (-0.628) \times (-0.128) \\ &\quad - 0.00051 \times 1.372 \times 0.372 \times (-0.628) \times (-1.628) \end{aligned}$$

$$= 0.37195 + 0.02315 - 0.00015 - 0.00027 = 0.39468$$

FRAME 54 (continued)  
 A third estimate,  $p_2$ , is obtained by using this value of  $p_1$  in the R.H.S. of (54.1). What do you get when you do this?  
 \*\*\*\*\*

0.395 23

54A

FRAME 55  
 Using this value in the R.H.S. of (54.1) produces no further change in the estimate of  $p$  and so this gives the value we want.

Then, as  $x = x_0 + ph$ ,  $x = 2.0 + 0.39523 \times 0.2 = 2.079046$ .

There is no reason why it has to be Bessel's formula which is used for this process. Repeat this example using Everett's formula (FRAME 18). ( $q$  must be replaced immediately by  $1 - p$ ).  
 \*\*\*\*\*

$$\begin{aligned} 0.08 &= (1 - p) \times 0.0739 + \frac{(2 - p)(1 - p)(-p)}{6} \times 0.0030 \\ &+ \frac{(3 - p)(2 - p)(1 - p)(-p)(-1 - p)}{24} \times (-0.0001) + p \times 0.0903 \\ &+ \frac{(p + 1)p(p - 1)}{6} \times 0.0035 + \frac{(p + 2)(p + 1)p(p - 1)(p - 2)}{24} \times 0.0005 \end{aligned} \quad \underline{55A}$$

Solving for  $p$  from the two linear terms,

$$\begin{aligned} p &= 0.37195 + p(p - 1)(p - 2)0.03049 - p(p^2 - 1)(p - 2)(p - 3)0.0003 \\ &- p(p^2 - 1)0.03557 - p(p^2 - 1)(p^2 - 4)0.0013 \end{aligned}$$

Successive estimates for  $p$  are 0.372, 0.39483, 0.39537, 0.39538.  
 $x$  is then 2.079076.

FRAME 56  
 In the last frame, the two values of  $p$  do not agree beyond the third decimal place. The main cause of this was the division by 0.0164, the first difference coefficient of  $p$ . (In 53A, 0.0164 appeared directly; in 55A it comes from  $0.0903 - 0.0739$ .) As this division is equivalent to multiplying by approximately 61, it can cause quite a difference to the final answer.

### Summary of Interpolation Formulae

For your convenience, the various interpolation formulae mentioned in this programme are listed below:

Newton-Gregory Forward

$$f_p = f_0 + \binom{p}{1} \Delta f_0 + \binom{p}{2} \Delta^2 f_0 + \binom{p}{3} \Delta^3 f_0 + \dots$$

Newton-Gregory Backward

$$f_p = f_0 + p \nabla f_0 + \binom{p+1}{2} \nabla^2 f_0 + \binom{p+2}{3} \nabla^3 f_0 + \dots$$

Bessel

FRAME 57 (continued)

$$\begin{aligned} f_p = \mu f_{\frac{1}{2}} + (p - \frac{1}{2}) \delta f_{\frac{1}{2}} + \frac{p(p-1)}{2!} \mu \delta^2 f_{\frac{1}{2}} + \frac{p(p-1)(p-\frac{1}{2})}{3!} \delta^3 f_{\frac{1}{2}} \\ + \frac{(p+1)p(p-1)(p-2)}{4!} \mu \delta^4 f_{\frac{1}{2}} + \dots \end{aligned}$$

Stirling

$$f_p = f_0 + p\mu \delta f_0 + \frac{p^2}{2!} \delta^2 f_0 + \frac{p(p^2-1)}{3!} \mu \delta^3 f_0 + \frac{p^2(p^2-1)}{4!} \delta^4 f_0 + \dots$$

Everett

$$\begin{aligned} f_p = \binom{q}{1} f_0 + \binom{q+1}{3} \delta^2 f_0 + \binom{q+2}{5} \delta^4 f_0 + \dots \\ + \binom{p}{1} f_1 + \binom{p+1}{3} \delta^2 f_1 + \binom{p+2}{5} \delta^4 f_1 + \dots \quad (q = 1 - p) \end{aligned}$$

Lagrange

$$\begin{aligned} \frac{f(x)}{(x-x_0)(x-x_1)\dots(x-x_n)} &= \frac{f(x_0)}{(x-x_0)(x_0-x_1)(x_0-x_2)\dots(x_0-x_n)} \\ &+ \frac{f(x_1)}{(x-x_1)(x_1-x_0)(x_1-x_2)\dots(x_1-x_n)} + \dots \\ &+ \frac{f(x_n)}{(x-x_n)(x_n-x_0)(x_n-x_1)\dots(x_n-x_{n-1})} \end{aligned}$$

FRAME 58Miscellaneous Examples

In this frame a collection of miscellaneous examples is given for you to try. Answers are provided in FRAME 59, together with such working as is considered helpful.

**Note:** The data from some of these questions will be used in subsequent programmes. You will find it helpful then to be able to refer quickly to the difference tables that you will now be forming.

1. The following readings of current,  $i$ , against deflection,  $\theta$ , were obtained for a certain galvanometer.

$\theta$	0.40	0.45	0.50	0.55	0.60	0.65
$i$	1.268	1.449	1.639	1.839	2.052	2.281

What will be the current when  $\theta = 0.536$ ?

2. i) A polynomial  $f(x)$  of low degree is tabulated as follows:

$x$	-3	-2	-1	0	1	2	3	4	5	6
$f(x)$	-14	-2	2	4	10	25	59	112	194	310

Errors in two values of  $f(x)$  are suspected. Locate and correct them.

ii) Derive the Newton interpolation formulae:

$$a) f_p = f_0 + \binom{p}{1} \Delta f_0 + \binom{p}{2} \Delta^2 f_0 + \binom{p}{3} \Delta^3 f_0 + \dots$$

$$b) f_p = f_0 + \binom{p}{1} \nabla f_0 + \binom{p+1}{2} \nabla^2 f_0 + \binom{p+2}{3} \nabla^3 f_0 + \dots$$

iii) Obtain the values of  $f(x)$  as given in (i) after correction  
when  $x = -4, -2.5, 5.5.$  (L.U.)

3. A fourth degree polynomial is tabulated as follows:

x   0	0.1	0.2	0.3	0.4
y   1.0000	0.9208	0.6928	0.3448	-0.0752
x   0.5	0.6	0.7	0.8	0.9
y   -0.5000	-0.8452	-0.9992	-0.8432	-0.2312

Show from a difference table that there is an error and use the corrected table with the Stirling interpolation formula

$$f_p = f_0 + \frac{1}{2} p(\delta f_{\frac{1}{2}} + \delta f_{-\frac{1}{2}}) + \frac{1}{2} p^2 \delta^2 f_0 + \frac{p(p^2 - 1)}{2(3!)} (\delta^3 f_{\frac{1}{2}} + \delta^3 f_{-\frac{1}{2}}) \\ + \frac{p^2(p^2 - 1)}{4!} \delta^4 f_0 + \dots$$

to find the value of  $y$  when  $x = 0.45.$

(L.U.)

(It was pointed out in FRAME 18 that interpolation formulae are not always quoted in exactly the same form. You should check that the form given in this question agrees with that in FRAME 18.)

4. The following table gives readings of the temperature ( $\theta^\circ$ ) recorded at given times ( $t$ ):

t   0	1	2	3	4	5	6	7	8	9	10
$\theta$   80.00 70.48 61.87 54.08 47.03 40.65 34.88 29.66 24.93 20.66 16.79										

Using (i) Bessel's formula, (ii) Everett's formula, find  $\theta$  at  $t = 4.3.$  At what time would you expect  $\theta$  to be 50?

5. The deflection,  $y$ , measured at various distances,  $x$ , from one end of a cantilever is given by

x   0.0	0.2	0.4	0.6	0.8	1.0
y   0.0000 0.0347 0.1173 0.2160 0.2987 0.3333					

For what value of  $x$  is  $y = 0.2?$

6. Write down the Lagrange interpolation polynomial which fits the points  $(0, y_0), (1, y_1), (2, y_2).$  Express  $y_1$  and  $y_2$  in terms of  $y_0$  and its differences and hence obtain the Gregory-Newton polynomial.

Write down the Lagrange polynomial which fits the points  $(1, 4), (3, 7), (4, 8), (6, 11)$  and use it to interpolate values of  $y$  at  $x = 2$  and  $x = 5.$  Check these values by differencing. (L.U.)

7. The following table gives values of the current  $i$  in a certain L,C,R circuit at various times  $t.$

t   0.000	0.002	0.004	0.006	0.008	0.010	0.012
i   0.000 00	0.015 63	0.024 63	0.029 31	0.031 23	0.031 41	0.030 54
t   0.014	0.016	0.018	0.020			
i   0.029 05	0.027 23	0.025 29	0.023 31			

Find i when  $t = 0.003, 0.0125$  and  $0.0184$  and t when  $i = 0.03000$ .

8. The following table contains one incorrect entry for  $f(x)$ . Locate the error; suggest a possible reason for its occurrence and a suitable correction. Using this correction, draw up a corrected difference table.

x   1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9
$f(x)$   5.743	3.959	2.511	1.486	0.969	1.046	1.800	3.341	5.673
x   2.0	2.1							
$f(x)$   8.965	13.274							

Use your corrected table and an interpolation formula to calculate  $f(1.45)$ . Any interpolation formula may be used but it should be clearly stated before use and all symbols defined. (L.U.)

### Answers to Miscellaneous Examples

1. 1.782

2. i) 25 and 59 should be 26 and 58 respectively.  
ii) -40, -6.625, 247.375. These three are obtained by extending the difference table back one step and by the use of formulae (ii) (a) and (ii) (b) respectively.

3. Corrected value:  $x = 0.6, y = -0.8432$   
When  $x = 0.45, y = -0.29195$ .

4. (i) 45.05 (ii) 45.05

Using the Newton-Gregory forwards difference formula (any other may be chosen) and solving iteratively for p, taking  $t_0 = 3$ , gives  $p = 0.57$ , and so  $t = 3.57$ .

5. 0.572

$$6. \frac{y}{x(x-1)(x-2)} = \frac{y_0}{2x} - \frac{y_1}{x-1} + \frac{y_2}{2(x-2)}$$

As  $x_0 = 0$  and  $h = 1, x = p$ . Using  $E = 1 + \Delta, y_1 = y_0 + \Delta y_0$ ,  $y_2 = y_0 + 2\Delta y_0 + \Delta^2 y_0$  and then  $y = y_0 + p\Delta y_0 + \binom{p}{2}\Delta^2 y_0$ ,

i.e., the first three terms of the Newton-Gregory formula.

$$\frac{y}{(x-1)(x-3)(x-4)(x-6)} = -\frac{2}{15(x-1)} + \frac{7}{6(x-3)} - \frac{4}{3(x-4)} + \frac{11}{30(x-6)}$$

TECNO When  $x = 2, y = 5.8$ .

When  $x = 5, y = 9.2$ .

## INTERPOLATION

### FRAME 59 (continued)

7.  $0.020\ 79, 0.030\ 22, 0.024\ 90; \quad 0.006\ 64, 0.012\ 80$

8. The difference table suggests that the last two digits of 3.341 are in the wrong order and that this figure should be 3.314. This points to a copying error. A revised difference table corroborates this.

As  $p = \frac{1}{2}$ , Bessel's formula is a reasonable choice. Using this gives  $f(1.45) = 1.159$ .

## Numerical Differentiation

### Introduction

FRAME 1

It has already been indicated in this book that you may sometimes need to find the value of a derivative at a point of some function  $y$  of  $x$ , even although the only information you are given (or can find experimentally) is a table showing values of  $y$  for specified values of  $x$ . If this happens, the analytical process of differentiation breaks down as, for this, it is necessary to know the functional relation between  $y$  and  $x$  in the form of an equation.

One way in which you can proceed to estimate a derivative in these circumstances is to plot the points on a graph, join them by a smooth curve, draw the tangent at the required point and measure its slope. This method is not entirely satisfactory as the best smooth curve would be to a certain extent open to conjecture and also drawing an exact tangent to a curve is not easy. It will be better if some numerical process can be evolved whereby the derivative can be actually calculated from the known values of  $y$ .

FRAME 2

Doubtless you have already met many cases where derivatives have been required in practical problems. So here we shall just be content with a few illustrations to indicate the type of problem where numerical differentiation might arise.

Freudenstein's equation  $R_1 \cos \theta - R_2 \cos \phi + R_3 - \cos(\theta - \phi) = 0$  for a certain crank mechanism was mentioned in Unit 1. Now suppose that values of  $\phi$ , the output lever angle, have been calculated for a series of values of  $\theta$ , the input crank angle. If the crank rotates with constant angular velocity  $\omega$ , what will be the angular velocity and acceleration of the output lever for the given values of  $\theta$ ? With the information now available, these can be found by analytical differentiation. An alternative method is to use a numerical approach for the actual differentiation itself. In this particular example, this has the advantage that the calculations are simpler although the results are not quite so accurate.

FRAME 3

The set of miscellaneous examples at the end of the programme on interpolation (see page 231) describe situations where numerical differentiation would be used to obtain rates of change. For the situation described in question 4, it might be necessary to find the rate of decrease of temperature with respect to time (i.e.  $-\frac{d\theta}{dt}$ ) when, say,

$t = 3.5$  or when  $t = 4.2$ . In the question (No. 5) on the cantilever, the slope at the point where  $x = 0.8$  might be required. Finally, in question 7 we may be asked to find the maximum current. This will

involve finding the time at which  $\frac{di}{dt} = 0$  and then interpolating for  $i$ .

## NUMERICAL DIFFERENTIATION

### A Basic Process

FRAME 4

If you turn back to FRAME 14, page 7, you will see that some estimates were obtained for  $\frac{d}{dx} \left( \frac{e^x}{x} \right)$  when  $x = 2$  by approximating  $f'(x)$  at  $x = a$ , i.e.  $f'(a)$ , to  $\frac{f(a+h) - f(a)}{h}$ . Four values of  $h$ , i.e., 0.2, 0.1, 0.05 and 0.01 were taken and it was seen that the estimate of  $f'(x)$  at  $x = 2$  was becoming more accurate as  $h$  was reduced. This is, of course, what one would expect from theory. A table can now be started, showing the various estimates of  $f'(2)$  for the different values of  $h$ . The following table shows these values and at the same time, extends the range of values of  $h$  taken.

$h$	0.2	0.1	0.05	0.01	0.005	0.002	0.001	0.0001
$f'(2)$	2.038	1.941	1.892	1.85	1.84	1.8	1.8	1

In calculating these values, exponential tables to four places of decimals were used. The only rounding that was done during the calculation was in the division of  $e^{a+h}$  by  $a+h$ , this rounding being to 4 decimal places. Now theoretically, calculus wise, the estimates should continue to improve as  $h$  is decreased. As the actual value of the derivative is 1.8473, you will notice that improvement only took place down to  $h = 0.01$ .

Taking the value of  $e^{2.0001}$  as 7.3898, work through the calculation giving  $f'(2)$  when  $h = 0.0001$ . Then suggest two reasons why the result is not as accurate as it should be.

\*\*\*\*\*

$$e^{a+h}/(a+h) = 3.6947, \quad \frac{e^{a+h}}{a+h} - \frac{e^a}{a} = 0.0001, \quad f'(2) \approx 1$$

$e^a/a = 3.6946$  and forming  $\frac{e^{a+h}}{a+h} - \frac{e^a}{a}$  thus involved the subtraction of two very nearly equal numbers. This introduced an error which was large in comparison with the true value. This error was then multiplied by 10 000 when the division by  $h (= 0.0001)$  was done.

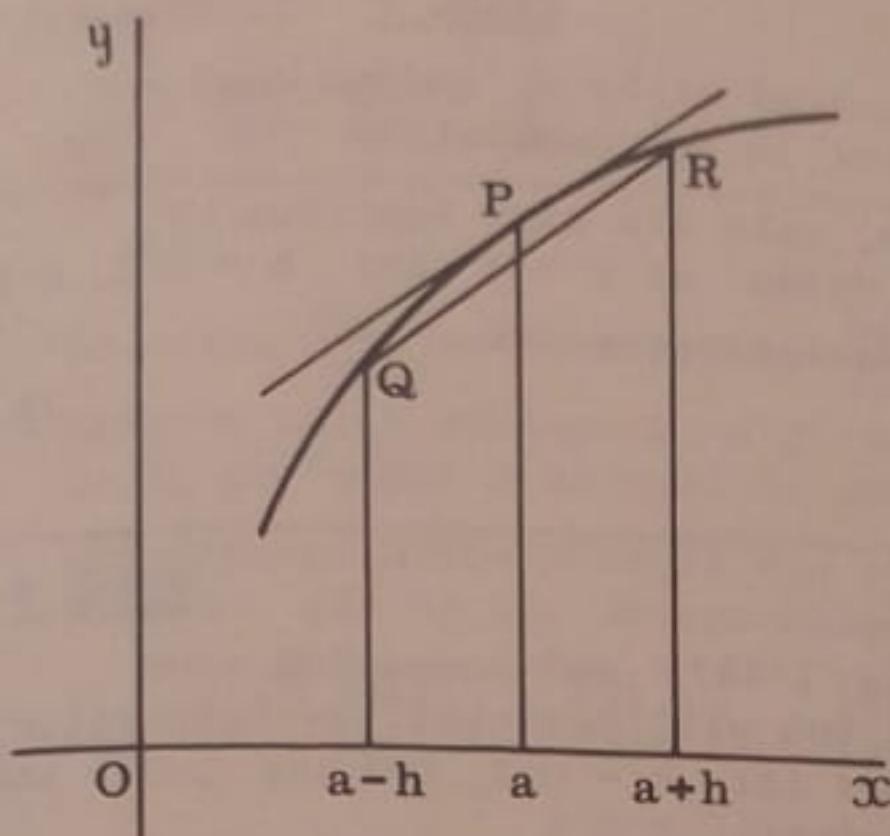
4A

FRAME 5

This example thus shows that, when working to a fixed number of decimal places, a stage is reached where accuracy cannot be improved just by decreasing the value of  $h$ . It is therefore necessary to look for some other means of increasing the accuracy. In practice, it is desirable to do this for another reason as well - if you have values of a function known only at regular intervals,  $h$  is fixed. Any attempt to decrease it would involve doing an interpolation calculation.

