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ON GENERALISED SIMPSON'S RULE
WITH END CORRECTIONS

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1. ABSTRACT

Presented in this note is an $O(h^8)$ generalised Simpson's rule with end corrections to evaluate

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

assuming the existence of Riemannian integration. This highly accurate formula demands only the knowledge of lower derivatives of $f(x)$. For $O(h^8)$ method knowledge of first and second derivatives of $f(x)$ is needed. For still higher accuracy, say, for $O(h^{10})$, we need upto third derivative; for $O(h^{12})$ we require the calculation of fourth derivatives along with first, second and third and so on. Methods of higher order can be developed but we must be very careful in doing this. This is because higher derivatives tend to behave increasingly badly so that despite the higher power of h , the error may not be less than that of even a fourth order method. A few numerical examples described in the subsequent pages illustrate this aspect. Also mentioned here are the bounds for truncation error for a few methods.

2. MATHEMATICS

We first choose a single interval of integration and then generalise it in the interval $[a, b]$. We assume

$$\int_{x_0-h}^{x_0+h} f(x) dx = h [af'(x_0-h) + bf(x_0) + af(x_0+h)] \\ + \sum_{i=1}^m h^{i+1} b_i \{ f^{(i)}(x_0-h) + (-1)^i f^{(i)}(x_0+h) \} \quad [1]$$

where $a, b, b_1, b_2, \dots, b_m$ are constants to be determined and m is any finite positive integer. In case $m=0$, the above assumption results in Simpson's rule for equidistant points without end correction. When $m=1$, the Simpson's rule is modified by an end correction term giving rise to $O(h^6)^{(1,2)}$ method. This is a particular case, usually in use, of our general assumption. When $m=2, 3, 4, \dots$ etc. the accuracy of numerical integration shoots up very rapidly within the limit of the precision of the computer.

The correction term in [1] involves the calculation of the derivatives of $f(x)$ at the end points of the interval $[x_0-h, x_0+h]$. The form of the expression, moreover, can be very simply justified by noting that the L.H.S. and hence the R.H.S. is an odd function of h (i.e. changes sign under the transformation $h \rightarrow -h$).

Expansion of left hand side of [1] gives

$$\int_{x_0-h}^{x_0+h} f(x) dx = F(x_0) + \sum_{i=1}^{\infty} \frac{h^i}{i!} f^{(i-1)}(x_0) - F(x_0) + \sum_{i=1}^{\infty} (-1)^{i-1} \frac{h^i}{i!} f^{(i-1)}(x_0)$$

where $f(x) \equiv dF(x)/dx$

On simplification

$$\int_{x_0-h}^{x_0+h} f(x) dx = 2 \sum_{i=0}^{\infty} \frac{h^{2i+1}}{(2i+1)!} f^{(2i)}(x_0) \quad [2]$$

Similarly expanding the right hand side of [1] for $m=2$, in series and equating the co-efficients of $f(x_0), f^{(2)}(x_0), \dots$ etc. with those of [2], we get

$$2a + b = 2$$

$$a - 2b_1 + 2b_2 = 1/3$$

$$\frac{a}{12} - \frac{b_1}{3} + b_2 = \frac{1}{60} \quad [3]$$

$$\frac{a}{360} - \frac{b_1}{60} + \frac{b_2}{12} = \frac{1}{2520}$$

On solving [3] we get

$$a = \frac{19}{35}, \quad b = \frac{32}{35}, \quad b_1 = \frac{4}{35}, \quad b_2 = \frac{1}{105} \quad [4]$$

For $m=1$, the values of a , b and b_1 becomes

$$a = \frac{7}{15}, \quad b = \frac{16}{15}, \quad b_1 = \frac{1}{15} \quad [5]$$

For $m=3$, we can determine a , b , b_1 , b_2 and b_3 in exactly the same way as above. For $m=4, 5, 6, \dots$ etc. the same procedure, however a lengthy one, can be followed to determine the constants a , b , b_1 , b_2 , \dots etc.

