Numerical Integration (20 pages; 31/3/20)

Contents

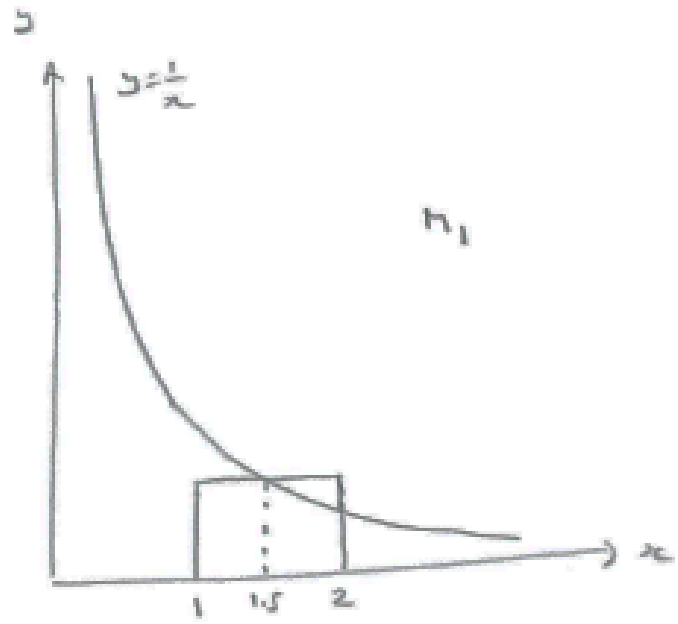
[Note: Because the expression 'absolute error' is now used to mean $x - A$ (where x is the observed value and A is the actual (ie true) value), as opposed to the 'relative error' $\frac{x-A}{A}$), I will use 'absolute size' of y to indicate $|y|$. However, this isn't a standard expression.]

(A) Midpoint rule (aka the mid-ordinate rule)

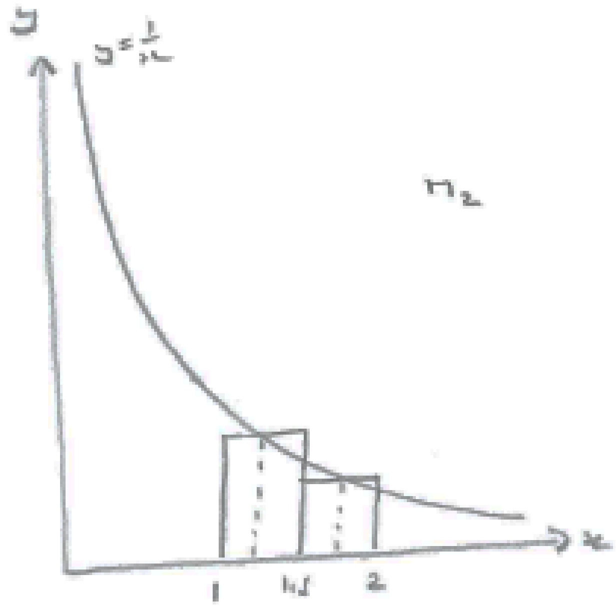
(1) M_n approximates the area under the curve by the sum of the areas of n rectangles, where the height of each rectangle is determined by the value of the function at the midpoint of the rectangle. This is shown below for $n = 1, 2$ & 3.

Example: $\int_1^2 \frac{1}{x}\, dx$

Exact value $= [lnx]_1^2 = ln2 - ln1 = ln2 = 0.69315$ (5dp)



$$M_1 = \frac{1}{1.5} \times 1 = 0.66667$$



$$M_2 = \left(\frac{1}{1.25} + \frac{1}{1.75}\right) \times 0.5 = 0.68571$$

$$M_3 = \left(\frac{1}{7/6} + \frac{1}{9/6} + \frac{1}{11/6}\right) \times \frac{1}{3} = 0.68975$$