FRAME 6

A variation of the basic process is shown in the accompanying figure. If the value of  $\frac{dy}{dx}$  at P is required, two points Q and R are taken, one on each side of P and equidistant from it x-wise. The slope of the chord



QR is then found, it being assumed that this chord is nearly parallel to the tangent at P. (It is certainly more so than the chord PR, whose slope the formula  $\frac{f(a+h) - f(a)}{h}$  finds.) This means that

$$\frac{f(a+h) - f(a-h)}{2h} \quad (6.1)$$

is taken as an estimate of  $f'(x)$  at  $x = a$ .

Now, if  $f(a+h)$  is expanded by means of Taylor's series, the original formula, i.e.  $\frac{f(a+h) - f(a)}{h}$  gives

$$\begin{aligned} & \left\{ f(a) + hf'(a) + \frac{h^2}{2!} f''(a) + \frac{h^3}{3!} f'''(a) + \dots \right\} - f(a) \\ &= f'(a) + \frac{h}{2} f''(a) + \frac{h^2}{6} f'''(a) + \dots \end{aligned}$$

and, assuming  $h$  small, the difference between this and  $f'(a)$  is approximately  $\frac{h}{2} f''(a)$ .

Now take the formula (6.1) and, treating this in a similar way, obtain the main term in the difference between it and  $f'(a)$ .

\*\*\*\*\*

6A

$$\begin{aligned} & \left[ \left\{ f(a) + hf'(a) + \frac{h^2}{2!} f''(a) + \frac{h^3}{3!} f'''(a) + \dots \right\} \right. \\ & \quad \left. - \left\{ f(a) - hf'(a) + \frac{h^2}{2!} f''(a) - \frac{h^3}{3!} f'''(a) + \dots \right\} \right] / 2h \\ &= f'(a) + \frac{h^2}{6} f'''(a) + \dots \end{aligned}$$

$$\text{Difference} = \frac{h^2}{6} f'''(a)$$

FRAME 7

This suggests that, for reasonably small  $h$ , the result should be more accurate than that obtained previously as the main term in the error now involves  $h^2$  instead of  $h$ . Consequently it should not be necessary to reduce  $h$  to the same degree as before to get a similar accuracy. This will have two advantages from the numerical point of view. Firstly, unless we are near a maximum or minimum, the difference between  $f(a+h)$  and  $f(a-h)$  will be larger than that between  $f(a+h)$  and  $f(a)$ .

FRAME 7 (continued)

Secondly the final division is by  $2h$  instead of by  $h$  and so does not magnify to quite the same extent any error in the numerator.

To test how well the formula (6.1) works, take the same function as before, i.e.  $y = e^x/x$ , and calculate  $dy/dx$  at  $x = 2$  for  $h = 0.2, 0.1, 0.05, 0.01$ .

\*\*\*\*\*

$1.8535, 1.849, 1.848, 1.85$

7A

FRAME 8

Remembering that the theoretical value is  $1.8473$  and comparing your results now with those given in FRAME 4, you will see that the best value is given by  $h = 0.05$  and that the values for  $h = 0.2, 0.1$  and  $0.05$  are all considerably better than they were before.

If  $h$  is further reduced, the table now corresponds completely to that given in FRAME 4 is

$h$	0.2	0.1	0.05	0.01	0.005	0.002	0.001	0.0001
$f'(2)$	1.8535	1.849	1.848	1.85	1.85	1.85	1.85	1.5

These figures corroborate very well the remarks made in FRAME 7.

FRAME 9

Even although the results obtained using formula (6.1) are an improvement over the previous ones, there are still some disadvantages inherent in the method. One of these has been mentioned before - the required values of the function may not be known and hence must be found by interpolation. Secondly, as the theoretical value will not be known in any actual example (otherwise we shouldn't be looking for an approximation to it) it will not be obvious which value of  $h$  will give the best answer. In view of these difficulties, other methods of numerical differentiation are more often used. These methods are based on the interpolation formulae that were given in the previous programme.

FRAME 10Differentiation Based on Equal Interval Interpolation Formulae

Effectively, an equal interval interpolation formula assumes that a curve can be adequately represented over a certain range of values by a polynomial in  $p$ . It is thus perhaps natural to enquire whether differentiation of the function represented by an interpolating polynomial formula can be achieved in some way by differentiation of the actual interpolating formula itself w.r.t.  $p$ .

Effectively this question means:

If  $y = f(x)$  is represented by  $y = F(p)$ , where  $x = x_0 + ph$ , can  $dy/dx$  be obtained from  $dy/dp$ ?

What will be the relation between  $\frac{dy}{dx}$  and  $\frac{dy}{dp}$ ?

\*\*\*\*\*

$$\frac{dy}{dx} = \frac{dy}{dp} \cdot \frac{dp}{dx} = \frac{dy}{dp} \cdot \frac{1}{h}$$

So, once  $\frac{dy}{dp}$  has been found,  $\frac{dy}{dx}$  follows immediately. You will notice that  $h$  still appears as a divisor and so there is good reason for its not being too small a decimal if possible (remember what happened in 4A). Any interpolation formula can be used for differentiation w.r.t.  $p$ . For example, taking the Newton-Gregory forward difference formula,

$$\begin{aligned} f_p &= f_0 + \binom{p}{1} \Delta f_0 + \binom{p}{2} \Delta^2 f_0 + \binom{p}{3} \Delta^3 f_0 + \binom{p}{4} \Delta^4 f_0 + \dots \\ &= f_0 + p \Delta f_0 + \frac{p(p-1)}{2} \Delta^2 f_0 + \frac{p(p-1)(p-2)}{6} \Delta^3 f_0 \\ &\quad + \frac{p(p-1)(p-2)(p-3)}{24} \Delta^4 f_0 + \dots \\ &= f_0 + p \Delta f_0 + \left( \frac{1}{2} p^2 - \frac{1}{2} p \right) \Delta^2 f_0 + \left( \frac{1}{6} p^3 - \frac{1}{2} p^2 + \frac{1}{3} p \right) \Delta^3 f_0 \\ &\quad + \left( \frac{1}{24} p^4 - \frac{1}{4} p^3 + \frac{11}{24} p^2 - \frac{1}{4} p \right) \Delta^4 f_0 + \dots \\ \therefore f'_p &= \Delta f_0 + \left( p - \frac{1}{2} \right) \Delta^2 f_0 + \left( \frac{1}{2} p^2 - p + \frac{1}{3} \right) \Delta^3 f_0 \\ &\quad + \left( \frac{1}{6} p^3 - \frac{3}{4} p^2 + \frac{11}{12} p - \frac{1}{4} \right) \Delta^4 f_0 + \dots \end{aligned}$$

and so  $f'(x_p) = \frac{1}{h} \left\{ \Delta f_0 + \left( p - \frac{1}{2} \right) \Delta^2 f_0 + \left( \frac{1}{2} p^2 - p + \frac{1}{3} \right) \Delta^3 f_0 + \left( \frac{1}{6} p^3 - \frac{3}{4} p^2 + \frac{11}{12} p - \frac{1}{4} \right) \Delta^4 f_0 + \dots \right\}$  (11.1)

Taking the data from the example in FRAME 8, page 209, the value of the derivative at  $x = 2.31$  is

$$\frac{1}{h} \left\{ 19 + \left( 0.31 - \frac{1}{2} \right) \times 18 + \left( \frac{1}{2} \times 0.31^2 - 0.31 + \frac{1}{3} \right) \times 6 \right\} \approx 19 - 3.42 + 0.428 = 16.008$$

In this example, the table represented the cubic  $x^3 + 2$ , the derivative of which is  $3x^2$ . When  $x = 2.31$ ,  $3x^2 \approx 16.008$  which agrees with the value just found.

Equation (11.1) takes on a particularly simple form if  $p = 0$ . Then

$$f'(x_0) = \frac{1}{h} \left( \Delta f_0 - \frac{1}{2} \Delta^2 f_0 + \frac{1}{3} \Delta^3 f_0 - \frac{1}{4} \Delta^4 f_0 + \dots \right) \quad (12.1)$$

What will this formula give for the derivative at  $x = 3$  of the function defined by the data in the example in FRAME 8, page 209?  
\*\*\*\*\*

Here it is necessary to take  $x_0 = 3$ , then

12A

$$f'(3) = \frac{1}{1} \left( 37 - \frac{1}{2} \times 24 + \frac{1}{3} \times 6 \right) = 27$$

Again this agrees with the value of  $3x^2$  when  $x = 3$ .

What will be the differentiation formula corresponding to the Newton-Gregory backward difference formula?

FRAME 13

\*\*\*\*\*

$$\begin{aligned} f_p &= f_0 + p \nabla f_0 + \left( \frac{1}{2}p^2 + \frac{1}{2}p \right) \nabla^2 f_0 + \left( \frac{1}{6}p^3 + \frac{1}{2}p^2 + \frac{1}{3}p \right) \nabla^3 f_0 \\ &\quad + \left( \frac{1}{24}p^4 + \frac{1}{4}p^3 + \frac{11}{24}p^2 + \frac{1}{4}p \right) \nabla^4 f_0 + \dots \end{aligned}$$

13A

$$\begin{aligned} \therefore f'(x_p) &= \frac{1}{h} \left\{ \nabla f_0 + \left( p + \frac{1}{2} \right) \nabla^2 f_0 + \left( \frac{1}{2}p^2 + p + \frac{1}{3} \right) \nabla^3 f_0 \right. \\ &\quad \left. + \left( \frac{1}{6}p^3 + \frac{3}{4}p^2 + \frac{11}{12}p + \frac{1}{4} \right) \nabla^4 f_0 + \dots \right\} \quad (13A.1) \end{aligned}$$

FRAME 14

If  $p = 0$ , this gives the very simple result

$$f'(x_0) = \frac{1}{h} \left( \nabla f_0 + \frac{1}{2} \nabla^2 f_0 + \frac{1}{3} \nabla^3 f_0 + \frac{1}{4} \nabla^4 f_0 + \dots \right)$$

What will be the slope, to 2 decimal places, of the cantilever in question 5, FRAME 58, page 232 when  $x = 0.8$ ?

\*\*\*\*\*

14A

0.32

FRAME 15

When interpolating, we used the forward difference formula when near the beginning of a difference table and the backward difference formula when near the end. A similar distinction has been followed when differentiating. But if you are working near the middle of a difference table, it is, as before, better to use a central difference formula. Any one of the central difference interpolation formulae can be used to give a central difference differentiation formula. What such formula will arise if Bessel's interpolation formula is used?

\*\*\*\*\*

15A

$$\begin{aligned} f_p &= \mu f_{\frac{1}{2}} + \left( p - \frac{1}{2} \right) \delta f_{\frac{1}{2}} + \left( \frac{1}{2}p^2 - \frac{1}{2}p \right) \mu \delta^2 f_{\frac{1}{2}} + \left( \frac{1}{6}p^3 - \frac{1}{4}p^2 + \frac{1}{12}p \right) \delta^3 f_{\frac{1}{2}} \\ &\quad + \left( \frac{1}{24}p^4 - \frac{1}{12}p^3 - \frac{1}{24}p^2 + \frac{1}{12}p \right) \mu \delta^4 f_{\frac{1}{2}} + \dots \end{aligned}$$

$$f'(x_p) = \frac{1}{h} \left\{ \delta f_{\frac{1}{2}} + \left( p - \frac{1}{2} \right) \mu \delta^2 f_{\frac{1}{2}} + \left( \frac{1}{2} p^2 - \frac{1}{2} p + \frac{1}{12} \right) \delta^3 f_{\frac{1}{2}} + \left( \frac{1}{6} p^3 - \frac{1}{4} p^2 - \frac{1}{12} p + \frac{1}{12} \right) \mu \delta^4 f_{\frac{1}{2}} + \dots \right\}$$

(15A.1)

If  $p = 0$ , this becomes

$$f'(x_0) = \frac{1}{h} \left( \delta f_{\frac{1}{2}} - \frac{1}{2} \mu \delta^2 f_{\frac{1}{2}} + \frac{1}{12} \delta^3 f_{\frac{1}{2}} + \frac{1}{12} \mu \delta^4 f_{\frac{1}{2}} + \dots \right) \quad (16.1)$$

It becomes even more simple if  $p$  happens to be  $\frac{1}{2}$ . Then

$$f'(x_{\frac{1}{2}}) = \frac{1}{h} \left( \delta f_{\frac{1}{2}} - \frac{1}{24} \delta^3 f_{\frac{1}{2}} + \dots \right) \quad (16.2)$$

Incidentally the next term in the brackets is  $\frac{3}{640} \delta^5 f_{\frac{1}{2}}$ .

You should now be able to find the rate of decrease of temperature at  $t = 3.5$  and at  $t = 4.2$  for the cooling curve given in question 4 of FRAME 58 on page 232.

\*\*\*\*\*

Using (16.2) with  $\theta_0 = 3$  gives  $\frac{d\theta}{dt} = -7.047$ .

Using (15A.1) with  $\theta_0 = 4$  and  $p = 0.2$  gives  $\frac{d\theta}{dt} = -6.572$ .

16A

FRAME 17

Let us now have a look at the last problem posed in FRAME 3. (The other two have now been dealt with.) As was mentioned there, it is necessary to find the time at which  $\frac{di}{dt}$  is zero. This can be done by forming a table showing the values of  $\frac{di}{dt}$  at various times and then using inverse interpolation to find  $t$  when  $\frac{di}{dt} = 0$ . Having found this value of  $t$ , ordinary interpolation will give us the required value of  $i$ .

Start by calculating the values of  $\frac{di}{dt}$  at  $t = 0.000, 0.002, 0.004$  and  $0.006$ , using differences up to the fourth. (The required table of values is given in question 7, FRAME 58, page 232.)

\*\*\*\*\*

17A

$9.95, 5.91, 3.26, 1.55$

FRAME 18

For the first two of these, the formula (12.1) (but for  $\frac{di}{dt}$  instead of  $\frac{dy}{dx}$ ) was used as we have been using a forward difference formula at the beginning of a difference table. For the other two we used (16.1). This is better than (12.1) as it depends less on the third and fourth differences. As  $h = 1/500$ , a multiplying factor of 500 is involved in

## NUMERICAL DIFFERENTIATION

the  $1/h$ . Any errors in the figures resulting from the terms inside the brackets in (12.1) and (16.1) are therefore multiplied by this amount. Consequently the final figures cannot be relied on to any great degree of accuracy and so have only been quoted to 2 decimal places.

### FRAME 18 (continued)

Continuing the calculation of the values of  $di/dt$  gives the following table:

$t$	0.000	0.002	0.004	0.006	0.008	0.010	0.012	0.014	0.016
$di/dt$	9.95	5.91	3.26	1.55	0.46	-0.22	-0.64	-0.85	-0.96
$t$	0.018	0.020							
$di/dt$	-0.98	-1.00							

$di/dt$  is obviously zero for a value of  $t$  between 0.008 and 0.010. It is also obvious from the original table for  $i$  that the maximum value of the current occurs when  $t$  is in the region of 0.010.

### FRAME 20

In order to use inverse interpolation to find  $t$  more accurately a difference table is necessary for  $di/dt$ . A section of this is shown below:

$t$	$\frac{di}{dt}$			
0.000	9.95			
		-404		
0.002	5.91		139	
		-265		-45
0.004	3.26		94	
		-171		-32
0.006	1.55		62	
		-109		-21
0.008	0.46		41	
		-68		-15
0.010	-0.22		26	
		-42		-5
0.012	-0.64		21	
		-21		-11
0.014	-0.85		10	
		-11		-1
0.016	-0.96		9	
		-2		-9
0.018	-0.98		0	
		-2		
0.020	-1.00			

It has only been taken as far as the third differences as these are fluctuating somewhat and consequently any more would not be reliable.

Now taking  $t_0 = 0.008$ , write down the appropriate equation for  $p$  when  $di/dt = 0$ , using Bessel's interpolation formula.

\*\*\*\*\*

$$O = O \cdot 12 + (p - \frac{1}{2})(-0 \cdot 68) + \frac{p(p-1)}{2} (0 \cdot 335) + \frac{p(p-1)(p-\frac{1}{2})}{6} (-0 \cdot 15)$$

20A

What value, to 2 decimal places, does this equation give for  $p$ ?  
\*\*\*\*\*

$$p = 0 \cdot 62$$

FRAME 21

The maximum value of the current therefore occurs at  $t = 0 \cdot 00924$  and then interpolation in the  $t - i$  table yields  $i = 0 \cdot 03150$ .

FRAME 22

### Differentiation Based on Lagrange's Interpolation Polynomial

You will remember that this formula has to be used for interpolation when a table is given at unequal intervals of  $x$ . It is also necessary, under similar circumstances, to use it for differentiation. For this purpose it is better to use it in the second form given in the previous programme, i.e., as

$$\begin{aligned} f(x) &= \frac{(x - x_0)(x - x_1) \dots (x - x_n)}{(x_0 - x_1)(x_0 - x_2) \dots (x_0 - x_n)} f(x_0) \\ &+ \frac{(x - x_0)(x - x_1)(x - x_2) \dots (x - x_n)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3) \dots (x_1 - x_n)} f(x_1) \\ &+ \frac{(x - x_0)(x - x_1)(x - x_2)(x - x_3) \dots (x - x_n)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)(x_2 - x_4) \dots (x_2 - x_n)} f(x_2) + \dots \\ &+ \frac{(x - x_0)(x - x_1) \dots (x - x_{n-1})}{(x_n - x_0)(x_n - x_1) \dots (x_n - x_{n-1})} f(x_n) \end{aligned} \quad (23.1)$$

Differentiation is now straightforward but, as you will realise, the general expression for  $f'(x)$  is rather cumbersome. Consequently we shall not obtain it here, but will just do one example for illustration purposes.