If these formulae are to be used for several adjacent intervals, the final formula using the values of a , b , b_1 and b_2 in [4] is

$$\begin{aligned} \int_a^b f(x) dx = & (h/35) [19f(x_0) + 32f(x_1) + 38f(x_2) + 32f(x_3) + 38f(x_4) + \dots \\ & + 32f(x_{2n-1}) + 19f(x_{2n})] + (4h^2/35) [f^{(1)}(x_0) - f^{(1)}(x_{2n})] \\ & + (h^3/105) [f^{(2)}(x_0) + 2f^{(2)}(x_1) + 2f^{(2)}(x_4) + \dots + 2f^{(2)}(x_{2n-2}) \\ & + f^{(2)}(x_{2n})] + (h^8) \quad [6] \end{aligned}$$

and that using the value of a , b , and b_1 in [5] is

$$\begin{aligned} \int_a^b f(x) dx = & (h/15) [7f(x_0) + 16f(x_1) + 14f(x_2) + 16f(x_3) + 14f(x_4) + \dots \\ & + 16f(x_{2n-1}) + 7f(x_{2n})] + (h^2/15) [f^{(1)}(x_0) - f^{(1)}(x_{2n})] + 0(h^6) \quad [7] \end{aligned}$$

where $b-a = 2nh$ and $f(x_0)$, $f(x_1)$, $f(x_2)$, \dots , $f(x_{2n})$ denote the ordinates at the points

$$x_0 = a, \quad x_1 (=x_0+h), \quad x_2 (=x_1+h), \quad \dots, \quad x_{2n} (=x_{2n-1}+h) = b$$

As an illustration of the fact that omission of the effect of even order derivatives leads to greater inaccuracy in the results we may notice approximating

$$\int_{x_0-h}^{x_0+h} f(x) dx$$

by

$$h[af(x_0-h) + bf(x_0) + af(x_0+h)] + \sum_{i=1}^m h^{2i} b_{2i-1} [f^{(2i-1)}(x_0-h) - f^{(2i-1)}(x_0+h)] \quad [8]$$

The actual difference between [8] and [1] lies in the absence of terms involving odd degrees of h . The similar series expansion of both sides produces, for $m=2$,

$$a = \frac{31}{63}, \quad b = \frac{64}{63}, \quad b_1 = \frac{5}{63}, \quad b_3 = -\frac{1}{945} \quad [9]$$

For $m=1$, the values of a , b and b_1 remain the same as in [5]. For several adjacent intervals, the final formula from the values of a , b , b_1 and b_3 in [9] is

$$\begin{aligned} \int_a^b f(x) dx &= \frac{h}{63} [31f(x_0) + 64f(x_1) + 62f(x_2) + 64f(x_3) + 62f(x_4) + \dots \\ &+ 64f(x_{2n-1}) + 31f(x_{2n})] + \frac{5}{63} h^2 [f^{(1)}(x_0) - f^{(1)}(x_{2n})] \\ &- \frac{1}{945} h^4 [f^{(3)}(x_0) - f^{(3)}(x_{2n})] + O(h^8) \end{aligned} \quad [10]$$

3. BOUNDS FOR TRUNCATION ERROR

For $m=1$, the truncation error bound determined by using Taylor's series expansion of both sides of [1] and then subtracting right hand side from left hand side is given by

$$E \simeq \left(\frac{2}{7!} - \frac{2}{6!} \cdot \frac{7}{15} + \frac{2}{5!} \cdot \frac{1}{15} \right) h^7 (\xi) f^{(6)}(\xi), \quad x_0 - h \leq \xi \leq x_0 + h$$

For n adjacent intervals

$$E \simeq (b-a) \cdot \frac{1}{360 \times 15} h^6 f^{(6)}(\xi), \quad a \leq \xi \leq b$$

For $m=2$ (formula 6), we give similarly the truncation error bound

$$E \simeq \left(\frac{2}{9!} - \frac{2}{8!} \cdot \frac{19}{35} + \frac{2}{7!} \cdot \frac{4}{35} - \frac{2}{6!} \cdot \frac{1}{105} \right) h^9 f^{(8)}(\xi), \quad x_0 - h \leq \xi \leq x_0 + h$$

For $m=2$ (formula 10), it becomes

$$E \simeq \left(\frac{2}{9!} - \frac{31}{63} \cdot \frac{2}{8!} + \frac{5}{63} \cdot \frac{2}{7!} - \frac{1}{945} \cdot \frac{2}{5!} \right) h^9 f^{(8)}(\xi), \quad x_0 - h \leq \xi \leq x_0 + h$$

4. NUMERICAL EXAMPLES

Calculations are carried out with 8 dit floating point arithmetic and the results are retained correct up to 7 significant figures. Because of the limited computational facility available to us, we could not carry out numerical experiments with higher precision. Rounding error depending on the nature of the integrand thus becomes dominant over the truncation error in most of the examples. These numerical examples, however, can still be noted for a rough comparative study for different end corrections. We have always taken h as .5 only.