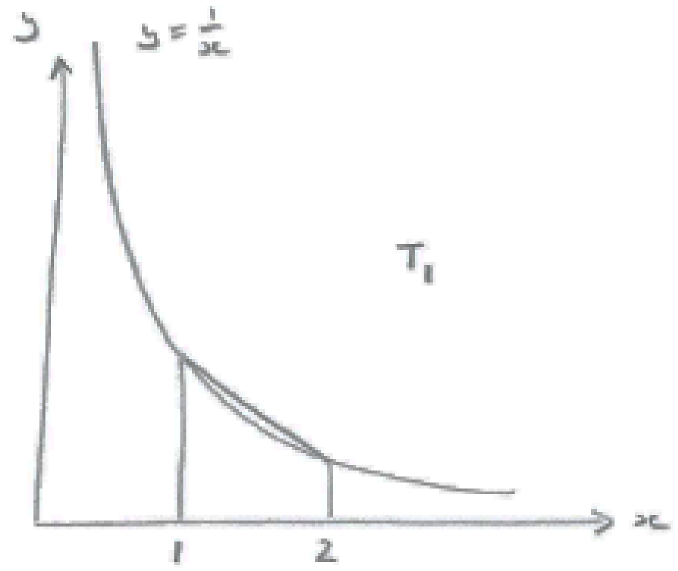
(2) The general formula is

$$M_n = h(f_{0.5} + f_{1.5} + \ldots + f_{n-0.5}),$$

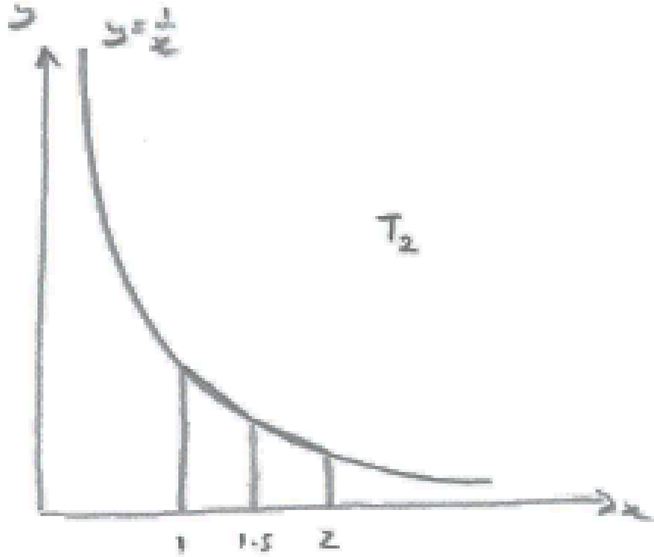
where h is the width of each rectangle.

(B) Trapezium rule

(1) T_n approximates the area under the curve by the sum of the areas of n trapezia, where the sides of each trapezium are the values of the function. This is shown below for $n = 1, 2$ & 3 (for the same example as for the midpoint rule, where the exact value was 0.69315).



$$T_1 = \frac{1}{2}\left(\frac{1}{1} + \frac{1}{2}\right) \times 1 = 0.75$$



$$T_2 = \frac{1}{2}(\frac{1}{1} + \frac{1}{1.5}) \times 0.5 + \frac{1}{2}(\frac{1}{1.5} + \frac{1}{2}) \times 0.5$$

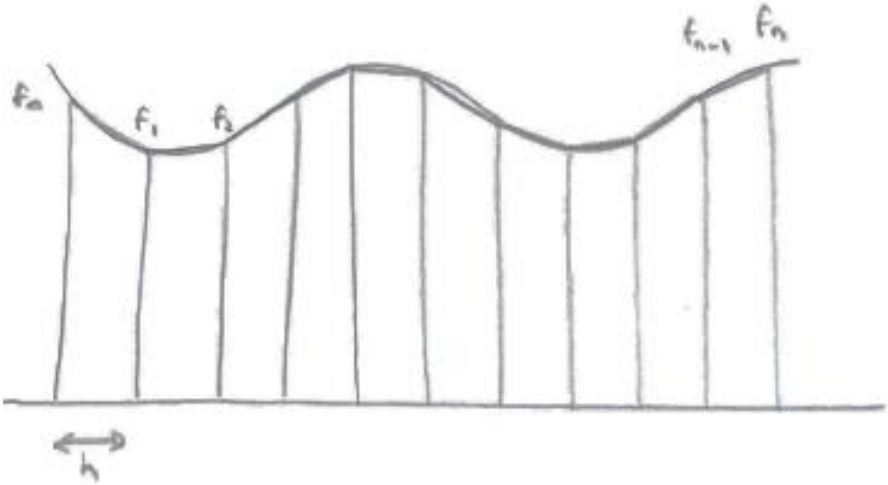
$$= \frac{1}{2}\ [\frac{1}{1} + \ \frac{1}{2} + 2\left(\frac{1}{1.5}\right)] = 0.70833$$

$$T_3 = \frac{1}{2}\ (\frac{1}{1} + \ \frac{1}{2} + 2\left(\frac{1}{4/3} + \frac{1}{5/3}\right)) \times \frac{1}{3} = 0.7$$

(2) The general formula is

$$T_n = \frac{1}{2} h\ \{ f_0 + f_n + 2(f_1 + f_2 + \cdots + f_{n-1})\},$$

where h is the width of each trapezium.



(C) Connections between the Trapezium and Midpoint rules

(1) It can be shown that $T_{2n} = ½\left(T_n + M_n\right)$

Proof

Let W be the width of the interval being considered.