FRAME 24

As an example, suppose that the value of  $f'(x)$  is required at  $x = 0 \cdot 12$ ,  $f(x)$  being given by the table

$x$	0.05	0.10	0.20	0.26
$f(x)$	0.0500	0.0999	0.1987	0.2574

Write down the equation resulting from applying (23.1) to this data.  
\*\*\*\*\*

$$\begin{aligned}
 f(x) &= \frac{0.0500(x - 0.10)(x - 0.20)(x - 0.26)}{(0.05 - 0.10)(0.05 - 0.20)(0.05 - 0.26)} \\
 &+ \frac{0.0999(x - 0.05)(x - 0.20)(x - 0.26)}{(0.10 - 0.05)(0.10 - 0.20)(0.10 - 0.26)} \\
 &+ \frac{0.1987(x - 0.05)(x - 0.10)(x - 0.26)}{(0.20 - 0.05)(0.20 - 0.10)(0.20 - 0.26)} \\
 &+ \frac{0.2571(x - 0.05)(x - 0.10)(x - 0.20)}{(0.26 - 0.05)(0.26 - 0.10)(0.26 - 0.20)}
 \end{aligned}$$


---

Before differentiating, it is a help to simplify this. It reduces to  
 $f(x) = -0.119x^3 - 0.025x^2 + 1.004x$  from which  
 $f'(x) = -0.357x^2 - 0.050x + 1.004$ .

When  $x = 0.12$ , this becomes 0.993.

### Higher Order Derivatives

All the methods used so far in this programme to obtain  $\frac{dy}{dx}$  can be extended to find the higher derivatives. Taking the first method (in FRAME 4),

$$f'(a) \approx \frac{f(a+h) - f(a)}{h} \quad (26.1)$$

$$\text{and so } f''(a) \approx \frac{f'(a+h) - f'(a)}{h} \quad (26.2)$$

If you can't see this, let  $f'(a) = F(a)$ , then  
 $f''(a) = F'(a) = \frac{F(a+h) - F(a)}{h} = \frac{f'(a+h) - f'(a)}{h}$ .

Now if, in (26.1),  $a$  is replaced by  $a + h$ ,

$$f'(a+h) \approx \frac{f(a+2h) - f(a+h)}{h}$$

Substituting into (26.2)

$$\begin{aligned}
 f''(a) &\approx \frac{1}{h} \left\{ \frac{f(a+2h) - f(a+h)}{h} - \frac{f(a+h) - f(a)}{h} \right\} \\
 &= \frac{1}{h^2} \{ f(a+2h) - 2f(a+h) + f(a) \} \quad (26.3)
 \end{aligned}$$

What will be the formula obtained for  $f''(a)$  when (6.1) is used for  $f'(a)$ ?  
\*\*\*\*\*

$$\begin{aligned}
 \frac{1}{2h} \{ f'(a+h) - f'(a-h) \} &\approx \frac{1}{2h} \left\{ \frac{f(a+2h) - f(a)}{2h} - \frac{f(a) - f(a-2h)}{2h} \right\} \\
 &= \frac{1}{4h^2} \{ f(a+2h) - 2f(a) + f(a-2h) \} \quad (26.4)
 \end{aligned}$$


---

FRAME 27

If  $h$  is small, what sources of error can you see in (26.3)?

---

\*\*\*\*\*

- i)  $f(a + 2h) + f(a)$  will be nearly equal to  $2f(a + h)$  and so the loss of significant figures consequent upon the subtraction of two nearly equal numbers will be involved.
- ii) The division by  $h^2$ .
- 

FRAME 28

Similar sources of error exist in (26A.1) but the effects are likely to be smaller due to the usually greater difference between functional values a distance  $2h$  apart over those only a distance  $h$  apart and also due to the presence of the 4 in the denominator.

Returning now to the expression used earlier, i.e.  $e^x/x$ , it can quite easily be shown analytically that  $\frac{d^2}{dx^2} \left( \frac{e^x}{x} \right)$  at  $x = 2$  is 1.8473. Use each of the formulae (26.3) and (26A.1) to estimate this derivative numerically, taking  $h = 0.1$ .

---

\*\*\*\*\*

28A

1.95, 1.85

FRAME 29

As you will notice, (26A.1) gives a more accurate result which, you will remember, was forecast in the last frame.

In FRAMES 10-22, differentiation formulae were obtained, based on equal interval interpolation formulae. There it was found that  $\frac{dy}{dx} = \frac{1}{h} \frac{dy}{dp}$ . Extending the ideas developed there enables us to find  $\frac{d^2y}{dx^2}$  from a knowledge of  $\frac{d^2y}{dp^2}$ .

What is the relation between  $\frac{d^2y}{dx^2}$  and  $\frac{d^2y}{dp^2}$ ?

---

\*\*\*\*\*

29A

$$\frac{d^2y}{dx^2} = \frac{d}{dx} \left( \frac{1}{h} \frac{dy}{dp} \right) = \frac{d}{dp} \left( \frac{1}{h} \frac{dy}{dp} \right) \frac{dp}{dx} = \frac{1}{h^2} \frac{d^2y}{dp^2}$$


---

FRAME 30

Then, using for example the Newton-Gregory forward difference formula,  $\frac{d^2y}{dx^2}$  can be obtained from (11.1) by differentiating its R.H.S. w.r.t.  $p$  and multiplying by  $1/h$ .

What will be the resulting formula for  $\frac{d^2y}{dx^2}$  and also the simplified version when  $p = 0$ ?

---

\*\*\*\*\*

NUMERICAL DIFFERENTIATION

$$\frac{1}{h^2} \left\{ \Delta^2 f_0 + (p - 1) \Delta^3 f_0 + \left( \frac{1}{2} p^2 - \frac{3}{2} p + \frac{11}{12} \right) \Delta^4 f_0 \dots \dots \dots \right\}$$


---


$$\frac{1}{h^2} \left( \Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12} \Delta^4 f_0 \dots \dots \dots \right)$$

30A

Using the data in the example in FRAME 8, page 209, what will be the value of  $\frac{d^2y}{dx^2}$  at (i)  $x = 2.31$ , (ii)  $x = 3$ ? FRAME 31

\*\*\*\*\*

$$i) \frac{1}{1^2} \{ 18 + (0.31 - 1) \times 6 \} = 13.86 \quad ii) \frac{1}{1^2} / 24 - 6 \} = 18$$

31A

As the table represented the polynomial  $x^3 + 2$ , you can immediately see that these values are correct analytically.

What expression will Bessel's interpolation formula give for  $\frac{d^2y}{dx^2}$ ? FRAME 32

\*\*\*\*\*

$$\frac{1}{h^2} \left\{ \mu \delta^2 f_{\frac{1}{2}} + \left( p - \frac{1}{2} \right) \delta^3 f_{\frac{1}{2}} + \left( \frac{1}{2} p^2 - \frac{1}{2} p - \frac{1}{12} \right) \mu \delta^4 f_{\frac{1}{2}} \dots \dots \dots \right\}$$

32A

You will notice that the first term in any of these formulae involves a second difference. When finding  $dy/dx$ , it involved a first difference. Similarly that for a third derivative would commence with a third difference and so on. Also the formula for a third difference would involve  $\frac{1}{h^3}$ . As

i) only the higher order differences are involved when calculating the higher derivatives,

ii) these differences are more subject to error when round-off is involved,

iii) division by a higher power of  $h$  takes place,

the values of the higher derivatives as found from these formulae are less accurate than those of the lower ones.

The following table gives the distance  $d$  travelled from rest by a car at various times  $t$ . What was the acceleration of the car when  $t = 0, 2.4, 4.6$ ? Work as far as 4th differences.

$t(s)$	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
$d(ms^{-1})$	0.00	0.07	0.53	1.60	3.61	6.61	10.62	15.62	21.54
$t(s)$	4.5	5.0							
$d(ms^{-1})$	28.09	35.00							

\*\*\*\*\*

1.08, 4.05, 0.04

33A

For the last of these results, we used the Newton-Gregory backward interpolation formula. From (13A.1) this gives

$$f''(x_p) = \frac{1}{h^2} \left\{ \nabla^2 f_0 + (p+1)\nabla^3 f_0 + \left( \frac{1}{2}p^2 + \frac{3}{2}p + \frac{11}{12} \right) \nabla^4 f_0 + \dots \right\}$$

FRAME 34

Lastly with respect to higher derivatives, we will mention the use of Lagrange's interpolation formula. As you saw in FRAME 25,  $f'(x)$  can be found directly once the formula has been used to produce  $f(x)$ . Obviously one can continue in order to find the higher derivatives. Taking the figures quoted in FRAME 24 and using  $f'(x)$  from FRAME 25,  $f''(x) = -0.714x - 0.050$  and so, when  $x = 0.12$ ,  $f''(x) = -0.136$ .

FRAME 35

### Miscellaneous Examples

In this frame a collection of miscellaneous examples is given for you to try. Answers are provided in FRAME 36, together with such working as is considered helpful.

1. Obtain formulae for  $\frac{dy}{dx}$  and  $\frac{d^2y}{dx^2}$  from the interpolation formula (due to Gauss)  $f_p = f_0 + \binom{p}{1} \delta f_{\frac{1}{2}} + \binom{p}{2} \delta^2 f_0 + \binom{p+1}{3} \delta^3 f_{\frac{1}{2}} + \binom{p+1}{4} \delta^4 f_0 + \dots$
2. The points  $(x_0, y_0), (x_1, y_1), (x_2, y_2)$  and  $(x_3, y_3)$ , the  $x$ 's being equally spaced, lie on a cubic curve. Show that (12.1) leads to  $-\frac{1}{6h}(y_3 - 6y_2 + 3y_1 + 2y_0)$  as the value of  $dy/dx$  at  $(x_1, y_1)$ . (This question illustrates that a derivative can be expressed in terms of functional values instead of differences.)
3. Express (16.2) in terms of functional values instead of differences, retaining the terms in (16.2) up to and including that involving  $\delta^3 f_{\frac{1}{2}}$ .
4. At what time will the rate of decrease of temperature be 8 for the cooling situation, given in question 4, FRAME 58, page 232?
5. Starting with Stirling's formula

$$f_p = f_0 + p\mu \delta f_0 + \frac{1}{2}p^2 \delta^2 f_0 + \frac{p(p^2 - 1)}{3!} \mu \delta^3 f_0 + \frac{p^2(p^2 - 1)}{4!} \delta^4 f_0 + \dots + \frac{p(p^2 - 1)(p^2 - 4)}{5!} \mu \delta^5 f_0 + \frac{p^2(p^2 - 1)(p^2 - 4)}{6!} \delta^6 f_0 + \dots$$

deduce that

$$hf'_0 = \mu \delta f_0 - \frac{1}{6} \mu \delta^3 f_0 + \frac{1}{30} \mu \delta^5 f_0 - \dots$$

$$h^2 f''_0 = \delta^2 f_0 - \frac{1}{12} \delta^4 f_0 + \frac{1}{90} \delta^6 f_0 - \dots$$

NUMERICAL DIFFERENTIATION

FRAME 35 (continued)

where  $hf'_p = h \frac{d}{dx} f(x_0 + ph) = \frac{d}{dp} f_p$ .

The following table gives the coordinates  $(x, y)$  of points on a certain polynomial curve.

x	0	0.2	0.4	0.6	0.8	1.0	1.2
y	0.710	1.175	1.811	2.666	3.801	5.292	7.232

Calculate the radius of curvature at the point  $x = 0.6$  (L.U.)

Note: In certain problems (e.g. deflection of beams, transition curves for railway tracks) the idea of curvature is used. The radius of curvature of a curve at a point is the radius of the circle which coincides with the curve over a very small length of arc at the point. The smaller the radius of curvature the sharper the bending. The radius of curvature is given by the formula

$$\left\{ 1 + \left( \frac{dy}{dx} \right)^2 \right\}^{3/2} / \frac{d^2y}{dx^2}$$

FRAME 36

Answers to Miscellaneous Examples

1. Gauss' formula can be written as

$$\begin{aligned} f_p &= f_0 + p\delta f_{\frac{1}{2}} + \frac{1}{2}p(p-1)\delta^2 f_0 + \frac{1}{6}(p+1)p(p-1)\delta^3 f_{\frac{1}{2}} \\ &\quad + \frac{1}{24}(p+1)p(p-1)(p-2)\delta^4 f_0 + \dots \\ &= f_0 + p\delta f_{\frac{1}{2}} + \left( \frac{1}{2}p^2 - \frac{1}{2}p \right) \delta^2 f_0 + \left( \frac{1}{6}p^3 - \frac{1}{6}p \right) \delta^3 f_{\frac{1}{2}} \\ &\quad + \left( \frac{1}{24}p^4 - \frac{1}{12}p^3 - \frac{1}{24}p^2 + \frac{1}{12}p \right) \delta^4 f_0 + \dots \end{aligned}$$

$$\begin{aligned} \frac{dy}{dx} &= \frac{1}{h} \left\{ \delta f_{\frac{1}{2}} + \left( p - \frac{1}{2} \right) \delta^2 f_0 + \left( \frac{1}{2}p^2 - \frac{1}{6} \right) \delta^3 f_{\frac{1}{2}} \right. \\ &\quad \left. + \left( \frac{1}{6}p^3 - \frac{1}{4}p^2 - \frac{1}{12}p + \frac{1}{12} \right) \delta^4 f_0 + \dots \right\} \end{aligned}$$

$$\frac{d^2y}{dx^2} = \frac{1}{h^2} \left\{ \delta^2 f_0 + p\delta^3 f_{\frac{1}{2}} + \left( \frac{1}{2}p^2 - \frac{1}{2}p - \frac{1}{12} \right) \delta^4 f_0 + \dots \right\}$$

2. The difference table is

$x_0$	$y_0$	$y_1 - y_0$		
$x_1$	$y_1$	$y_2 - y_1$	$y_2 - 2y_1 + y_0$	$y_3 - 3y_2 + 3y_1 - y_0$
$x_2$	$y_2$	$y_3 - y_2$	$y_3 - 2y_2 + y_1$	*
$x_3$	$y_3$			

At  $(x_1, y_1)$ , (12.1) gives  $dy/dx$  to be

FRAME 36 (continued)

$$\frac{1}{h} \left\{ (y_2 - y_1) - \frac{1}{2}(y_3 - 2y_2 + y_1) + \frac{1}{3}(y_3 - 3y_2 + 3y_1 - y_0) \right\}$$

= quoted result.

Note that the formula requires the use of the starred difference. As the curve is a cubic, all third order differences are the same and so that immediately above \* has been used in its place.

$$\begin{aligned} 3. \quad \delta^3 f_{\frac{1}{2}} &= \delta^2 f_1 - \delta^2 f_0 \\ &= (\delta f_{1\frac{1}{2}} - \delta f_{\frac{1}{2}}) - (\delta f_{\frac{1}{2}} - \delta f_{-\frac{1}{2}}) \\ &= \delta f_{1\frac{1}{2}} - 2\delta f_{\frac{1}{2}} + \delta f_{-\frac{1}{2}} \\ &= (f_2 - f_1) - 2(f_1 - f_0) + (f_0 - f_{-1}) \\ \text{or} \quad &= f_2 - 3f_1 + 3f_0 - f_{-1} \end{aligned}$$

$$\begin{aligned} \delta^3 f_{\frac{1}{2}} &= (E^{\frac{1}{2}} - E^{-\frac{1}{2}})^3 f_{\frac{1}{2}} \\ &= (E^{1\frac{1}{2}} - 3E^{\frac{1}{2}} + 3E^{-\frac{1}{2}} - E^{-1\frac{1}{2}}) f_{\frac{1}{2}} \\ &= f_2 - 3f_1 + 3f_0 - f_{-1} \end{aligned}$$

$$\begin{aligned} \frac{df}{dx} &= \frac{1}{h} \left\{ f_1 - f_0 - \frac{1}{24}(f_2 - 3f_1 + 3f_0 - f_{-1}) \right\} \\ &= \frac{1}{24h} (-f_2 + 27f_1 - 27f_0 + f_{-1}) \end{aligned}$$

4. Calculating  $d\theta/dt$  and differencing gives the table

0	-10.008	959			
1	-9.049	863	-96		
2	-8.186	778	-85	11	-1
3	-7.408	703	-75	10	2
4	-6.705	640	-63	12	
5	-6.065				

It is not necessary to take this table any further for the result required. Using inverse interpolation leads to  $p = 0.23$  where  $t_0 = 2$ . Hence required  $t = 2.23$ .

5. At  $x = 0.6$ ,  $\frac{dy}{dx} = 4.918$ ,  $\frac{d^2y}{dx^2} = 6.969$ , radius of curvature = 18.1.

Note that the leading term in the expression quoted for  $hf_0'$  effectively gives (6.1) and that in the expression for  $h^2f_0''$  leads to (26.3).

# Numerical Integration

FRAME 1

## Introduction

You have no doubt already learnt how to integrate a variety of functions and seen how integration results from a number of different physical situations. We shall commence this programme by looking at some problems which involve integrals but which either cannot be solved by analytical techniques or, even if they can, are more easily done by other means.

The first problem is this:

A coach accelerates from rest to 100 km/h in 90 s. Its speed,  $v$  km/h, measured at five second intervals, is given by the table

t	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80
v	0	5	19	22	32	40	43	52	61	65	66	71	77	85	90	95	98

t	85	90
v	99	100

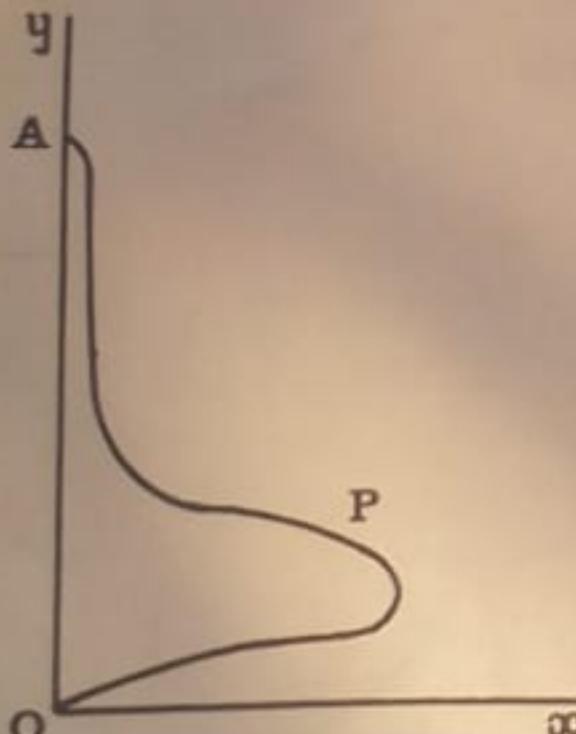
What distance will it travel in this time?