Example 1.
$$\int_1^2 (a^2 - x^2)^{3/2} dx$$

<i>a</i>	<i>Simpson</i>	<i>Simpson with end corrections</i>			<i>Exact soln.</i>
		Formula [7]	Formula [6]	Formula [10]	
3	$.1732597 \times 10^2$	$.1732374 \times 10^2$	$.1732376 \times 10^2$	$.1733059 \times 10^2$	$.1732376 \times 10^2$
5	$.1079753 \times 10^3$	$.1079745 \times 10^3$	$.1079745 \times 10^3$	$.1079768 \times 10^3$	$.1079745 \times 10^3$
10	$.9652340 \times 10^3$	$.9652336 \times 10^3$	$.9652336 \times 10^3$	$.9652346 \times 10^3$	$.9652336 \times 10^3$
50	$.1248250 \times 10^6$	$.1248250 \times 10^6$	$.1248250 \times 10^6$	$.1248250 \times 10^6$	$.1248250 \times 10^6$

Example 2.
$$\int_1^2 (x^2 + a^2)^{-1/2} dx$$

<i>a</i>	<i>Simpson</i>	<i>Simpson with end corrections</i>			<i>Exact soln.</i>
		Formula [7]	Formula [6]	Formula [10]	
3	$.2976912 \times 10^0$	$.2976949 \times 10^0$	$.2976950 \times 10^0$	$.2976857 \times 10^0$	$.2976950 \times 10^0$
5	$.1913454 \times 10^0$	$.1913452 \times 10^0$	$.1913452 \times 10^0$	$.1913458 \times 10^0$	$.1913452 \times 10^0$
10	$.9885605 \times 10^{-1}$	$.9885603 \times 10^{-1}$	$.9885603 \times 10^{-1}$	$.9885610 \times 10^{-1}$	$.9885603 \times 10^{-1}$
50	$.1999067 \times 10^{-1}$	$.1999067 \times 10^{-1}$	$.1999067 \times 10^{-1}$	$.1999067 \times 10^{-1}$	$.1999068 \times 10^{-1}$

Example 3.
$$\int_1^2 x^3 e^{ax} dx$$

<i>a</i>	<i>Simpson</i>	<i>Simpson with end corrections</i>			<i>Exact soln.</i>
		Formula [7]	Formula [6]	Formula [10]	
3	$.7437912 \times 10^3$	$.6797358 \times 10^3$	$.6845516 \times 10^3$	$.9431624 \times 10^3$	$.6843475 \times 10^3$
5	$.3346145 \times 10^5$	$.2533536 \times 10^5$	$.2668410 \times 10^5$	$.7233888 \times 10^5$	$.2655516 \times 10^5$
10	$.6542460 \times 10^9$	$.1676159 \times 10^9$	$.3908840 \times 10^9$	$.6218249 \times 10^{10}$	$.3354416 \times 10^9$

Example 4. $\int_1^2 \sin hx \, dx$

Simpson	Simpson with end corrections			Exact soln.
	Formula [7]	Formula [6]	Formula [10]	
$.2219863 \times 10^4$	$.2219111 \times 10^4$	$.2219115 \times 10^4$	$.2221317 \times 10^4$	$.2219115 \times 10^4$

Example 5. $\int_1^2 e^{-x} \, dx$

Simpson	Simpson with end corrections			Exact soln.
	Formula [7]	Formula [6]	Formula [10]	
$.2326226 \times 10^0$	$.2325438 \times 10^0$	$.2325442 \times 10^0$	$.2327749 \times 10^0$	$.2325442 \times 10^0$

It can be roughly noted that in all the above examples Formula [6] produces the best results of all. Formula [10], however, becomes worse than even Simpson's rule, thereby warning us to be very careful in developing high order method. Example 3 indicates the rounding error as a very dominant factor over the truncation error because of the use of low precision of 8 dit. Example 1, on the other hand, shows the stability for larger a . This is because of the fact that the variation in the value of the integrand over the specified interval is very small for greater a .

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