As $T_n = \frac{1}{2}h\,\{ f_0 + f_n + 2(f_1 + f_2 + \cdots + f_{n-1})\}$,

$T_{2n} = \frac{1}{2}\left(\frac{W}{2n}\right)\{ f_0 + f_{2n} + 2(f_1 + f_2 + \cdots + f_{2n-1})\}$

(noting that f_1, f_2 etc are now defined differently).

Using the definitions of f_1, f_2 that appear in T_{2n},

T_n becomes $\frac{1}{2}\left(\frac{W}{n}\right)\{ f_0 + f_{2n} + 2(f_2 + f_4 + \cdots + f_{2n-2})\}$.

Also, M_n becomes $\left(\frac{W}{n}\right)(f_1 + f_3 + \ldots + f_{2n-1})$,

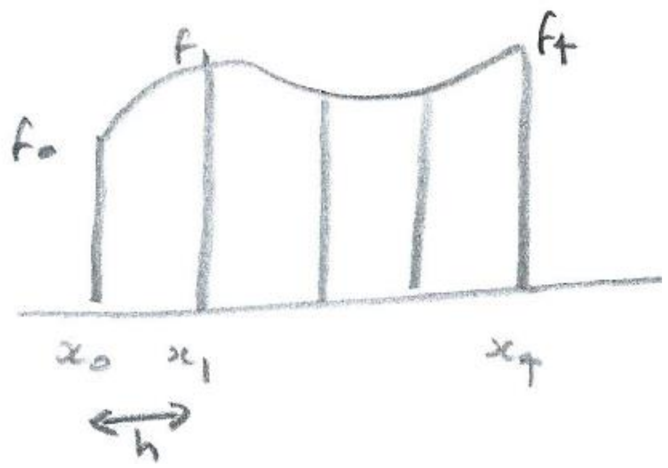
and so $T_n + M_n = \frac{1}{2}\left(\frac{W}{n}\right)\{f_0 + f_{2n} + + 2(f_2 + f_4 + \cdots + f_{2n-2})$

$+2(f_1 + f_3 + \ldots + f_{2n-1})\}$

$= 2T_{2n}$, as required.

(2) Exercise: Demonstrate that $T_4 = ½\left(T_2 + M_2\right)$

Solution



$T_2 = \frac{1}{2}(2h)(f_0 + 2f_2 + f_4)$

$M_2 = (2h)(f_1 + f_3)$

$\Rightarrow \frac{1}{2}(T_2 + M_2) = \frac{1}{2}h([f_0 + 2f_2 + f_4] + [2f_1 + 2f_3])$

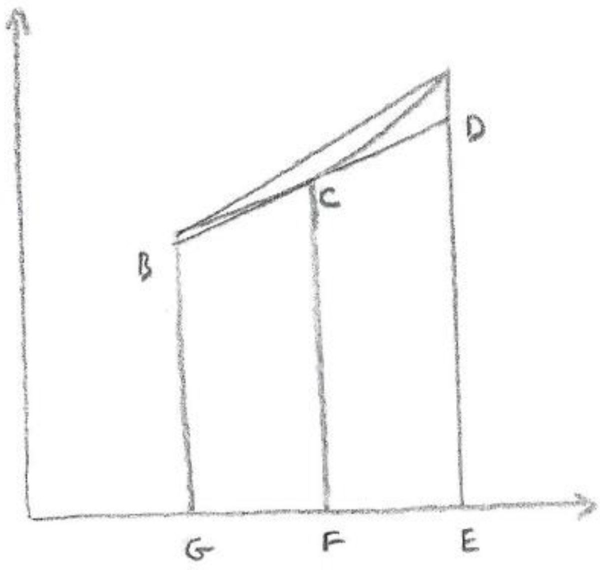
$= \frac{1}{2}h(f_0 + 2[f_1 + f_2 + f_3] + f_4) = T_4$

(3) Comparison of values from Trapezium & Midpoint rules (from the earlier example of $y = \frac{1}{x}$)

n	T_n	M_n	$\frac{T_n - A}{A} \times 100\%$	$\frac{M_n - A}{A} \times 100\%$
A(actual)	0.69315	0.69315		
1	0.75	0.66667	8.202%	−3.820%
2	0.70833	0.68571	2.190%	−1.073%
3	0.7	0.68975	0.988%	−0.491%

(4) In the table above, the T_n fall towards the actual value, whilst the M_n rise. $y = \frac{1}{x}$ is an example of a convex function. The diagram below shows the Midpoint and Trapezium rules being applied to a general convex function.

[A convex function is one such as $y = e^x$ (think of $conve^x$), whilst a concave function is one such as $y = -x^2$. (See "Convexity and concavity" note.)]



For a convex function, $M_n < A < T_n$,

where A is the actual value of the area under the curve.