As  $v = \frac{ds}{dt}$ ,  $s = \int_0^{90} v dt$  and difficulty arises in that the formula for  $v$  in terms of  $t$  is not known. Note that, in this formula,  $v$  must be in km/s.

FRAME 2

The second problem is:

A solid, made of material of density  $0.02 \text{ g/mm}^3$  is formed by rotating the shape shown through  $360^\circ$  about OA. If O is taken to be the origin and the coordinates of P are  $(x, y)$ , the following pairs of values of  $x$  and  $y$  are known.



y(mm)	0	5	10	15	20	25	30	35	40
x(mm)	0	22	48	50	49	45	30	11	7

y	45	50	55	60	65	70	75	80	85
x	5	5	5	5	5	5	5	4	0

What is the moment of inertia of the solid about OA? If you are familiar with the ideas involved in moments of inertia, then, by way of revision, find the integral formula for this M. of I., remembering that  $k^2$  for a circle of radius  $a$

about its axis is  $\frac{1}{2}a^2$ . If you are not familiar with moments of inertia, proceed directly to FRAME 3.

\*\*\*\*\*

2A

Taking a slice, perpendicular to Oy, thickness  $\delta y$ ,

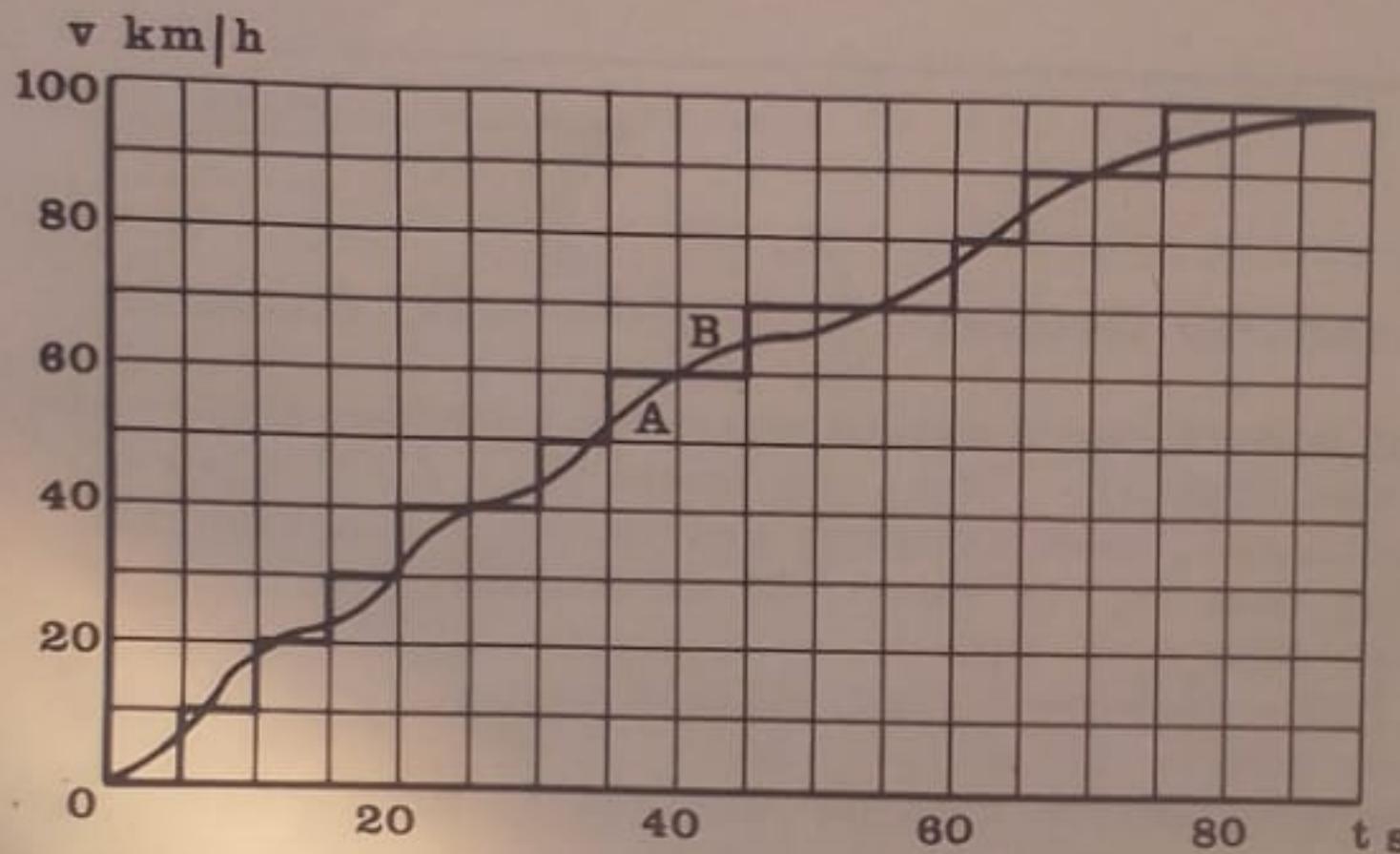
Volume of slice  $= \pi x^2 \delta y$ , Mass of slice  $\approx 0.02\pi x^2 \delta y$

M. of I. of slice  $\approx (0.02\pi x^2 \delta y) \frac{1}{2}x^2 = 0.01\pi x^4 \delta y$

$$\text{Total M. of I. of solid} = \int_0^{85} 0.01\pi x^4 dy = 0.01\pi \int_0^{85} x^4 dy.$$

In the first example (in FRAME 1) the distance travelled is given, with a suitable conversion of units, by the area under the distance-time graph. In the second example the final integral is not the area contained by the  $x$ - $y$  graph but can be interpreted as the area enclosed by the graph of  $X$  and the  $y$ -axis where  $X = x^4$ . Similarly any integral can be interpreted as representing an area, even although it may be giving us something else, for example, a first or second moment. It is the purpose of this programme to obtain methods of estimating definite integrals of functions for which either analytical formulae are not known or, even if they are, it is desirable to proceed by non-analytical methods. The methods that will be described are those of NUMERICAL INTEGRATION, or, as it is often known, QUADRATURE.

### Counting Squares



This method you may have learnt at school and the figure shows the original curve and the squares that would be included in the count for the coach problem in FRAME 1, assuming squares of the size shown. What would be the estimate of the distance travelled by this method?

\*\*\*\*\*

Number of squares = 108.

Each square represents 5 s horizontally and  $10 \text{ km/h} = \frac{1}{360} \text{ km/s}$  vertically,  
i.e. a distance  $\frac{1}{72} \text{ km}$ . Total distance  $\approx 1.5 \text{ km}$ .

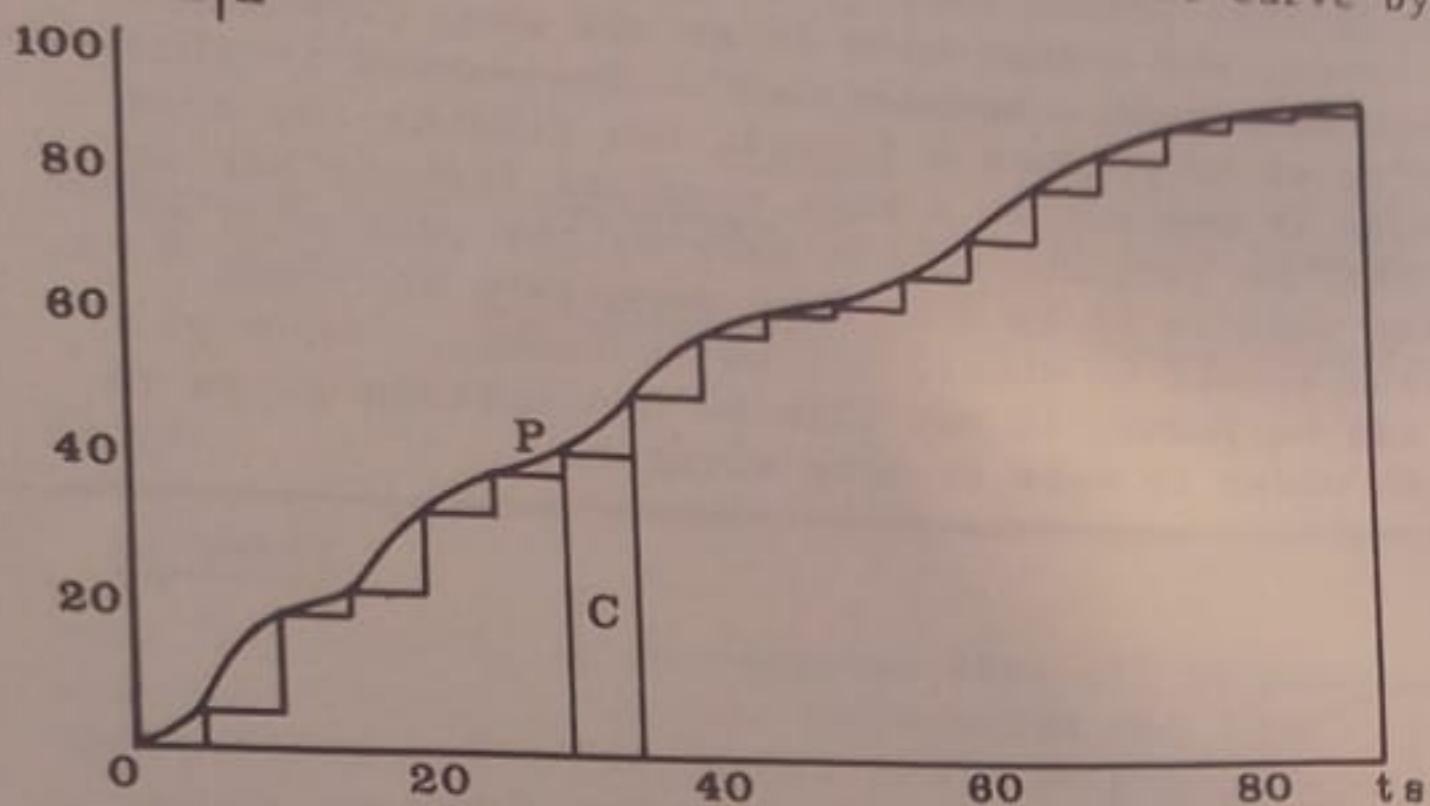
This result is not accurate as some squares, e.g. A, have contributed more to the total than they should, while others, e.g. B, have been totally ignored. It is, of course, hoped that these 'gains' and 'losses' cancel each other out reasonably well so that the net result is not too far out.

Effectively this method replaces the actual curve by a step function, and the area under this step function found instead of that actually required.

The Rectangular Rule

An alternative way of replacing the true curve by a step function is the

v km/h



RECTANGULAR RULE which is illustrated in the accompanying diagram.

For each tabular point P (except the final one) a rectangle C is constructed as shown. The sum of the areas of these rectangles is then taken as the required area. As the conversion factor from km/h to km/s is  $1/3600$ , the result will now be given by

$$5 \times \frac{0 + 5 + 19 + 22 + 32 + 40 + 43 + 52 + 61 + 65 + 66 + 71 + 77 + 85 + 90 + 95 + 98 + 99}{3600}$$

$$= \frac{5 \times 1020}{3600} = 1.417 \text{ km.}$$

The answer obtained previously was 1.50. Which of these two figures do you think is more accurate and why?

\*\*\*\*\*

9A

1.50. A certain amount of compensation was effected in this calculation by including squares like A and excluding those like B in the diagram in FRAME 7. In the second calculation all rectangles C were under-estimates.

FRAME 10

Will it always happen, for any curve, that rectangles such as C will be under-estimates?

\*\*\*\*\*

10A

No. They might always be over-estimates as in Fig. (i) or a mixture of over- and under-estimates as in Fig. (ii).

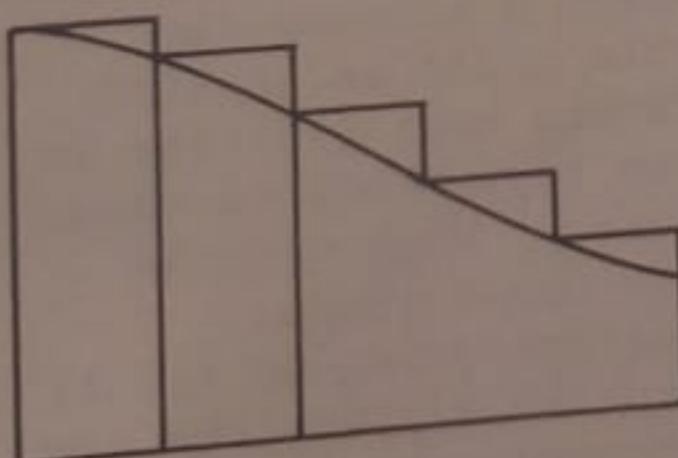


Fig (i)

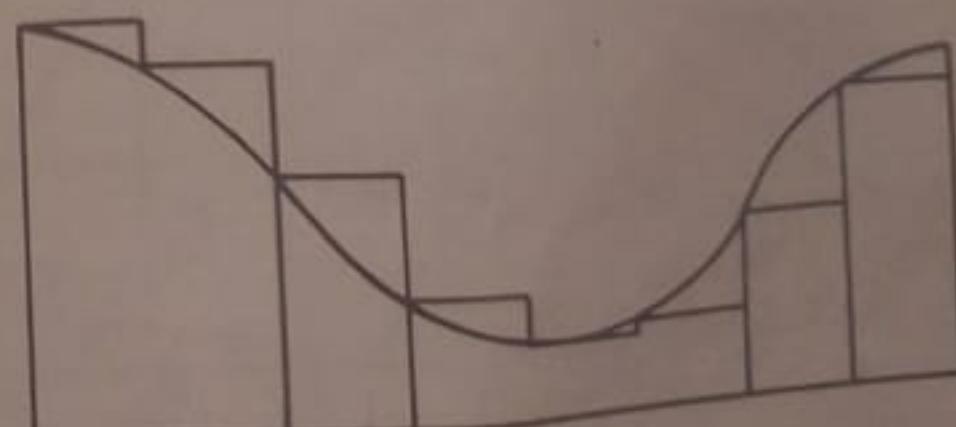
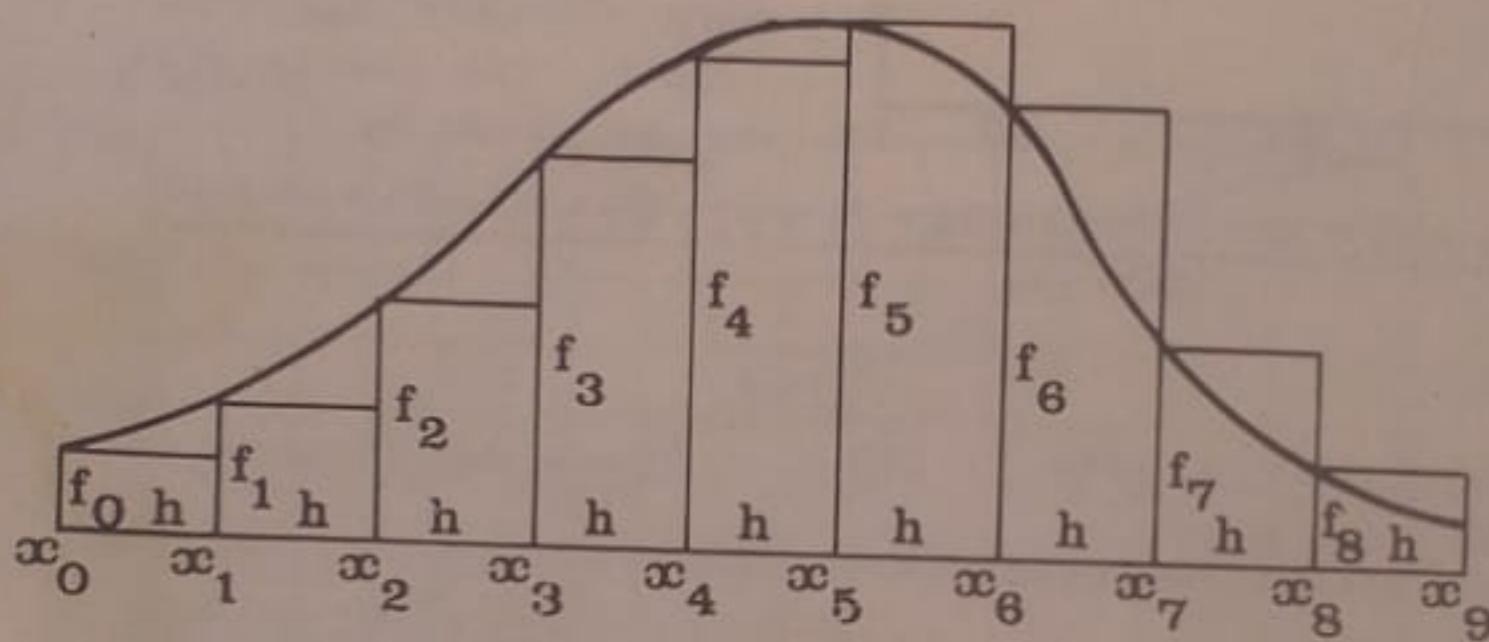


Fig (ii)

It is therefore only in cases similar to that shown in Fig.(ii) that any sort of compensation is produced by this method. You might then very well ask the question - "If this method only gives any sort of compensation in certain cases, why bother with it at all when counting squares will very often produce some compensation?" The answer to this question is that it enables us to produce a formula for finding the area under a curve. Admittedly it may not be a very accurate formula but it will have the advantage that no judgment on the part of the user will be necessary. When counting squares it is sometimes necessary to judge whether a particular square should or should not be included. Once we have seen how a formula can be found, it may then be possible to go on to incorporate refinements in order to make it more accurate.

FRAME 11



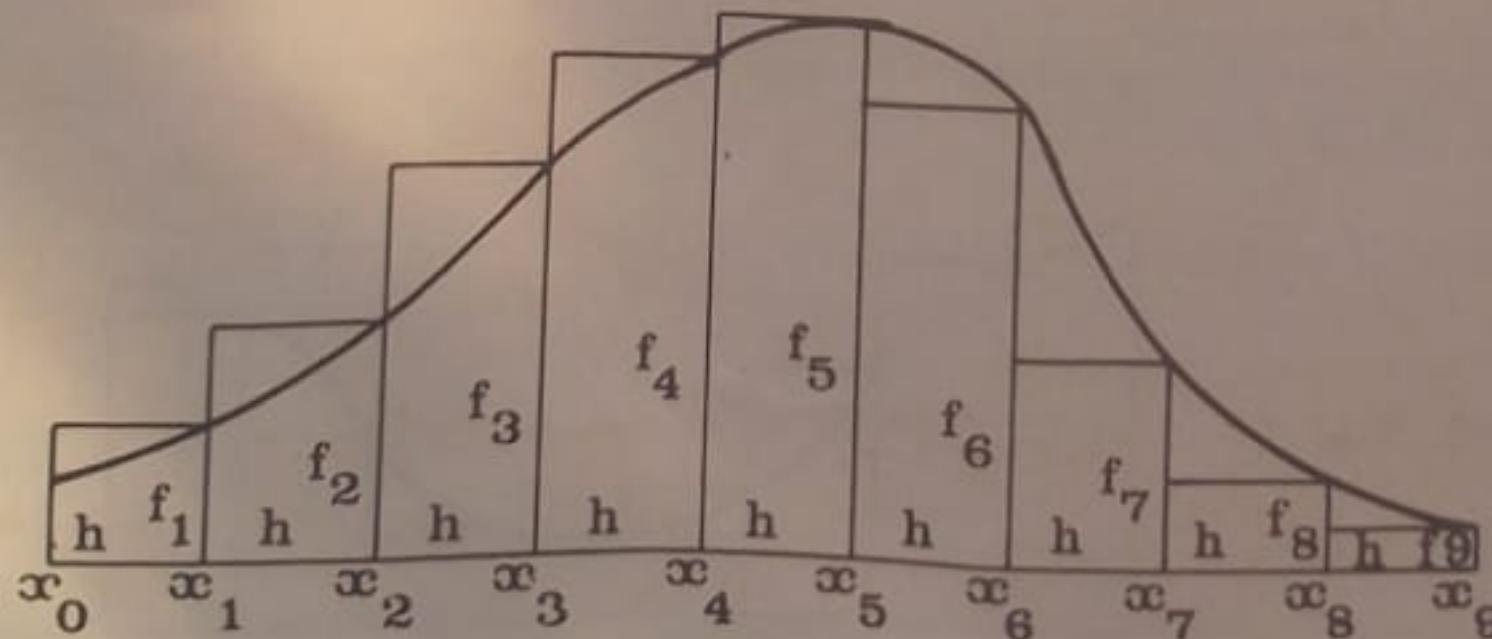
If ordinates are drawn to the curve as shown at  $x_0, x_1, x_2, \dots$ , the distance between consecutive  $x$ 's being constant at  $h$ , then the area under the stepped function is given by

$$h(f_0 + f_1 + \dots + f_n) \quad (12.1)$$

More generally, if there are  $n + 1$  points taken along the  $x$ -axis,  $x_0, x_1, \dots, x_n$ , all distance  $h$  apart, the formula will become  $h(f_0 + f_1 + \dots + f_{n-1})$  i.e.,

$$h \sum_{r=0}^{n-1} f_r \quad (12.2)$$

FRAME 13



An alternative way in which a rectangular rule could be applied to the area depicted in the last frame is shown here. What will be the new formulae, corresponding to (12.1) and (12.2), for the new stepped area if this is done?

\*\*\*\*\*

$$\frac{h}{n} (f_1 + f_2 + \dots + f_n)$$

$$h \sum_{r=1}^n f_r$$

(13A.1)

(13A.2)

13A

What will this alternative rectangular rule give as the answer to the coach problem? FRAME 14

\*\*\*\*\*

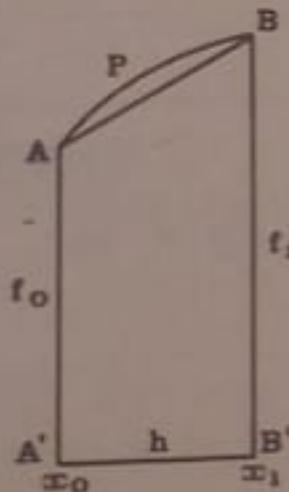
1.556

14A

Now, in FRAME 9, it so happened that all rectangles such as C were under-estimates. If you constructed the diagram corresponding to that in FRAME 13, all the rectangles would be over-estimates. It would, therefore, seem logical to take the average of the two figures 1.417 and 1.556 as being more likely than either of them. This would give the result 1.486. If this is done then we are effectively applying what is known as the TRAPEZIUM RULE (or very frequently, but less accurately, the TRAPEZOIDAL RULE) as will be seen shortly.

FRAME 15

### The Trapezium Rule

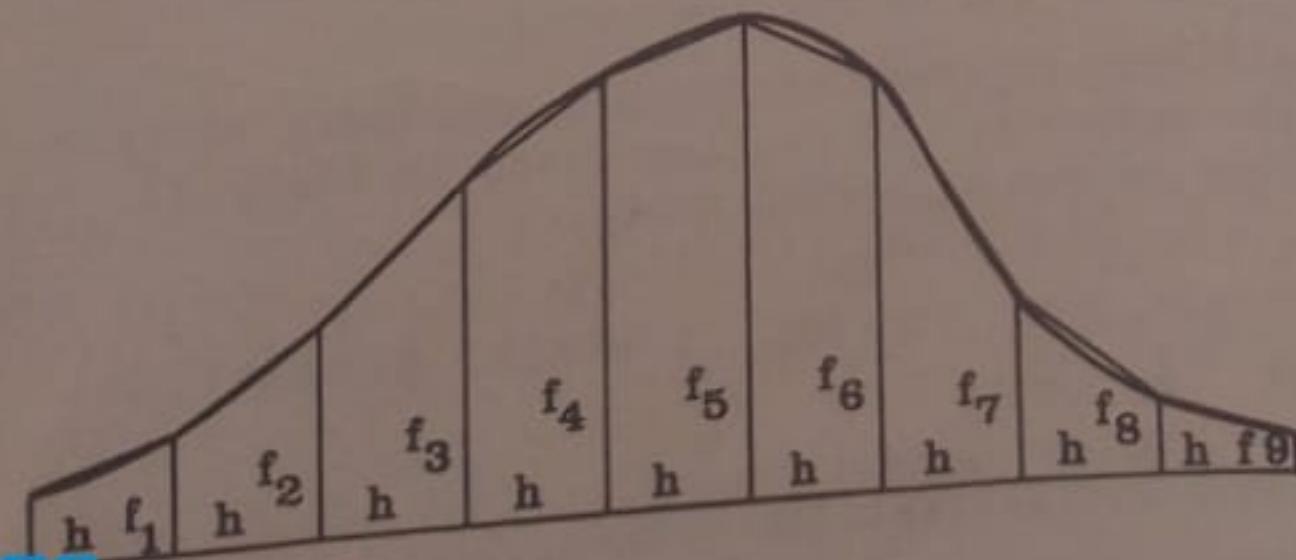


In this rule, the area under the curve APB between the two ordinates at  $x_0$  and  $x_1$  is replaced by that under the chord AB, i.e., by the trapezium A'ABB'. One would naturally expect this to be a better approximation than either of the two

rectangles used previously. If  $f_0$  and  $f_1$  are the corresponding ordinates, then

$$\text{area} = \frac{h}{2} (f_0 + f_1) \quad (16.1)$$

$h$  having the same meaning as before.



To apply this rule to finding an area such as that shown in FRAMES 12 and 13, the area is first replaced by a number of trapezia as shown here. The rule is then applied to each trapezium in turn and the results added together.

FRAME 17 (continued)

What will be the formula for the complete area shown here when you do this? Having obtained this formula verify that it is the average of formulae (12.1) and (13A.1).

\*\*\*\*\*

$$\frac{h}{2} (f_0 + 2f_1 + 2f_2 + 2f_3 + 2f_4 + 2f_5 + 2f_6 + 2f_7 + 2f_8 + f_9)$$

17AFRAME 18

Extending the formula to  $n$  (instead of nine) intervals and writing it in a slightly different form gives

$$h(\frac{1}{2}f_0 + f_1 + f_2 + f_3 + \dots + f_{n-2} + f_{n-1} + \frac{1}{2}f_n) \quad (18.1)$$

Now use formulae (12.2), (13A.2) and (18.1) to find estimates of the area under the curves, from  $x = 0$  to  $x = 10$ , given by the following tables:

i)	x	0	2	4	6	8	10
	y	0	12	48	108	192	300

ii)	x	0	1	2	3	4	5	6	7	8	9	10
	y	0	3	12	27	48	75	108	147	192	243	300

\*\*\*\*\*

18A

i) 720, 1320, 1020

ii) 855, 1155, 1005

Note that, for each table,  $f_0 = 0$ .

FRAME 19

The figures in the previous frame were taken from the curve  $y = 3x^2$ .

$$\text{The actual area} = \int_0^{10} 3x^2 dx = \left[ x^3 \right]_0^{10} = 1000$$

Two things are noticeable from the results:

- a) In both cases (i) and (ii), (18.1) gives the best answer.
- b) Each answer in (ii) is better than the corresponding one in (i).

From what has been said previously (a) was to be expected. (b) is also to be expected because in (i),  $h = 2$  but in (ii)  $h = 1$ . It has been remarked in earlier programmes that, unless other considerations are involved, the smaller the value of  $h$  the better the result.

What is the value, to 4 significant figures, of the best estimate you can expect to obtain so far for the answer to the problem given in FRAME 2? The values of  $x^4 (=X)$  are given in the following table.

y	0	5	10	15	20	25	30
$x^4 (=X)$	0	234 256	5308 416	6250 000	5764 801	4100 625	810 000
y	35	40	45 - 75	80 85			
$x^4 (=X)$	14 641	2401	625	256 0			

\*\*\*\*\*

$$0.01\pi \times 5 \times 22486021 \approx 3532000 \text{ g mm}^2$$

19A

(using the trapezium rule)

FRAME 20Integration Formulae via Interpolation Formulae

An alternative method will now be used to obtain (16.1). This method may seem to be very complicated in comparison with that used in FRAME 16 but it will show us a way which can be extended to get other, more accurate, formulae than those we have already.

The Newton-Gregory forward difference interpolation formula was obtained in the programme on Interpolation and is

$$y = f_0 + \binom{p}{1} \Delta f_0 + \binom{p}{2} \Delta^2 f_0 + \binom{p}{3} \Delta^3 f_0 + \dots$$

$$\text{or } y = f_0 + p \Delta f_0 + \frac{p(p-1)}{2} \Delta^2 f_0 + \frac{p(p-1)(p-2)}{6} \Delta^3 f_0 + \dots \quad (20.1)$$

$$\text{where } x = x_0 + ph.$$

What will be the connection between  $\int y dx$  and  $\int y dp$ ?

\*\*\*\*\*

20A

$$\int y dx = \int y \frac{dx}{dp} dp = h \int y dp$$

FRAME 21

Referring to the figure in FRAME 16, what will be the values of  $p$  corresponding to  $A'$  and  $B'$ ?

\*\*\*\*\*

21A0 and 1.FRAME 22

$$\begin{aligned} \text{Thus } \int_{x_0}^{x_1} y dx &= h \int_0^1 y dp \\ &= h \int_0^1 \left\{ f_0 + p \Delta f_0 + \frac{p^2 - p}{2} \Delta^2 f_0 + \frac{p^3 - 3p^2 + 2p}{6} \Delta^3 f_0 + \dots \right\} dp \\ &= h \left[ p f_0 + \frac{1}{2} p^2 \Delta f_0 + \left( \frac{1}{6} p^3 - \frac{1}{4} p^2 \right) \Delta^2 f_0 \right. \\ &\quad \left. + \left( \frac{1}{24} p^4 - \frac{1}{6} p^3 + \frac{1}{6} p^2 \right) \Delta^3 f_0 + \dots \right]_0^1 \\ &= h \left\{ f_0 + \frac{1}{2} \Delta f_0 - \frac{1}{12} \Delta^2 f_0 + \frac{1}{24} \Delta^3 f_0 + \dots \right\} \end{aligned}$$

Now, as you know, for well behaved curves, the higher order differences are small compared with the lower ones. Round-off errors do, of course, get things, but differences rendered unreliable because of these errors

FRAME 25 (continued)

Taking the first three terms of this formula, what will the result be when expressed in terms of functional values only?

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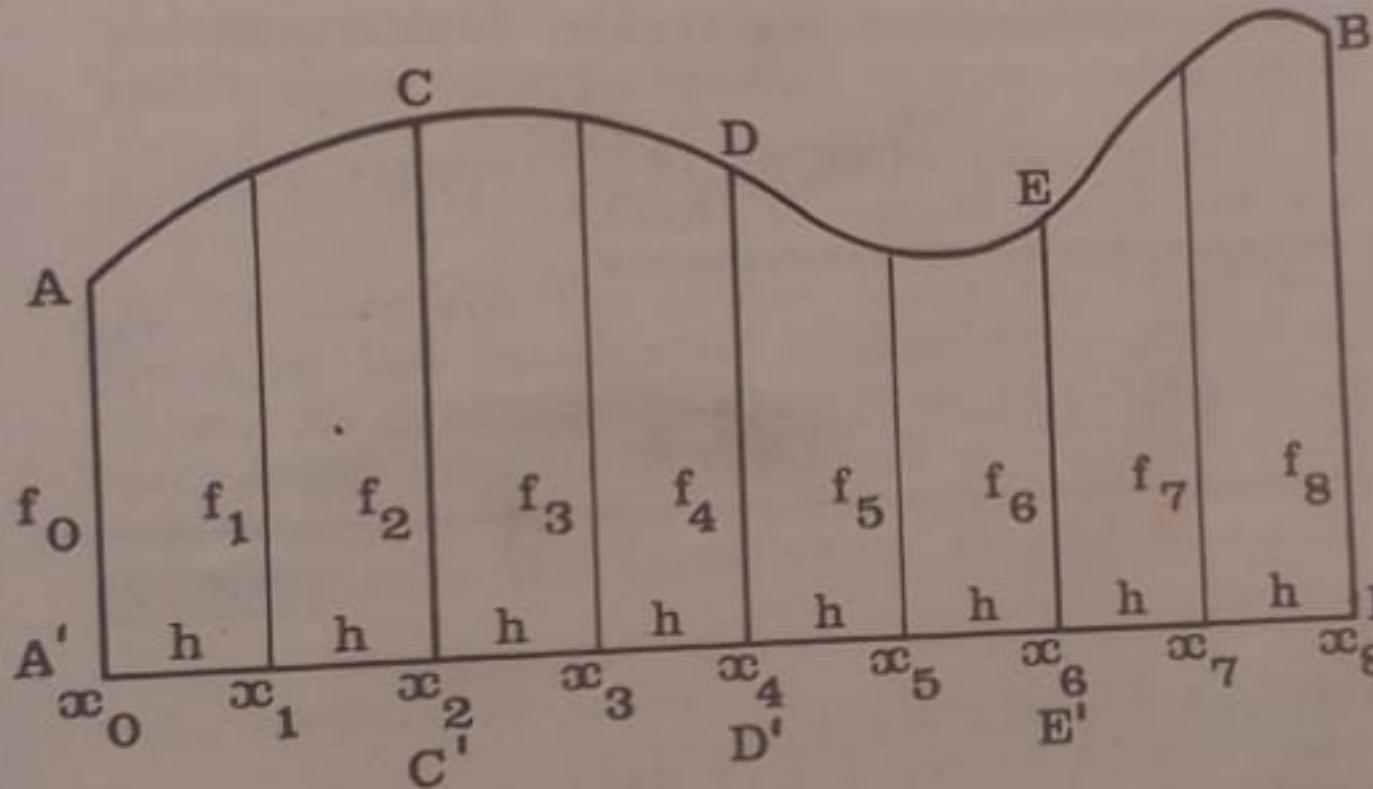
$$h \left\{ 2f_0 + 2(f_1 - f_0) + \frac{1}{3}(f_2 - 2f_1 + f_0) \right\} = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

25A

(This formula can also be obtained from Taylor's series. This was done in our "Mathematics for Engineers and Scientists" Vol. 1 as an illustration of one of the uses of that series.)

FRAME 26

The first term neglected now is that involving  $\Delta^4 f_0$  due to the coefficient of  $\Delta^3 f_0$  being zero. It can be shown that the  $\Delta^4$  term is  $-\frac{h}{90}\Delta^4 f_0$  and so it is to be expected that Simpson's rule gives a much more accurate result than the trapezium rule.

FRAME 27

If the range of integration is large, then  $h$  will also be large. The figure shows how such an integral can be split up into a number of sub-integrals, for each of which  $h$  is smaller. Making  $h$  smaller means that you expect the result to be more accurate. In the figure as shown, the area

A'ABB' has been divided into four smaller areas A'ACC', C'CDD', D'DEE' and E'EBB'. This has been done in such a way that the width of each area is the same. The formula that you obtained in 25A is now applied to each of these smaller areas in turn. What will you get when you do this for the three areas C'CDD', D'DEE' and E'EBB'?

\*\*\*\*\*

27A

$$\frac{h}{3}(f_2 + 4f_3 + f_4), \quad \frac{h}{3}(f_4 + 4f_5 + f_6), \quad \frac{h}{3}(f_6 + 4f_7 + f_8)$$

FRAME 28

The total area is thus

$$\begin{aligned} & \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) + \frac{h}{3}(f_4 + 4f_5 + f_6) + \frac{h}{3}(f_6 + 4f_7 + f_8) \\ &= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + 2f_6 + 4f_7 + f_8) \end{aligned}$$

FRAME 28 (continued)

It is easy to see how this can be extended to an area subdivided into a different number of small sections. As each sub-area has to be divided into two, it follows that the total number of strips must be even (8 in the example just done). If this number is  $n$  the formula becomes

$$\frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \dots + 4f_{n-3} + 2f_{n-2} + 4f_{n-1} + f_n)$$

Alternatively, it can be written as

$$\frac{h}{3} \left\{ f_0 + f_n + 4(f_1 + f_3 + \dots + f_{n-1}) + 2(f_2 + f_4 + \dots + f_{n-2}) \right\} \quad (28.1)$$

To illustrate the rule, if it is applied to the coach problem in FRAME 1, the distance travelled is

$$\frac{5}{3} \left\{ \frac{(0+100) + 4(5+22+40+52+65+71+85+95+99) + 2(19+32+43+61+66+77+90+98)}{3600} \right\}$$

$$= 1.485 \text{ km.}$$

In this example  $h = 5$  and you remember that the factor  $1/3600$  is necessary to change km/h into km/s.