$A < T_n$ is clear from the diagram

To see why $M_n < A$, we draw the tangent to the curve at the midpoint C (the line BCD in the diagram). As the function is convex, the curve lies above the tangent on both sides of C, so that the trapezium BCDEFG has an area smaller than A. This trapezium has the same area as the rectangle in the mid-point rule, with base GE and height FC.

As the number of strips is increased, the M_n will approach A from below, whilst the T_n will approach A from above. An interval estimate is also provided by (M_n, T_n).

Similarly for a concave function, $T_n < A < M_n$.

In practice, a curve may need to be split up into convex and concave parts.

(5) In the table above, the absolute size of the relative error for T_n

is seen to be approximately twice that for M_n;

ie $\left|\frac{T_n - A}{A} \times 100\right| \approx 2\left|\frac{M_n - A}{A} \times 100\right|$

This leads to: $|T_n - A| \approx 2|M_n - A|$

For a convex function, $T_n - A \approx 2(A - M_n)$

and for a concave function, $A - T_n \approx 2(M_n - A)$

Proof for the concave case (where $T_n < A < M_n$)

$T_{2n} = ½\,(T_n + M_n)$ and $T_{2n} - A \approx \frac{1}{4}(T_n - A)$

so that $½\left(T_n + M_n\right) - A \approx \frac{1}{4}(T_n - A)$

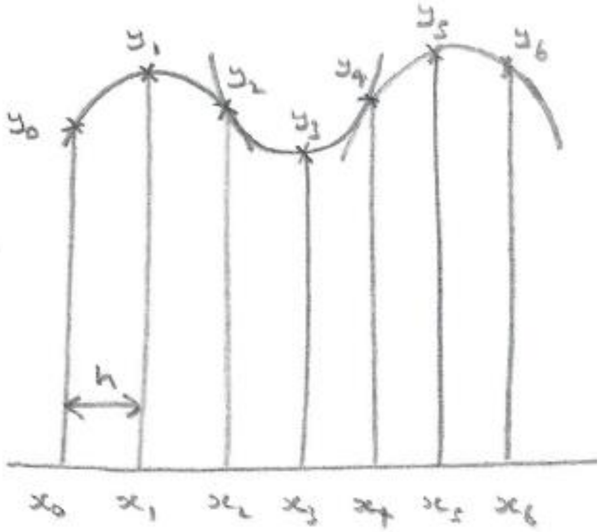
$\Rightarrow\ 2T_n + 2M_n - 4A \approx T_n - A$

$\Rightarrow\ T_n - A \approx 2A - 2M_n$

$\Rightarrow\ A - T_n \approx 2(M_n - A)$

(D) Simpson's Rule

(1) Given a number of points on the curve, Simpson's rule is derived by fitting a series of overlapping quadratic curves to the points. (Note that, unless they lie on a straight line, a quadratic curve can be found that passes through any 3 points.)



[Note: The diagram doesn't show the original curve; just the points on it and the quadratic curves fitted to those points.]

Referring to the diagram above, if $y_0, y_1, \ldots, y_6$ are the given y values (or 'ordinates'), then the first quadratic curve is fitted to the points (x_0, y_0), (x_1, y_1) & (x_2, y_2); the second quadratic curve is fitted to the points (x_2, y_2), (x_3, y_3) & (x_4, y_4) , and so on.

Integration is then used to find the areas under the quadratic curves, and these are added to give the final formula, which for the above example is:

$S_6 = \frac{h}{3}\left(y_0 + y_6 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)\right)$

(to be proved shortly)

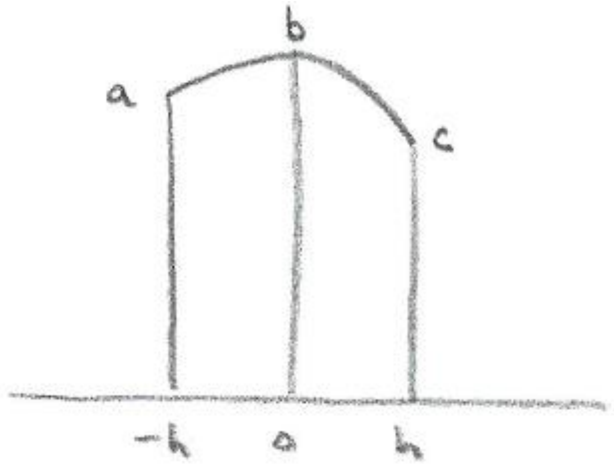
Notes

(i) This is the notation that is now used in the MEI exams. The 6 in S_6 is the number of strips. In an alternative notation, S_3 is written instead of S_6. (With the S_3 notation, the formula $S_3 = \frac{2M_3+T_3}{3}$ is obtained (see below), as opposed to $S_6 = \frac{2M_3+T_3}{3}$ under the new MEI notation.) For Edexcel and AQA, it would seem that the S_n

and S_{2n} notations are avoided (instead they say, for example, "Use Simpson's rule with 8 strips").