Now apply the formula to set (ii) of data in FRAME 18. Compare your answers with those in 18A and the exact figure of 1000.

\*\*\*\*\*

28A

$$\frac{1}{3} \left\{ (0+300) + 4(3+27+75+147+243) + 2(12+48+108+192) \right\} = 1000$$

FRAME 29

Two questions now:

- Why do you think the answer is exactly right?
- Why couldn't you apply the formula to set (i) of data in FRAME 18?

\*\*\*\*\*

29A

- The data came from a quadratic, for which all differences higher than the second are zero. Thus all the terms ignored in arriving at the formula are zero in this case.
- The number of strips into which the area is divided is odd (5).

FRAME 30

- can be partially overcome by using the formula for the first four strips and applying the trapezium rule to the fifth. What will be the answer if you do this?

\*\*\*\*\*

30A

$$\frac{2}{3} \left\{ (0 + 192) + 4(12 + 108) + 2 \times 48 \right\} + \frac{2}{2}(192 + 300) = 512 + 492 = 1004$$

Alternatively the trapezium rule could have been used for the first strip and Simpson's for the other four. The result would then also have worked

out to 1004. Usually one would expect different answers in the two cases. They are equal here because it happens to be a parabola you are working with.

30A (continued)

A flow diagram for evaluating  $\int_a^b f(x)dx$  by Simpson's rule using n strips (n assumed even) is shown on page 262.

FRAME 31The Three-Eighths RuleFRAME 32

The basic trapezium rule  $\left\{ \frac{h}{2}(f_0 + f_1) \right\}$  involves the use of two functional values,  $f_0$  and  $f_1$ . The basic Simpson's rule involves the use of three such values,  $f_0$ ,  $f_1$  and  $f_2$ . Because of this, the trapezium rule is called a two-point formula and Simpson's rule a three-point formula. Other formulae for numerical integration exist which use more functional values. One of these is the THREE-EIGHTHS RULE which uses four functional values in its basic form and so is a four-

point formula. It gives  $\int_{x_0}^{x_3} ydx$  which is equivalent to  $h \int_0^3 ydp$ .

In working out the latter integral, it is necessary to retain one more term in the integrated interpolation formula than for Simpson's rule. Thus, in finding the trapezium rule from an interpolation formula, it is necessary to retain the first difference term. For Simpson's rule it is necessary to retain the first two difference terms. For the three-eighths rule the first three difference terms must be kept.

See if you can obtain this rule, expressing the result in terms of  $h$  and the functional values  $f_0$ ,  $f_1$ ,  $f_2$  and  $f_3$ .

\*\*\*\*\*

32A

$$h \left[ pf_0 + \frac{1}{2}p^2 \Delta f_0 + \left( \frac{1}{6}p^3 - \frac{1}{4}p^2 \right) \Delta^2 f_0 + \left( \frac{1}{24}p^4 - \frac{1}{6}p^3 + \frac{1}{6}p^2 \right) \Delta^3 f_0 + \dots \right]_0^3 \\ = h \left\{ 3f_0 + \frac{9}{2}\Delta f_0 + \frac{9}{4}\Delta^2 f_0 + \frac{3}{8}\Delta^3 f_0 + \dots \right\}$$

Retaining terms up to and including  $\Delta^3$  gives

$$h \left\{ 3f_0 + \frac{9}{2}(f_1 - f_0) + \frac{9}{4}(f_2 - 2f_1 + f_0) + \frac{3}{8}(f_3 - 3f_2 + 3f_1 - f_0) \right\} \\ = \frac{3}{8}h(f_0 + 3f_1 + 3f_2 + f_3)$$

FRAME 33

It can be shown that the dominant term in the error in this formula is  $-\frac{3}{80}h^5 f_0$ . It is therefore not quite so accurate as Simpson's Rule, but on the other hand it enables us to find the value of an integral for which

It is easy to see how this can be different number of small sectors into two, it follows that the example just done).

$$\frac{h}{3}(f_0 + 4f_1 + 2f_2)$$

Alternatively, it

$$\frac{h}{3} \{ f_0 + f_1 + 4f_2 + f_3 + \dots + f_{n-1} + 2f_n \}$$

To ill.

5

the value of the integral is given by the formula:

$\int_a^b f(x) dx = \frac{h}{3} [f_0 + 4f_1 + 2f_2 + \dots + f_{n-1} + 4f_n]$

where  $a$  and  $b$  are the limits of integration,  $f(x)$  is the function being integrated,  $n$  is the number of subintervals, and  $h$  is the width of each subinterval.

The width of each subinterval is given by:

$h = \frac{b-a}{n}$

The subintervals are defined by:

$x_i = a + ih$  for  $i = 0, 1, 2, \dots, n$

The function values at these points are given by:

$f_i = f(x_i)$  for  $i = 0, 1, 2, \dots, n$

$f(x)$  is defined only by modular values they would be read here using subscript notation.

The notation being used is  $f_1 = f(a+h)$ ,  $f_m = f(a+mh)$  etc.

This "loop" forms the sums:

$$P = f_1 + f_3 + f_5 + \dots + f_{n-1}$$

$$Q = f_2 + f_4 + \dots + f_{n-2}$$

The formula to be used here for  $I$ , the value of the integral, is

$$\frac{1}{3}h \{ f(a) + 4P + 2Q + f(b) \}$$

(Programs for evaluating integrals by Simpson's Rule can be found in references (2), (4), (5), (6), (7) and (9).)

FRAME 33 (continued)

the corresponding area is split into three strips instead of only two. It can be extended to any area which is split into a multiple of three strips.

What will it become for an area split into 9 strips?

\*\*\*\*\*

$$\begin{aligned} & \frac{3}{8}h(f_0 + 3f_1 + 3f_2 + f_3) + \frac{3}{8}h(f_3 + 3f_4 + 3f_5 + f_6) + \frac{3}{8}h(f_6 + 3f_7 + 3f_8 + f_9) \\ &= \frac{3}{8}h(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + 3f_7 + 3f_8 + f_9) \end{aligned}$$

33AFRAME 34

Now use a combination of Simpson's and the three-eighths rules to obtain an estimate of the moment of inertia of the solid described in FRAME 2. (The required definite integral is in 2A and the table of values of  $x^4$  in FRAME 19.) It is suggested that you use Simpson's rule for the first fourteen strips and the three-eighths rule for the remaining three.

\*\*\*\*\*

34A

$$\begin{aligned} \int_0^{8.5} x^4 dy &= \frac{5}{3} \{ 0 + 625 + 4(234\ 256 + 6250\ 000 + 4100\ 625 + 14\ 641 + 625 \\ &\quad + 625 + 625) + 2(5308\ 416 + 5764\ 801 + 810\ 000 + 2401 \\ &\quad + 625 + 625) \} + \frac{3 \times 5}{8} \{ 625 + 3(625 + 256) + 0 \} \\ &= 110\ 299\ 915 + 6128 = 110\ 306\ 043 \end{aligned}$$

$$M. \text{ of } I. \approx 3465\ 000 \text{ g mm}^2.$$

FRAME 35Other Integration Formulae

You will realise that the way in which the Newton-Gregory forward difference formula is used can be varied by integrating between other sets of limits. We have integrated w.r.t. p between 0 and 1, 0 and 2, 0 and 3 to give, respectively, the trapezium rule, Simpson's rule and the three-eighths rule.

BOOLE'S RULE is obtained by integrating between 0 and 4, retaining differences up to the fourth. It gives

$$\begin{aligned} \int_{x_0}^{x_4} y dx &= h \int_0^4 y dp \\ &= \frac{2h}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \end{aligned}$$

This is a five-point formula and as the coefficient of  $\Delta^5 f_0$  turns out to be zero, the leading term omitted is that involving  $\Delta^6 f_0$ . It is actually  $-\frac{8h}{945} \Delta^6 f_0$ .

**TECNO** WEDDLE'S RULE is obtained by integrating between 0 and 6, retaining differences up to the sixth. But in order to give a simple formula, only

FRAME 35 (continued)

part of the sixth difference is retained. The rest is included in the error. The formula, which is a seven-point one, is

$$\begin{aligned} \int_{x_0}^{x_6} y dx &= h \int_0^6 y dp \\ &= \frac{3h}{10}(f_0 + 5f_1 + f_2 + 6f_3 + f_4 + 5f_5 + f_6) \end{aligned}$$

The part of the sixth difference term omitted is  $- \frac{h}{140} \Delta^6 f_0$ .

Each of these formulae can be extended to areas split into more strips. The number of strips will have to be a multiple of four in the case of Boole's rule and a multiple of six for Weddle's.

FRAME 36

In the moment of inertia problem there were 17 strips. These were divided in FRAME 34 into seven twos and a three. Another way in which they could be split is into two sixes, a three and a two. Using this split, Weddle's rule can be used for the two sixes, the three-eighths rule for the three and Simpson's rule for the two.

The total area will then be

$$\begin{aligned} \frac{3 \times 5}{10} \{ &(0 + 5 \times 234\ 256 + 5308\ 416 + 6 \times 6250\ 000 + 5764\ 801 + 5 \times 4100\ 625 \\ &+ 810\ 000) + (810\ 000 + 5 \times 14\ 641 + 2401 + 6 \times 625 + 625 + 5 \times 625 \\ &+ 625) \} + \frac{3 \times 5}{8} (625 + 3 \times 625 + 3 \times 625 + 625) + \frac{5}{3} (625 + 4 \times 256 + 0) \\ &= 106\ 598\ 556 \\ \therefore M. \text{ of I.} &\approx 3349\ 000 \text{ g mm}^2 \end{aligned}$$

What result do you get for the coach problem using Weddle's rule?  
\*\*\*\*\*

36A

1.482 km.

FRAME 37

From the nature of the formulae, one would expect the last two results to be more accurate than those obtained previously. In practice this is unlikely to be so as Weddle's rule takes into account higher order differences than, say, Simpson's rule. From the natures of the two problems these higher differences are probably not very reliable.

Generally speaking, it is reasonable to say that Simpson's rule will probably give you sufficient accuracy in most problems. If the number of strips is not even, then a combination of Simpson and three-eighths will generally suffice. You will only need to use Boole and Weddle if you have very accurate data and require a similarly very accurate result.

Errors

So far all that has been done about errors has been to give an estimate of the predominant term omitted from an interpolation formula when finding a basic integration formula. Taking, for example, Simpson's rule this term is  $-\frac{1}{90}h\Delta^4 f_0$ . But when the basic formula is extended as in FRAMES 27 and 28, then a similar error is introduced on each application of this basic formula. Taking the situation described in FRAME 27, the leading term in the error will be

$$-\frac{1}{90}h\Delta^4 f_0 \quad \text{on finding A'ACC'}$$

$$-\frac{1}{90}h\Delta^4 f_2 \quad \text{on finding C'CDD'}$$

$$-\frac{1}{90}h\Delta^4 f_4 \quad \text{on finding D'DEE'}$$

$$\text{and } -\frac{1}{90}h\Delta^4 f_6 \quad \text{on finding E'EBB'}$$

An estimate of the magnitude of the total error introduced is thus  $\frac{1}{90}h(|\Delta^4 f_0| + |\Delta^4 f_2| + |\Delta^4 f_4| + |\Delta^4 f_6|)$ , the modulus signs being introduced as the differences may be positive or negative.

Now the contents of the brackets will be less than four times the value of the maximum term inside them and so an estimate of the magnitude of the total error is

$$\frac{1}{90}h \times 4M$$

where  $M$  is the maximum absolute value of the fourth differences of the function. Now  $4h = \frac{1}{2}(x_8 - x_0)$  and so the maximum absolute error is

$$\frac{M(x_8 - x_0)}{180}$$

In a similar way, for the more general formula (28.1), an estimate of the maximum absolute error is

$$\frac{M(x_n - x_0)}{180}. \quad (38.1)$$

Sometimes it may be more convenient, as, for example, if the analytical formula for the function is known, to express the error in terms of a derivative instead of a difference.

$$\text{Now } f'(x_0) = \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h} = \lim_{h \rightarrow 0} \frac{\Delta f_0}{h}$$

and so, approximately,  $\Delta f_0 = hf'(x_0)$ .

In a similar way  $\Delta^2 f_0 \approx h^2 f''(x_0)$ ,  $\Delta^3 f_0 \approx h^3 f'''(x_0)$ ,  $\Delta^4 f_0 \approx h^4 f^{iv}(x_0)$ , and so an approximate value for the maximum fourth difference of a function

in a given range is  $h^4 \times$  the maximum value of the fourth derivative of the function in the range. An alternative expression for (38.1) is therefore

$$\frac{mh^4(x_n - x_0)}{180} \quad (39.1)$$

where  $m$  is the maximum absolute value of  $f^{(iv)}(x)$  in the range.

In a similar manner, results corresponding to (38.1) and (39.1) can be obtained for each of the other integration formulae.

FRAME 39 (continued)

As an example on the use of this, let us look at the following problem:

Determine numerically  $\int_0^{\frac{1}{4}\pi} \sin x dx$  using Simpson's rule with a step length so chosen that the truncation error is less than 0.001. Find a bound for the round-off error in your answer. (C.E.I.)

First of all, it is obvious that Simpson's rule is not really necessary to find  $\int_0^{\frac{1}{4}\pi} \sin x dx$ , as this can be done directly. However, an easy example like this will serve to illustrate the ideas involved.

To start with, the maximum value of the fourth derivative of  $\sin x$  in the range 0 to  $\frac{1}{4}\pi$  is required. What will this be?

\*\*\*\*\*

40A

$\frac{d^4}{dx^4}(\sin x) = \sin x$ . This increases steadily from 0 to  $1/\sqrt{2}$  as  $x$  increases from 0 to  $\pi/4$ .

Thus  $m = 1/\sqrt{2} = 0.7071$ .

Note that the greatest value of  $\sin x$  in this range is not at a turning point and hence cannot be found by putting its first derivative equal to zero.

FRAME 41

For the error to be less than 0.001 requires  $\frac{0.7071 h^4 \left\{ \frac{\pi}{4} - 0 \right\}}{180} < 0.001$ , using (39.1). From this  $h < 0.76$ .

The least number of strips that can be used in Simpson's rule is 2. If this number is used, then, as the range of integration is  $\frac{\pi}{4} = 0.7854$ ,  $h = 0.3927$  and this satisfies the required condition.

A table of values is then

$x$	0	0.3927	0.7854
$\sin x$	0	0.3827	0.7071

Using these figures, what does Simpson's rule give for the integral?

\*\*\*\*\*

$$\frac{0.3927}{3} (0 + 4 \times 0.3827 + 0.7071) = 0.2929$$

41A

Finally, what will be a bound for the round-off error introduced?

FRAME 42

\*\*\*\*\*

Maximum error in each decimal = 0.00005

42A

Maximum error in contents of brackets in 41A =  $4 \times 0.00005 + 0.00005$

$$= 0.00025$$

Maximum error in multiplication  $\approx 0.4 \times 0.00025 + 2.2 \times 0.00005 = 0.00021$

Maximum error on division by 3  $\approx 0.00007$ .

### Summary of Integration Formulae

FRAME 43

<u>Rule</u>	<u>Formula</u>	<u>Leading Error Term</u>
Trapezium	$\int_{x_0}^{x_1} y dx = \frac{h}{2}(f_0 + f_1)$	$-\frac{1}{12}h\Delta^2 f_0$
Simpson	$\int_{x_0}^{x_2} y dx = \frac{h}{3}(f_0 + 4f_1 + f_2)$	$-\frac{1}{90}h\Delta^4 f_0$
Three-Eighths	$\int_{x_0}^{x_3} y dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$	$-\frac{3}{80}h\Delta^4 f_0$
Boole	$\int_{x_0}^{x_4} y dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$	$-\frac{8}{945}h\Delta^6 f_0$
Weddle	$\int_{x_0}^{x_6} y dx = \frac{3h}{10}(f_0 + 5f_1 + f_2 + 6f_3 + f_4 + 5f_5 + f_6)$	$-\frac{1}{140}h\Delta^6 f_0$

These are all examples of what are known as formulae of the NEWTON-COTES type.

FRAME 44

### Romberg Integration

If the integral of a linear function is required between given limits, the trapezium rule will give it exactly. Similarly, for a quadratic or cubic function, Simpson's rule is exact. The other integral formulae which have been found are exact for certain other polynomial curves. Otherwise the use of a numerical integration formula leads to an error. The magnitude of the error may be reduced by making  $h$  smaller but this is not always desirable. For example, if tabular values are given, any reduction in  $h$  involves a number of interpolations. An alternative

method, popular for computer work, of increasing the accuracy is known as ROMBERG INTEGRATION.

FRAME 44 (continued)

This method starts off with the trapezium rule, which, in view of the fact that this rule is not generally very accurate, may seem surprising. But the process then adopted rapidly gives rise to a very accurate answer.

It will be illustrated by applying it to find  $\int_0^2 e^x dx$ , which we know to be  $[e^x]_0^2 = 6.389\ 056$  to 6 decimal places.

The following table gives the value of the function  $e^x$  for  $x = 0(0.125)2$ .

$x$	0	0.125	0.25	0.375	0.5	0.625
$e^x$	1	1.133 148	1.284 025	1.454 991	1.648 721	1.868 246
$x$	0.75	0.875	1	1.125	1.25	1.375
$e^x$	2.117 000	2.398 875	2.718 282	3.080 217	3.490 343	3.955 077
$x$	1.5	1.625	1.75	1.875	2	
$e^x$	4.481 689	5.078 419	5.754 603	6.520 819	7.389 056	

The values of  $x$  chosen may appear to be unusual, but they have been selected so that the interval  $0 - 2$  can be taken as a whole or divided into 2, 4, 8 or 16 parts. This will be equivalent to taking  $h = 2, 1, 0.5, 0.25$  or  $0.125$ , i.e., successively halving its value. Obviously one could take this halving further, but it only entails more work and may not be necessary. Indeed, we may discover that we have gone further than necessary already.

FRAME 46

The trapezium rule (16.1) and its extended form (18.1) are now used to give estimates of the integral, taking, in turn, the values of  $h$  in the last frame.

What results will you get when  $h = 2$  and  $1$ ?