(ii) The quadratic functions can be found by either Newton's Forward Difference method or Lagrange's method (see separate notes).

(2) Proof



Let the quadratic function in the above diagram be

$y = px^2 + qx + b$

The area under the curve is $\int_{-h}^{h} px^2 + qx + b\, dx$

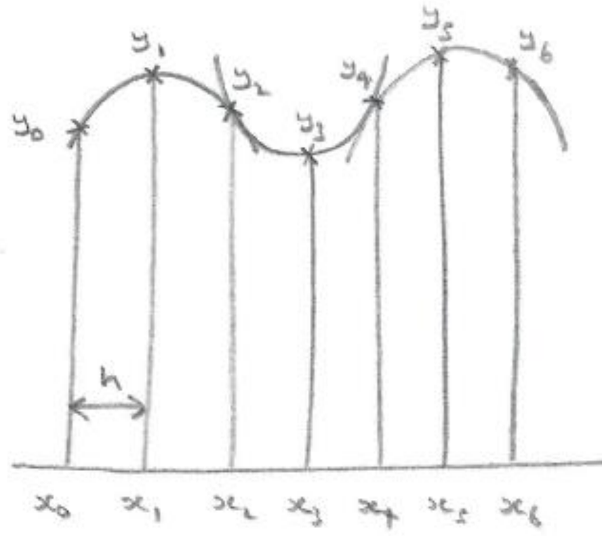
$= \left[\frac{px^3}{3} + \frac{qx^2}{2} + bx\right]_{-h}^{h} = \frac{2ph^3}{3} + 2bh \quad (1)$

Also $ph^2 - qh + b = a$ (2) and $ph^2 + qh + b = c$ (3)

Adding (1) & (2) gives $2ph^2 + 2b = a + c$ (4)

Then from (1) & (4),

Area $= \frac{h}{3}(a + c - 2b + 6b) = \frac{h}{3}(a + 4b + c)$



For 3 quadratic curves, the area is therefore

$S_6 = \frac{h}{3}([y_0 + 4y_1 + y_2] + [y_2 + 4y_3 + y_4] + [y_4 + 4y_5 + y_6])$

$= \frac{h}{3}\left(y_0 + y_6 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)\right)$, as required.

(3) This extends to the following general formula:

$S_{2n} = \frac{1}{3}h\{ f_0 + f_{2n} + 4(f_1 + f_3 + \cdots + f_{2n-1})$

$+2(f_2 + f_4 + \cdots + f_{2n-2})\}$,

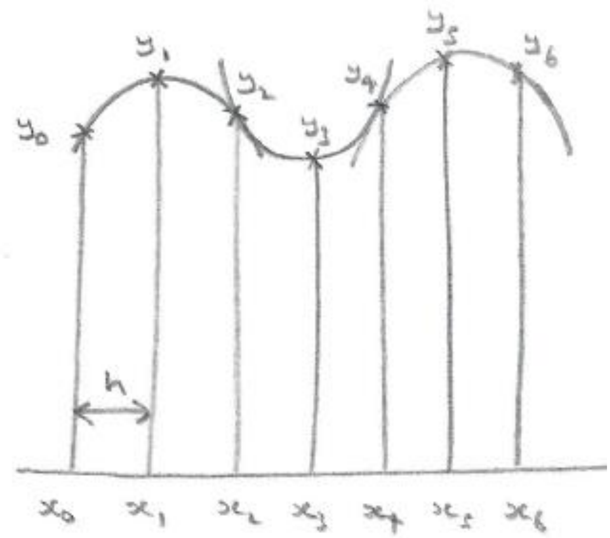
where the odd ordinates are multiplied by 4, and the even ones (except the first and last) are multiplied by 2.

(E) Connections between Simpson's rule and the Trapezium and Midpoint rules

(1) $S_{2n} = \frac{2M_n+T_n}{3}$

This result is not approximate. In practice, it will usually be more convenient to find S_{2n} in this way, rather than from the basic definition.