\*\*\*\*\*

46A

$$h = 2, \quad (16.1) \text{ gives } \frac{2}{2}(1 + 7.389\ 056) = 8.389\ 056$$

$$h = 1, \quad (18.1) \text{ gives } 1(0.5 + 2.718\ 282 + 3.694\ 528) = 6.912\ 810$$

FRAME 47

Continuing, a table can be built up:

$h$	Estimate of Integral
2	8.389 056
1	6.912 810
0.5	6.521 610
0.25	6.422 298
0.125	6.397 373

As you would expect, the estimates are increasing in accuracy as one goes down the table.

FRAME 47 (continued)

Now, in FRAMES 38 and 39, you saw that an estimate of the maximum error for an integral obtained by Simpson's rule is  $mh^4(x_n - x_0)/180$ . By a similar process, find the corresponding expression for an integral obtained by the trapezium rule.

\*\*\*\*\*

The leading error term for the first strip is  $-\frac{1}{12}h\Delta^2f_0$ .

47A

The formula corresponding to (38.1) is  $M(x_n - x_0)/12$ . That corresponding to (39.1) is  $mh^2(x_n - x_0)/12$ . This is the required result.

FRAME 48

For a given function and for fixed values of  $x_0$  and  $x_n$ ,  $m$  will be fixed and so this formula is equivalent to a constant times  $h^2$ . Now this is only an estimate of the maximum error. It can be shown, but not very easily, that the actual error itself is of the form  $Ah^2 + Bh^4 + Ch^6 + \dots$  The most important term in this expression, unless  $h$  is large, is  $Ah^2$ . As true value - estimated value = error we now write, approximately,

$$I - I_{\text{est}} = Ah^2 \quad (48.1)$$

If the five successive estimates given in the previous frame are labelled  $I_1$ ,  $I_2$  etc., then, as  $h = 2, 1, \frac{1}{2}$  etc., in turn,

$$I - I_1 = 4A \quad (48.2)$$

$$I - I_2 = A \quad (48.3)$$

$$I - I_3 = A/4 \quad (48.4)$$

What will be the other equations in this list?

\*\*\*\*\*

48A

$$I - I_4 = A/16 \quad \text{and} \quad I - I_5 = A/64$$

FRAME 49

The next step is to eliminate  $A$  between (48.2) and (48.3). Doing this gives

$$\frac{I - I_1}{I - I_2} = 4 \quad (49.1) \quad \text{i.e.} \quad I = (4I_2 - I_1)/3$$

$$\text{or alternatively} \quad I = I_2 + (I_2 - I_1)/3 \quad (49.2)$$

Note that the denominator here is one less than the number on the R.H.S. of (49.1).

What will you get for  $I$  when you eliminate  $A$  between (48.3) and (48.4)?

\*\*\*\*\*

49A

$I = (4I_3 - I_2)/3$  which can also be written as  $I = I_3 + (I_3 - I_2)/3$

(49A.1)

Similarly, also,

$$I = I_4 + (I_4 - I_3)/3 \quad (50.1)$$

$$\text{and } I = I_5 + (I_5 - I_4)/3 \quad (50.2)$$

Now owing to the fact that equation (48.1) is only an approximation, the  $I$  in it will not be exactly the true value of the integral. This means that the  $I$  in all equations of the type (49.2) is not quite exact. What we do find, however, is that the  $I$  in (49.2) is a better approximation than either  $I_1$  or  $I_2$ . Similarly, the  $I$  in (49A.1) is a better approximation than either  $I_2$  or  $I_3$  and so on. What will be the values of  $I$ , to 6 decimal places, as given by (49.2) and (49A.1).  
\*\*\*\*\*

6.420 728 and 6.391 210

The other two values of  $I$ , as found from (50.1) and (50.2) are 6.389 194 and 6.389 065. The table in FRAME 47 can now be extended to read

2	8.389 056	
1	6.912 810	6.420 728
0.5	6.521 610	6.391 210
0.25	6.422 298	6.389 194
0.125	6.397 373	6.389 065

Looking to see what was done in (49.2) to give 6.420 728, a relatively small amount was subtracted from 6.912 810. This amount can be regarded as a correction to the value 6.912 810 and so the result has been placed on the same level. Similar remarks apply to the other values obtained at this stage.

In FRAME 47 it was remarked that the estimates there were increasing in accuracy as one went down the table. You will notice that the values in the latest column we have now formed are doing exactly the same.

If we denote the latest estimates by  $J_1, J_2, J_3, J_4$ , then

$$J_1 = I_2 + (I_2 - I_1)/3$$

$$J_2 = I_3 + (I_3 - I_2)/3 \text{ etc.}$$

These equations can all be embraced by the single equation

$$J_i = I_{i+1} + (I_{i+1} - I_i)/3 \quad (52.1)$$

where  $i$  here takes the values 1, 2, 3, and 4, but can go higher or stop earlier as necessary.

When using a computer, this is a very simple equation to program, incorporating an easy DO loop. But when you are doing examples manually, you may prefer to re-write the equation (52.1) as

improved value = more accurate value

$$+ (\text{more accurate value} - \text{less accurate value})/3 \quad (52.2)$$

FRAME 53

The next step in the process is to use the four values in the J column to obtain three, still more improved, estimates of the integral. These are obtained on the basis that all  $h^2$  terms in the errors have now been taken care of and so equation (48.1) is replaced by

$$I - I_{\text{est}} = Bh^4$$

and the  $I_{\text{est}}$  terms are now given by  $J_1$ ,  $J_2$ , etc.

By a process similar to that in FRAMES 48-50, still further improved estimates  $K_1$ ,  $K_2$  and  $K_3$  are found to be given by

$$\begin{aligned} K_1 &= J_2 + (J_2 - J_1)/15 \\ K_2 &= J_3 + (J_3 - J_2)/15 \\ K_3 &= J_4 + (J_4 - J_3)/15 \end{aligned}$$

The 15's occur (instead of 3's as previously) due to the use of  $h^4$  instead of  $h^2$ , the ratio of two successive  $h^4$ 's being 16 instead of 4. Similarly, if you use the form (52.2) the 3 in the denominator is replaced by 15.

Find the values of the 3 K's and then extend the table in FRAME 51 to include the K column.

\*\*\*\*\*

53A

$6 \cdot 389 \ 242$	$6 \cdot 389 \ 060$	$6 \cdot 389 \ 056$	
2	$8 \cdot 389 \ 056$		
1	$6 \cdot 912 \ 810$	$6 \cdot 420 \ 728$	
0.5	$6 \cdot 521 \ 610$	$6 \cdot 391 \ 210$	$6 \cdot 389 \ 242$
0.25	$6 \cdot 422 \ 298$	$6 \cdot 389 \ 194$	$6 \cdot 389 \ 060$
0.125	$6 \cdot 397 \ 373$	$6 \cdot 389 \ 065$	$6 \cdot 389 \ 056$

FRAME 54

If you examine the K values you will see that, once again, the further one goes down the column, the better the estimate of the integral. Not only that, but the column as a whole contains much better values than previous columns.

From the 3 K values, two more estimates can be obtained,  $L_1$  and  $L_2$ .  $Ch^6$  is now used instead of  $Bh^4$  and the equations for the L's are

$$\begin{aligned} L_1 &= K_2 + (K_2 - K_1)/63 \\ L_2 &= K_3 + (K_3 - K_2)/63 \end{aligned}$$

(Note that 64 is the ratio of two successive  $h^6$ 's.)

From them, we get  $L_1 = 6 \cdot 389 \ 057$  and  $L_2 = 6 \cdot 389 \ 056$ .

FRAME 55

From the two L's, one further estimate,  $M_1$ , can be obtained by using the equation

$$M_1 = L_2 + (L_2 - L_1)/255$$

(256 is the ratio of two successive  $h^8$ 's.)

This is found to be  $6 \cdot 389 \ 056$  and the table is now

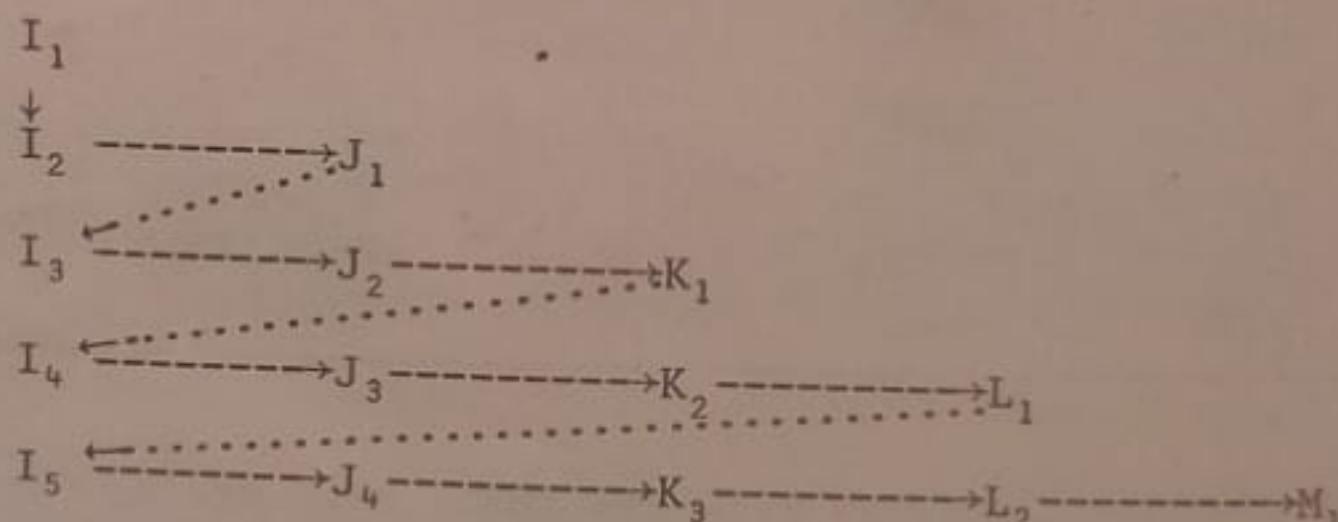
2	8.389 056					
1	6.912 810	6.420 728				
0.5	6.521 610	6.391 210	6.389 242			
0.25	6.422 298	6.389 194	6.389 060	6.389 057		
0.125	6.397 373	6.389 065	6.389 056	6.389 056	6.389 056	

Now it has already been pointed out that, for the various columns, as one goes down each column, the estimate of the integral is increasing in accuracy, and it eventually converges to the actual value required. Further, the estimates in the columns on the right are, taking them as a whole, better than those in the columns on the left. These facts give the clue as to how much or how little of the table is necessary and, also, as to the final value taken for the integral.

In deriving the process, the table was completed as much as possible for the values of  $h$  chosen. In order to obtain more entries, it would be necessary to take the next value of  $h$ , i.e. 0.0625. In practice, one wants to stop, for obvious reasons, as soon as possible. For this purpose, the entries are calculated in the order

$$I_1; I_2, J_1; I_3, J_2, K_1; I_4, J_3, K_2, L_1; \text{ etc.}$$

i.e., in rows as indicated by the arrows.



This can be continued if necessary by calculating next  $I_6$ , then  $J_5$ ,  $K_4$  and so on. One stops when two successive entries in the same column are equal or differ by not more than a pre-specified degree of tolerance, for example, 1 in the last place of decimals. The lower in position of the two entries concerned, rounded as necessary, gives the value of the integral. In our case  $L_1$  and  $L_2$  are so close that  $L_2$  can be taken as the value required and the table could stop here.

Working on the same basis, round off the entries at the top of the  $I$  column to 3 decimal places and form the table as far as is necessary so that two consecutive entries in a column do not differ by more than 0.001. Form the entries in the order indicated.

\*\*\*\*\*

56A

8.389			
6.913	6.421		
6.522	6.392	6.390	
6.422	6.389	6.389	

The numbers enclosed indicate the result as 6.389, which, rounding off to 2 decimal places, is 6.39.

Now find, by this method,  $\frac{1}{\pi} \int_0^{\frac{1}{2}\pi} \sin x dx$ , given the following values:

x	0	$\pi/32$	$\pi/16$	$3\pi/32$	$\pi/8$
y	0	0.098 017	0.195 090	0.290 284	0.382 683
x	$5\pi/32$	$3\pi/16$	$7\pi/32$	$\pi/4$	$9\pi/32$
y	0.471 396	0.555 570	0.634 394	0.707 107	0.773 010
x	$5\pi/16$	$11\pi/32$	$3\pi/8$	$13\pi/32$	$7\pi/16$
y	0.831 470	0.881 922	0.923 880	0.956 940	0.980 785
x	$15\pi/32$	$\pi/2$			
y	0.995 184	1			

\*\*\*\*\*

$\pi/2$	0.25			
$\pi/4$	0.301 777	0.319 036		
$\pi/8$	0.314 209	0.318 353	0.318 307	
$\pi/16$	0.317 287	0.318 313	0.318 310	0.318 310
$\pi/32$	0.318 054	0.318 310	0.318 310	0.318 310

Integral  $\approx 0.318 31$ . (To 7 decimal places, the value of the integral obtained analytically, is 0.318 3099.)

If the table formed in a Romberg integration is very extensive, the notation that has been adopted for the entries becomes rather unwieldy. As the table looks something like a matrix, a double suffix notation such as the following is frequently adopted for labelling the entries:

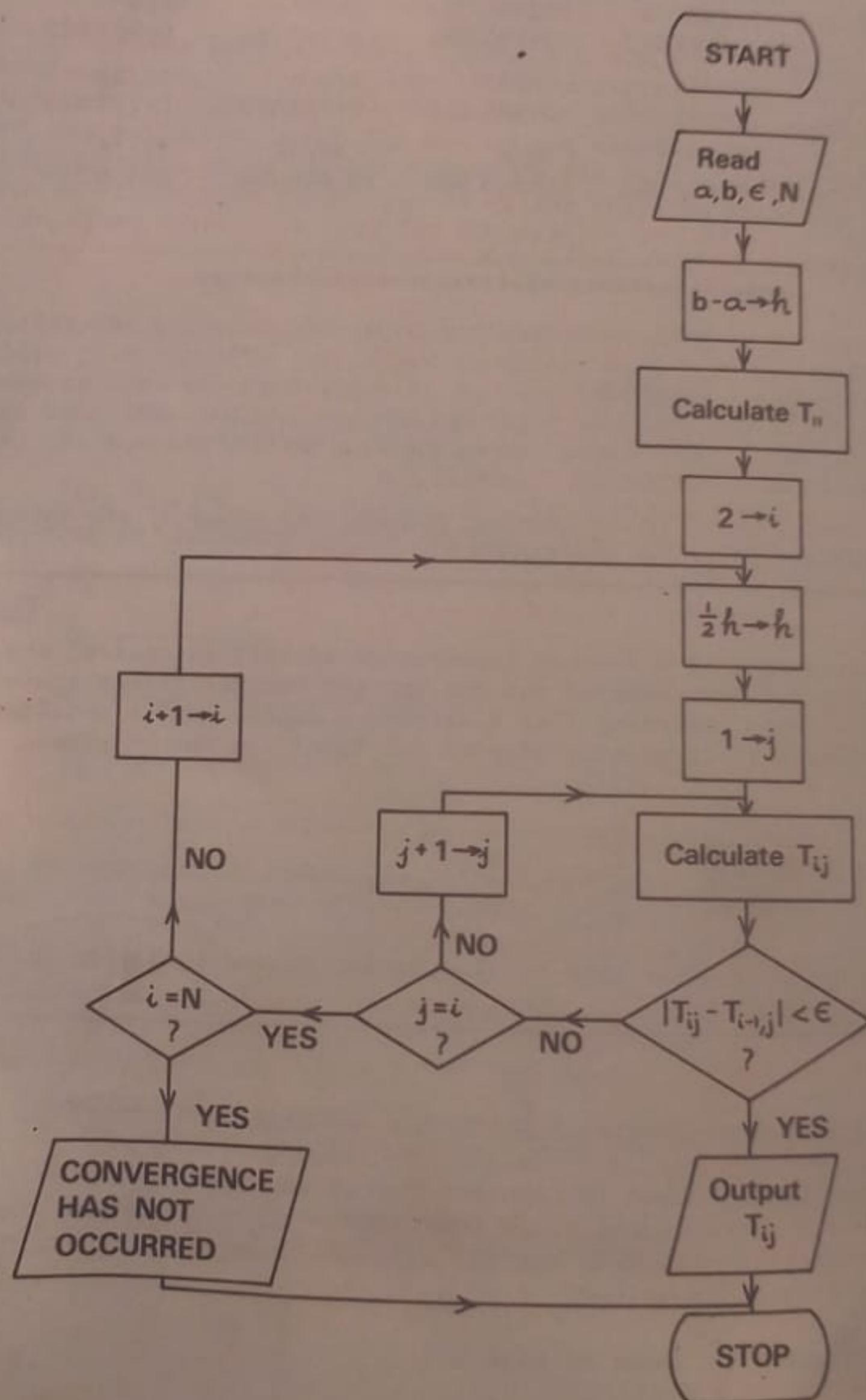
$$\begin{matrix} T_{11} & & & & \\ T_{21} & T_{22} & & & \\ T_{31} & T_{32} & T_{33} & & \\ T_{41} & T_{42} & T_{43} & T_{44} & \\ T_{51} & T_{52} & T_{53} & T_{54} & T_{55} \end{matrix}$$

etc. A notation such as this is also easier to use in a flow chart and for computer purposes.

A flow diagram for evaluating  $\int_a^b f(x)dx$  by Romberg's method is as

shown. The Romberg table is computed row by row and stops when a value is sufficiently close to the value immediately above it in the same column. If this convergence criterion has not been met when N rows have been formed, the process is halted.

(This flow diagram is shown on page 274.)



{ Programs for Romberg integration can be found in references (2), (3),  
(8) and (9). }

Unequally Spaced Data - Use of Lagrange's Interpolation Formula

If the points given are not equally spaced in the x-direction, then Lagrange's interpolation formula can be used to estimate an integral. You will remember that it was used in the last programme, under similar circumstances, to estimate the value of a derivative. Turn to FRAME 24, page 243 and find  $\int_{0.05}^{0.25} f(x)dx$  for the function  $f(x)$  given in the table in that frame.