Demonstration for S_6:



We are dealing with 3 trapezia and 3 rectangles here, with bases of $2h$:

$T_3 = \frac{2h}{2}(y_0 + y_6 + 2(y_2 + y_4))$

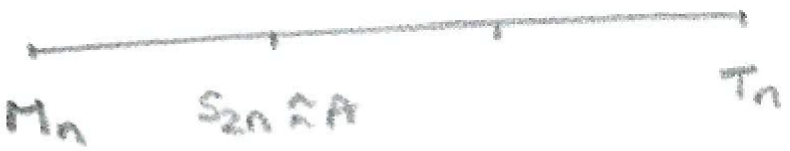
$M_3 = 2h(y_1 + y_3 + y_5)$

So $\frac{2M_3+T_3}{3} = \frac{h}{3}(4(y_1 + y_3 + y_5) + (y_0 + y_6 + 2(y_2 + y_4)))$

$= \frac{h}{3}\left(y_0 + y_6 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)\right) = S_6$

(2) It was seen earlier that the absolute size of the relative error for T_n is approximately twice that for M_n. This is consistent with the formula $S_{2n} = \frac{2M_n+T_n}{3}$: S_{2n} is more accurate than the other two methods (with the quadratic function producing a better fit), and can therefore be taken to be approximately equal to A, the actual value. Then, from the formula, A is approximately the given weighted average of M_n and T_n (see diagram below), with

$T_n - A \approx 2(A - M_n)$ (if $T_n > M_n$).

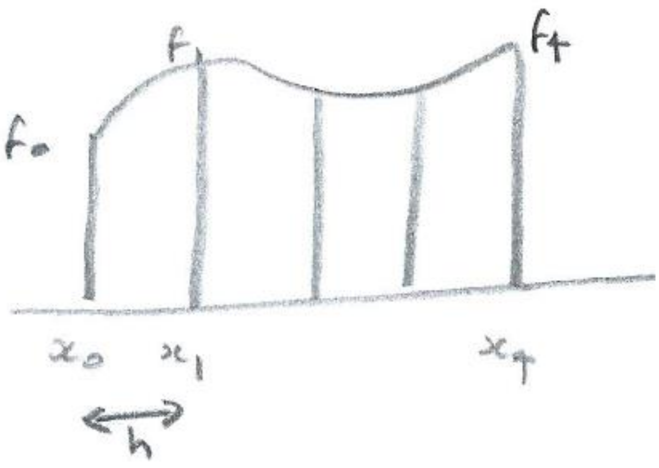


Thus M_n is more accurate than T_n, and S_{2n} is more accurate than M_n.

(3) Exercise

Show that $S_4 = \frac{2M_2+T_2}{3}$, from the basic definitions.

Solution



$\frac{2M_2+T_2}{3}=\frac{2}{3}(2h)(f_1+f_3)+\frac{1}{3}.\frac{1}{2}(2h)(f_0+2f_2+f_4)$

$=\frac{h}{3}(4f_1+4f_3+f_0+2f_2+f_4)$

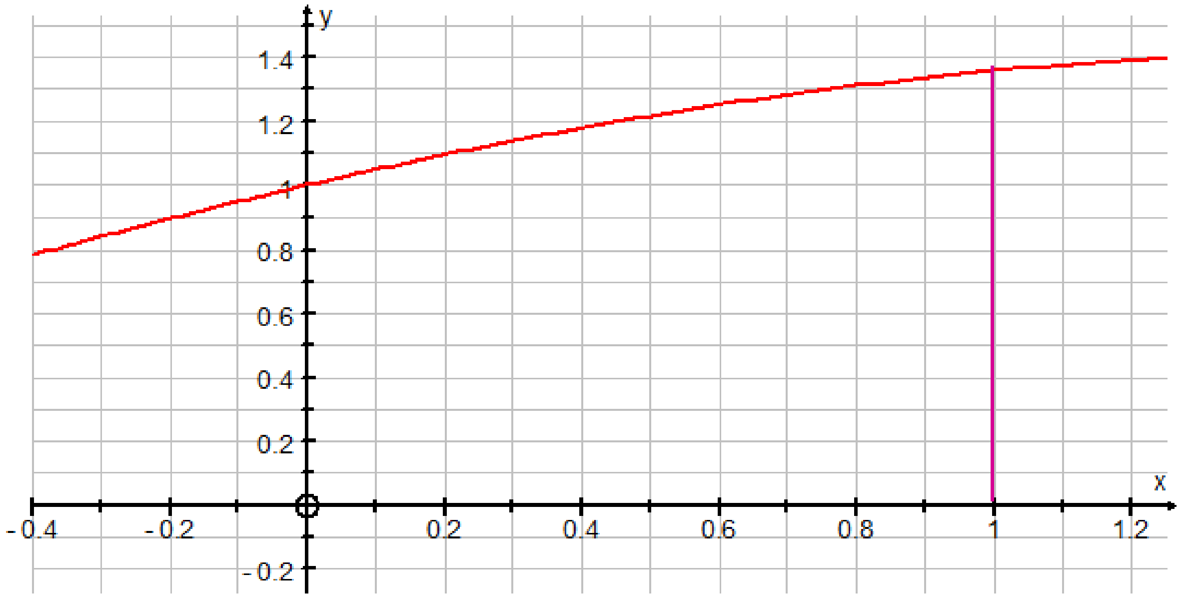
$=\frac{h}{3}(f_0+f_4+4(f_1+f_3)+2f_2)$

$=S_4$

(4) The table below applies this relation to the $y=\frac{1}{x}$ example earlier on, and shows that the Simpson's rule estimate is much closer to the exact value.

	A	B	C	D
1				
2	n	T_n	M_n	$S_{2n}=\frac{2}{3}M_n+\frac{1}{3}T_n$
3				
4	1	0.75	0.66667	0.69445
5	2	0.70833	0.68571	0.69325
6	3	0.7	0.68975	0.69317
7				
8	Exact	0.69315	0.69315	0.69315

(5) Example: $\int_0^1 \sqrt{sinx + 1}\, dx$



$M_2 = 0.5\big(f(0.25) + f(0.75)\big)$

$f(0.25) = \sqrt{\sin(0.25) + 1} = 1.11687$

$f(0.75) = \sqrt{\sin(0.75) + 1} = 1.29678$

$M_2 = 0.5(1.11687 + 1.29678) = 1.20683$

$T_n = \frac{1}{2}h\{\mathrm{f}_0 + f_n + 2(f_1 + f_2 + \cdots + f_{n-1})\}$

$T_2 = \frac{1}{2}(0.5)\{f(0) + f(1) + 2f(0.5)\}$

$f(0) = \sqrt{\sin(0) + 1} = 1$

$f(0.5) = \sqrt{\sin(0.5) + 1} = 1.21632$

$f(1) = \sqrt{\sin(1) + 1} = 1.35701$

$T_2 = \frac{1}{2}(0.5)\{1 + 1.35701 + 2(1.21632)\} = 1.19741$

$S_4 = \frac{2M_2+T_2}{3} = \frac{2(1.20683\ )+1.19741}{3} = 1.20369$

$T_{2n} = \frac{1}{2}(T_n + \ M_n)$

$T_4 = \frac{1}{2}(T_2 + \ M_2) = \frac{1}{2}(1.19741 + 1.20683) = 1.20212$

$M_4 = 0.25\big(f(0.125) + f(0.375) + f(0.625) + f(0.875\ )\big)$

$= 0.25(1.06051 + 1.16888 + 1.25901 + 1.32949)$

$= 1.20447$

$S_8 = \frac{2M_4+T_4}{3} = \frac{2(1.20447)+1.20212}{3} = 1.20369$

(6) $S_{2n} = \frac{4T_{2n}-T_n}{3}$

Proof

$S_{2n} = \frac{2M_n+T_n}{3}$ and $T_{2n} = ½\ (T_n + \ M_n)$

$\Rightarrow\ S_{2n} = \frac{2(2T_{2n}-T_n)+T_n}{3} = \frac{4T_{2n}-T_n}{3}$

(F) Speed of convergence

(1) A sequence is said to have 1st order convergence if

$e_{r+1} \approx ke_r$ (where $|k| < 1$), where $e_r = x_r - \alpha$

2nd order convergence is when $e_{r+1} \approx k{e_r}^2$ (again, with $|k| < 1$)

In the case of 1st order convergence, we can show that

$\frac{x_{r+1}-x_r}{x_r-x_{r-1}}$ (the 'ratio of differences') $\approx k$

Proof

$e_r = x_r - \alpha$ and $e_{r+1} = x_{r+1} - \alpha$

$e_r \approx ke_{r-1}$ and $e_{r+1} \approx ke_r$

So $\frac{x_{r+1}-x_r}{x_r-x_{r-1}} = \frac{(\alpha+e_{r+1})-(\alpha+e_r)}{(\alpha+e_r)-(\alpha+e_{r-1})} = \frac{e_{r+1}-e_r}{e_r-e_{r-1}} = \frac{ke_r-ke_{r-1}}{e_r-e_{r-1}} \approx k$

(2) For the Midpoint & Trapezium rules, it can be shown that the absolute size of the error (ie $|M_n - A|$ or $|T_n - A|$) is approximately proportional to h^2.

The Midpoint & Trapezium rules are accordingly described as '2nd order' methods.

So the absolute size of the error in $M_n \approx \lambda h^2$ and the absolute size of the error in $M_{2n} \approx \lambda \left(\frac{h}{2}\right)^2$ (and similarly for the Trapezium rule).

Hence $\frac{absolute\ size\ of\ error\ in\ M_{2n}}{absolute\ size\ of\ error\ in\ M_n} \approx \frac{\lambda\left(\frac{h}{2}\right)^2}{\lambda h^2} = \frac{1}{4}$

and the absolute size of error in $M_{2n} \approx \frac{1}{4} \times$ absolute size of error in M_n (and similarly for the Trapezium rule).