\*\*\*\*\*

60A

The Lagrangian Interpolation formula is given in FRAME 25, page 244. Integrating gives

$$\left[ -0.0298x^4 - 0.0083x^3 + 0.502x^2 \right]_{0.05}^{0.25} \approx 0.0299$$

Miscellaneous Examples

In this frame a collection of miscellaneous examples is given for you to try. Answers are supplied in FRAME 62, together with such working as is considered helpful.

1. A particle moves along a straight line so that at time  $t$  its distance  $s$  from a fixed point of the line is given by  $\frac{ds}{dt} = t\sqrt{8 - t^3}$ .

Use Simpson's rule with 8 strips to calculate the approximate distance travelled by the particle from  $t = 0$  to  $t = 2$ . (L.U.)

2. The coordinates of points on a curve are given in the following table

x	0	0.2	0.4	0.6	0.8	1.0	1.2
y	1	1.1	1.3	1.5	1.6	1.4	1.3

Find, using Simpson's rule, the volume of revolution obtained when the area under this curve bounded by the lines  $x = 0$ ,  $x = 1.2$  and the x-axis is rotated through  $2\pi$  radians about the x-axis.

Obtain the coordinates of the centroid of this volume. (L.U.)

3. Evaluate numerically  $\int_0^{\frac{1}{2}\pi} \cos x dx$  using the trapezium rule with step length so chosen that the truncation error is less than 0.01. Find a bound for the round-off error in your answer. (C.E.I.)

(HINT: You will find in 47A the formula you require for the truncation error.)

4. It was mentioned earlier in this programme that

$$\int_0^{x_0} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

occurs in a certain heat capacity problem. From the following table of the function  $y = \frac{x^4 e^x}{(e^x - 1)^2}$ , evaluate this integral when  $x_0 = 0.7$  by a combination of Boole's rule for the section from  $x = 0$  to  $0.4$  and the three-eighths rule for the rest.

x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
y	0	0.0010	0.0399	0.0893	0.1579	0.2449	0.3494	0.4705

5. The solutions of certain problems in various topics, e.g., gravitational potential, fluid flow, non-linear springs, lead to the use of what are known as elliptic functions. A simple example of such a function is  $\int_0^{2\pi} \frac{1}{\sqrt{1 - \frac{1}{2} \sin^2 \theta}} d\theta$ . Find, using Weddle's rule, the value of this integral from the following table of values of  $\theta$  and  $y$  where  $y = \frac{1}{\sqrt{1 - \frac{1}{2} \sin^2 \theta}}$ .

$\theta$	0	$\pi/24$	$\pi/12$	$\pi/8$	$\pi/6$	$5\pi/24$	$\pi/4$	$7\pi/24$
y	1	1.0043	1.0172	1.0388	1.0690	1.1079	1.1547	1.2080
$\theta$	$\pi/3$	$3\pi/8$	$5\pi/12$	$11\pi/24$	$\pi/2$			
y	1.2649	1.3208	1.3692	1.4023	1.4142			

6. Starting from Everett's interpolation formula:

$$y_p = qy_0 + \frac{q(q^2 - 1^2)}{6} \delta^2 y_0 + \frac{q(q^2 - 1^2)(q^2 - 2^2)}{120} \delta^4 y_0 + \dots$$

$$+ py_1 + \frac{p(p^2 - 1^2)}{6} \delta^2 y_1 + \frac{p(p^2 - 1^2)(p^2 - 2^2)}{120} \delta^4 y_1 + \dots$$

where  $q = 1 - p$ , derive the formula

$$\frac{1}{h} \int_{x_0}^{x_1} y dx = \mu y_{\frac{1}{2}} - \frac{1}{12} \mu \delta^2 y_{\frac{1}{2}} + \frac{11}{720} \mu \delta^4 y_{\frac{1}{2}} - \dots$$

for integrating over one table interval, and deduce the formula

$$\frac{1}{h} \int_{x_0}^{x_n} y dx = \frac{1}{2} y_0 + y_1 + \dots + y_{n-1} + \frac{1}{2} y_n - \frac{1}{12} (\mu \delta y_n - \mu \delta y_0)$$

$$+ \frac{11}{720} (\mu \delta^3 y_n - \mu \delta^3 y_0) + \dots$$

for integrating over  $n$  table intervals.

Use the table provided to evaluate  $\int_0^{0.5} e^{-x^2} dx$ .

x	$y = e^{-x^2}$	$\Delta y$	$\Delta^2 y$	$\Delta^3 y$
0	1.000 000		-19 900	
0.1	0.990 050	-9950	-19 311	589
0.2	0.960 789	-29 261	-17 597	1714
0.3	0.913 931	-46 858	-14 929	2668
0.4	0.852 144	-61 787	-11 556	3373
0.5	0.778 801	-73 343	-7782	3774
0.6	0.697 676	-81 125	-3925	3857
0.7	0.612 626	-85 050	-284	3641

(L.U.)

[There are certain points to notice about this question:

a) In the programme, all integration formulae obtained by integrating an interpolation formula used the Newton-Gregory interpolation formula. As this question illustrates, other interpolation formulae can be used equally as well.

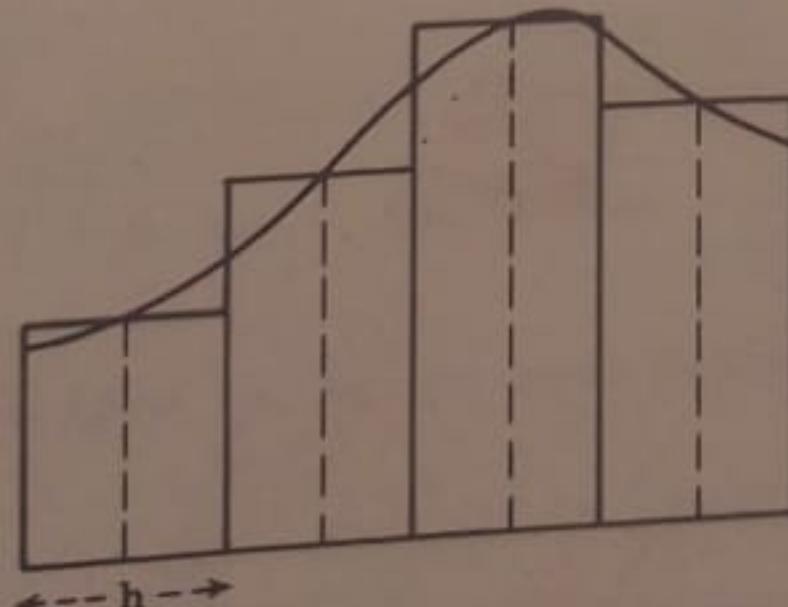
b) When integrating the interpolation formula you will find it easier to leave it in terms of p and q than to convert it all into terms of p, and, for the q terms, use

$$\int f(q) dp = \int f(q) \frac{dp}{dq} dq = -\int f(q) dq, \quad \text{as } \frac{dp}{dq} = -1.$$

c) You will find it necessary to extend the table slightly backwards in order to get all the necessary differences. As the function  $e^{-x^2}$  is symmetrical about  $x = 0$ , this will be quite easy.]

7. Using the values given in question 6 together with  $y = 0.527 292$  when  $x = 0.8$ , find  $\int_0^{0.8} e^{-x^2} dx$  by Romberg integration.

8.



The MID-ORDINATE RULE approximates an area to the sum of a number of rectangles, the height of each rectangle being that of the height of the ordinate in the centre of each strip. Use this rule to find

$\int_0^{1.0} 3x^2 dx$ , taking  $h = 2$ . (You will find the values of  $3x^2$  given in FRAME 18.)

Answers to Miscellaneous Examples

Page 10

1.	$t$	0	0.25	0.50	0.75	1	1.25	1.50	1.75	2
	$\frac{ds}{dt}$	0	0.706	1.403	2.065	2.646	3.074	3.225	2.844	0
	$s = 4.109$									

2. Volume =  $\int_0^{1.2} \pi y^2 dx$

First moment about plane passing through origin and perpendicular to  $Ox = \int_0^{1.2} \pi xy^2 dx$ . Integrals required by numerical means are  $\int_0^{1.2} y^2 dx$  and  $\int_0^{1.2} xy^2 dx$ .

These two integrals give 2.19133 and 1.44560.

Volume  $\approx 6.8843$      $\bar{x} \approx 0.6597$      $\bar{y} = 0$  from symmetry.

3. For error to be less than that given,  $\frac{h^2}{12} \times \frac{\pi}{4} < 0.01$ ;  $h < 0.3909$ . As range of integration = 0.7854, it is therefore necessary to take 3 strips and so  $h = 0.2618$ .

Trapezium rule then gives value of integral = 0.7031.

Round-off error bound  $\approx 0.0002$ .

4. 0.1116

5. 1.8541

6. Integrating w.r.t.  $p$  gives

$$\int y_p dp = -\frac{q^2}{2} y_0 - \frac{\frac{q^4}{4} - \frac{q^2}{2}}{6} \delta^2 y_0 - \frac{\frac{q^6}{6} - \frac{5q^4}{4} + 2q^2}{120} \delta^4 y_0 - \dots$$

$$+ \frac{p^2}{2} y_1 + \frac{\frac{p^4}{4} - \frac{p^2}{2}}{6} \delta^2 y_1 + \frac{\frac{p^6}{6} - \frac{5p^4}{4} + 2p^2}{120} \delta^4 y_1 + \dots$$

Limits of  $p$  are 0 and 1. Those of  $q$  are 1 and 0 as  $q = 1 - p$ . The first integration formula results.

The corresponding formula for the integral from  $x_1$  to  $x_2$  will be

$$\frac{1}{h} \int_{x_1}^{x_2} y dx = \mu y_{1\frac{1}{2}} - \frac{1}{12} \mu \delta^2 y_{1\frac{1}{2}} + \frac{11}{720} \mu \delta^4 y_{1\frac{1}{2}} - \dots$$

and similarly for the other intervals up to that for  $x_{n-1}$  to  $x_n$ .

Then  $\frac{1}{h} \int_{x_0}^{x_n} y dx = \frac{1}{h} \left\{ \int_{x_0}^{x_1} y dx + \int_{x_1}^{x_2} y dx + \dots + \int_{x_{n-1}}^{x_n} y dx \right\}$

Adding the first terms in each integral gives

$$\begin{aligned} \mu y_{\frac{1}{2}} + \mu y_{1\frac{1}{2}} + \mu y_{2\frac{1}{2}} + \dots + \mu y_{n-\frac{1}{2}} \\ = \frac{1}{2}(y_0 + y_1) + \frac{1}{2}(y_1 + y_2) + \frac{1}{2}(y_2 + y_3) + \dots + \frac{1}{2}(y_{n-1} + y_n) \\ = \frac{1}{2}y_0 + y_1 + y_2 + \dots + y_{n-1} + \frac{1}{2}y_n \end{aligned}$$

Adding the second terms gives

$$\begin{aligned} & -\frac{1}{12} \left( \mu \delta^2 y_{\frac{1}{2}} + \mu \delta^2 y_{1\frac{1}{2}} + \dots + \mu \delta^2 y_{n-1\frac{1}{2}} + \mu \delta^2 y_{n-\frac{1}{2}} \right) \\ &= -\frac{1}{12} \left( \frac{1}{2} \delta^2 y_0 + \delta^2 y_1 + \dots + \delta^2 y_{n-1} + \frac{1}{2} \delta^2 y_n \right) \\ &= -\frac{1}{12} \left\{ \frac{1}{2} \left( \delta y_{\frac{1}{2}} - \delta y_{-\frac{1}{2}} \right) + \left( \delta y_{1\frac{1}{2}} - \delta y_{\frac{1}{2}} \right) + \left( \delta y_{2\frac{1}{2}} - \delta y_{1\frac{1}{2}} \right) + \dots \right. \\ &\quad \left. + \left( \delta y_{n-1\frac{1}{2}} - \delta y_{n-2\frac{1}{2}} \right) + \left( \delta y_{n-\frac{1}{2}} - \delta y_{n-1\frac{1}{2}} \right) + \frac{1}{2} \left( \delta y_{n+\frac{1}{2}} - \delta y_{n-\frac{1}{2}} \right) \right\} \\ &= -\frac{1}{12} \left\{ \left( -\frac{1}{2} \delta y_{-\frac{1}{2}} - \frac{1}{2} \delta y_{\frac{1}{2}} \right) + \left( \frac{1}{2} \delta y_{n-\frac{1}{2}} + \frac{1}{2} \delta y_{n+\frac{1}{2}} \right) \right\} \\ &= -\frac{1}{12} \left( -\mu \delta y_0 + \mu \delta y_n \right) \end{aligned}$$

The term  $\frac{11}{720} (\mu \delta^3 y_n - \mu \delta^3 y_0)$  follows similarly by adding the third terms in each integral.

Extending the quoted difference table backwards slightly,

-0.2	0.960 789	29 261		
-0.1	0.990 050	9950	-19 311	-589
0	1.000 000	-9950	-19 900	589

$$\begin{aligned} \frac{1}{0.1} \int_0^{0.5} e^{-x^2} dx &= \frac{1}{2} \times 1.000 000 + 0.990 050 + 0.960 789 + 0.913 931 \\ &\quad + 0.852 144 + \frac{1}{2} \times 0.778 801 - \frac{1}{12} (-0.077 234 - 0) \\ &\quad + \frac{11}{720} (0.003 816 - 0) \end{aligned}$$

$$\therefore \int_0^{0.5} e^{-x^2} dx = 0.461 281$$

You will recognise the first part of the integration formula i.e.  $h(\frac{1}{2}y_0 + y_1 + \dots + y_{n-1} + \frac{1}{2}y_n)$  as being the trapezium rule extended

## NUMERICAL INTEGRATION

FRAME 62 (continued)  
 to several intervals. As you know, this is not an accurate formula for an area. The complete formula derived in this question increases the accuracy by including higher order difference terms. These are omitted when the straightforward simple trapezium rule is used.

$e^{-x^2}$  is a function whose indefinite integral cannot be found. Integrals of this kind are needed when finding the area under the normal curve in probability and also when finding the values of what is known as the error function.

7.  $0.8 \quad 0.610\ 9168$

$0.4 \quad 0.646\ 3160 \quad 0.658\ 1157$

$0.2 \quad 0.654\ 8510 \quad 0.657\ 6960 \quad 0.657\ 6680$

$0.1 \quad 0.656\ 9663 \quad 0.657\ 6714 \quad 0.657\ 6698 \quad 0.657\ 6698$

Integral  $\approx 0.657\ 67$

8. 990

---

1. The acceleration,  $a$ , of a rocket at time  $t$ , measured from launching, is given by the table

$t$	$s$	0	10	20	30	40	50	60	70
$a \text{ ms}^{-2}$		30.0	31.7	33.6	35.7	38.0	40.7	43.7	47.1
Find the rocket's velocity and height at $t = 70$ .									

2. An air cooled engine cylinder is simulated by a cooling fin placed in an air stream, the fin being heated at its centre. The temperature

ToC of the fin at various distances  $r$  cm from the centre is given by the table.

$r$	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0	22.5
T	58.9	59.3	59.8	60.8	61.9	63.1	64.5	65.7	66.8
$r$	25.0	27.5							
T	67.2	67.5							

Find the least squares law of the form  $T = a_0 + a_1 r + a_2 r^2 + a_3 r^3$ .

$$3. \text{ Prove that } \Delta \sqrt{f_k} = \frac{\Delta f_k}{\sqrt{f_k} + \sqrt{f_{k+1}}}$$

4. Use Romberg integration to find  $\int_0^1 \frac{\tan^{-1} x}{x} dx$ , correct to four decimal places, from the following table of values of  $y = \frac{\tan^{-1} x}{x}$ .

x	0	0.0625	0.125	0.1875	0.25	0.3125
y	1	0.99870	0.99484	0.98852	0.97836	0.96923
x	0.375	0.4375	0.5	0.5625	0.625	0.6875
y	0.95672	0.94265	0.92729	0.91091	0.89379	0.87605
x	0.75	0.8125	0.875	0.9375	1	
y	0.85800	0.83977	0.82152	0.80336	0.78540	

5. Find, to 5 decimal places,  $f'(0.6)$  for the function given by the following table:

x	0.45	0.50	0.55	0.60	0.65
$f(x)$	4.069057	4.053474	4.035500	4.014994	3.991775
x	0.70	0.75			
$f(x)$	3.965615	3.936218			

6. Find the value of the normal distribution function,  $\phi(x)$ , for  $x = 2.0673$  from the following table:

x	2.00	2.05	2.10	2.15	2.20	2.25
$\phi(x)$	0.97725	0.97982	0.98214	0.98422	0.98610	0.98778
x	2.30					
$\phi(x)$	0.98928					

7. Find the value of  $\coth 0.10276$  from the table

$x$	0.100	0.101	0.102	0.103	0.104
$\coth x$	10.03331	9.93463	9.83790	9.74305	9.65003
$x$	0.105				
$\coth x$	9.55878				

using (i) Bessel's formula (ii) Stirling's formula.

8. The points  $(-1, 8)$ ,  $(0, 5)$ ,  $(1, 4)$ ,  $(3, 56)$  lie on a certain polynomial curve,  $y = f(x)$ . Find the value of  $y$  when  $x = 2$ , assuming that  $f(x)$  is of the lowest degree possible.

9. For what value of  $x$ , to 6 decimal places, will the function  $f(x)$  given below take the value 5?

$x$	1.595	1.600	1.605	1.610	1.615
$f(x)$	4.928329	4.953032	4.977860	5.002811	5.027888
$x$	1.620	1.625			
$f(x)$	5.053090	5.078419			

10. Use (i) Simpson's rule, (ii) Boole's rule to obtain the integral given in question number 4.

#### ANSWERS

1.  $2618 \text{ ms}^{-1}$ ,  $84.75 \text{ km}$ . [In order to find the height, it is necessary to complete a table of velocities for  $t = 0(10)^70$ .]

2.  $T = 59.3 - 0.260r + 0.0519r^2 - 0.001150r^3$

$$3. \Delta\sqrt{f_k} = \sqrt{f_{k+1}} - \sqrt{f_k} = \frac{f_{k+1} - f_k}{\sqrt{f_{k+1}} + \sqrt{f_k}} = \frac{\Delta f_k}{\sqrt{f_{k+1}} + \sqrt{f_k}}$$

4. 0.9159
5. -0.43658
6. 0.98065
7. 9.76565 in each case.
8. 17
9. 1.609438
10. 0.9159 in each case.