This means that the Midpoint & Trapezium rules both have 1st order convergence.

[Note the confusing terminology: 2nd order method, but 1st order convergence.]

Also, it can be shown that, for the Simpson's rule:

absolute size of error in $S_{2n} \approx \lambda h^4$

so that $\frac{absolute\ size\ of\ error\ in\ S_{4n}}{absolute\ size\ of\ error\ in\ S_{2n}} \approx \frac{\lambda\left(\frac{h}{2}\right)^4}{\lambda h^4} = \frac{1}{16}$

Simpson's rule is a 4th order method, but again having 1st order convergence, as

$absolute\ size\ of\ error\ in\ S_{4n}$

$\approx \frac{1}{16} \times absolute\ size\ of\ error\ in\ S_{2n}$

(3) Obtaining a better estimate of the integral by extrapolation

The result $\frac{x_{r+1}-x_r}{x_r-x_{r-1}} \approx k$ in the case of 1st order convergence can be applied to M_n (and also T_n and S_{2n}). Here the sequence is $M_1, M_2, M_4, \ldots$ (ie $x_3 = M_4$) and $\frac{M_4-M_2}{M_2-M_1}, \frac{M_8-M_4}{M_4-M_2}, \frac{M_{16}-M_8}{M_8-M_4}$ .... $\approx \frac{1}{4}$

Similarly, $\frac{T_4-T_2}{T_2-T_1}, \frac{T_8-T_4}{T_4-T_2}, \frac{T_{16}-T_8}{T_8-T_4}$ .... $\approx \frac{1}{4}$

and $\frac{S_8-S_4}{S_4-S_2}, \frac{S_{16}-S_8}{S_8-S_4}$ .... $\approx \frac{1}{16}$ (note that S_1 isn't defined)

Then, for the Trapezium rule (for example):

$T_{32} - T_{16} \approx \frac{1}{4}\,(T_{16} - T_8)$ (1)

and hence $T_{32} \approx T_{16} + \frac{1}{4}\,(T_{16} - T_8)$ (1')

ie given T_8 & T_{16}, we can estimate T_{32} (which will be a better estimate for the integral A)

Similarly $T_{64} \approx T_{32} + \frac{1}{4}\,(T_{32} - T_{16})$ (1'')

So, from (1') & (1),

$T_{64} \approx \left[T_{16} + \frac{1}{4}(T_{16} - T_8)\right] + \frac{1}{4}.\frac{1}{4}(T_{16} - T_8)$ (2)

And $T_{128} \approx T_{64} + \frac{1}{4}(T_{64} - T_{32})$ (3)

so that, from (3) & (2)

$T_{128} \approx \left[T_{16} + \frac{1}{4}(T_{16} - T_8) + \frac{1}{4^2}(T_{16} - T_8)\right] + \frac{1}{4}.\frac{1}{4}(T_{32} - T_{16})$,

as $T_{64} - T_{32} \approx \frac{1}{4}(T_{32} - T_{16})$, from (1'')

So $T_{128} \approx T_{16} + \frac{1}{4}(T_{16} - T_8) + \frac{1}{4^2}(T_{16} - T_8) + \frac{1}{4^3}(T_{16} - T_8)$, from (1)

and, repeating this process,

$A \approx T_{16} + \frac{1}{4}(T_{16} - T_8) + \frac{1}{4^2}(T_{16} - T_8) + \frac{1}{4^3}(T_{16} - T_8) + \cdots$

$\approx T_{16} + \frac{1}{4}(T_{16} - T_8)\frac{1}{1-\frac{1}{4}}$

$= T_{16} + \frac{1}{3}(T_{16} - T_8)$

Naturally we would use the best pair of T_n & T_{2n} available,

when $A \approx T_{2n} + \frac{1}{3}(T_{2n} - T_n)$ or $\frac{4T_{2n}}{3} - \frac{T_n}{3}$

Note: The same result can be obtained more simply as follows:

$T_{2n} - A \approx \frac{T_n - A}{4} \Rightarrow T_{2n} - \frac{T_n}{4} \approx \frac{3A}{4}$

$\Rightarrow A \approx \frac{4T_{2n}}{3} - \frac{T_n}{3}$

The same result applies to the Midpoint rule.

For Simpson's rule,

$$A \approx S_{32} + \frac{1}{16}\ (S_{32} - S_{16})\left(\frac{1}{1-\frac{1}{16}}\right) = S_{32} + \frac{1}{15}\ (S_{32} - S_{16})\ \text{etc}$$

and generally: $A \approx S_{4n} + \frac{1}{15}\ (S_{4n} - S_{2n})$ or $\frac{16S_{4n}}{15} - \frac{S_{2n}}{15}$