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ON ESTIMATES OF ERROR IN NUMERICAL INTEGRATION

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INTRODUCTION

In order to determine numerical approximations for definite integrals, the principal methods used are the trapezoidal rule and Simpson's rule. In this paper, upper bounds are established for the errors obtained by these two methods. The error resulting from use of the trapezoidal rule is expressed in terms of the second derivative of the integrand, and that incurred in Simpson's rule is expressed in terms of the fourth derivative. A difference formula, analogous to Taylor's formula with remainder, is established. This relation is then used to derive expressions for the errors in terms of second and fourth differences respectively.

ERROR IN TERMS OF DERIVATIVES

The procedure is based on the Fundamental Theorem of the integral calculus. Let a subdivision of the interval from $x = a$ to $x = b$ into n parts be given by the points $a = x_o, x_1, \ldots, x_n = b$, with $x_{i+1} - x_i = 2\delta$. The midpoint of the subinterval from x_i to x_{i+1} is designated by $\bar{x}_i$. From the formula $f(x) = f(\bar{x}_i) + (x-\bar{x}_i)f'(\bar{x}_i) + \frac{(x-\bar{x}_i)^2 f''(\xi)}{2!}$ with ξ between x and $\bar{x}_i$, it follows that

$$\int_{x_i}^{x_{i+1}} f(x)dx = [f(\bar{x}_i)]\ 2\delta + E_1, \text{ with } E_1 \leq \frac{\delta^3}{3} \text{Max } |f''(x)|.$$

For one subdivision, the approximate area, A, as defined by the trapezoidal rule is

$$A = \frac{1}{2}\ [f(x_i) + f(x_{i+1})]\ 2\delta. \tag{1.1}$$

Hence A is given by this rule as

$$A = [f(\bar{x}_i)]\ 2\delta + E_2, \text{ where } E_2 \leq \delta^3 \text{ Max } |f''(x)|. \tag{1.2}$$

From (1.1) and (1.2) it follows that, in one subdivision, the actual error of the trapezoidal rule satisfies the inequality

$$E \leq E_1 + E_2 = \frac{4}{3}\ \delta^3 \text{Max } |f''(x)|. \tag{1.3}$$

But $2\delta = w$, the width of one subdivision, so that $\delta = \frac{w}{2}$. Hence

$$E \leq \frac{1}{6}\ w^3 \text{Max } |f''(x)|. \tag{1.4}$$

Then, for n subdivisions, the total error obtained in the trapezoidal rule is

$$\frac{E_t \leq n\ w^3 \text{Max } |f''(x)|}{6}\ , \tag{1.5}$$

and since $nw = b-a$

$$\frac{E_t \leq (b-a)\ w^2 \text{Max } |f''(x)|}{6} \tag{1.6}$$

The error resulting from Simpson's Rule can be lumped into an expression containing the fourth derivative. Developing the expansion of f(x) for two more terms, the result is

$$f(x) = f(\bar{x}_i) + (x-\bar{x}_i)f'(\bar{x}_i) + \frac{(x-\bar{x}_i)^2 f''(\bar{x}_i)}{2!} + \frac{(x-\bar{x}_i)^3 f'''(\bar{x}_i)}{3!} + \frac{(x-\bar{x}_i)^4 f^{IV}(\bar{x})}{4!}$$

with $\bar{x}$ between x and $\bar{x}_i$.

For the two subdivisions from x_{i-1} to x_i and from x_i to x_{i+1}, we have

$$\int_{x_{i-1}}^{x_{i+1}} f(x)\,dx = [f(\bar{x}_i)]\ 4\delta + \frac{8\delta^3 f''(\bar{x}_i)}{3} + E_3\ , \qquad (2.1)$$

where $$E_3 \leq \frac{8\ \delta^5}{15}\ \text{Max}\ |f^{IV}(x)|.$$

In these two subdivisions, A, as defined by Simpson's rule is

$$A = \frac{2\delta}{3}\,[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})]$$

$$= \frac{2\delta}{3}\,[f(\bar{x}_i - 2\delta) + 4f(\bar{x}_i) + f(\bar{x}_i + 2\delta)]\ ,\ \text{and since}$$

$$[f(\bar{x}_i - 2\delta) + 4f(\bar{x}_i) + f(\bar{x}_i + 2\delta)] = 6f(\bar{x}_i) + \frac{8\delta^2}{2!}f''(\bar{x}_i) + \frac{16\delta^4}{4!}\,[f^{IV}(\bar{x}_i + \theta_1 2\delta) + f^{IV}(\bar{x}_i - \theta_2 2\delta)]$$

$$0 < \theta_1 < 1,\ \ 0 < \theta_2 < 1,$$

the value for A is

$$A = 4\delta\ [f(\bar{x}_i)] + \frac{8}{3}\,\delta^3\ f''(\bar{x}_i) + E_4 \qquad (2.2)$$

with $$E_4 \leq \frac{8}{9}\ \delta^5\ \text{Max}\ |f^{IV}(x)|.$$

From (2.1) and (2.2) it follows that an upper bound for the actual error in Simpson's rule for the two subdivisions is given by

$$E \leq E_3 + E_4 = \frac{64}{45}\ \delta^5 \text{Max}\ |f^{IV}(x)|. \qquad (2.3)$$

Hence, when expressed in terms of w, $E \leq \frac{2}{45}\,w^5 \text{Max}\ |f^{IV}(x)|.$ (2.4)

For the entire interval, the error in Simpson's rule is then bounded as follows:

$$E_s \leq \frac{2}{45}\,w^5 \text{Max}\ |f^{IV}(x)|\,\frac{n}{2}\ ,\ \text{and, as } nw = b-a,$$

$$E_s \leq \frac{(b-a)\,w^4 \text{Max}\ |f^{IV}(x)|}{45} \qquad (2.5)$$

Thus E_t and E_s give upper bounds in terms of derivatives for the trapezoidal rule and Simpson's rule respectively.

DIFFERENCE INTERPOLATION FORMULA WITH REMAINDER

When it is difficult to obtain the derivatives of the integrand, Taylor's Formula with remainder may be replaced by a difference interpolation formula with remainder. An expression for the remainder after one term (Mean Value Theorem for differences) for the difference interpolation formula will be extablished. Likewise, an expression for the remainder after two terms will be determined.

THEOREM. If the function $f(x)$ is continuous in the interval $a \leq x \leq a+p\delta$, then with each value of x in that interval there is associated a value η satisfying $|\eta| \leq |p|$ such that

$$f(a+p\delta) = f(a) + p\,\Delta\,f(a) + \frac{p(p-1)}{2!}\,\Delta^2 f(a) + \ .\ .\ .\ + \frac{p(p-1)\ .\ .\ .(p-n+1)}{n!}\,\Delta^n f(a+\eta\delta).$$

PROOF. The following equations are valid:

$$f(a+p\delta) - f(a) = \sum_{n=1}^{p} \{f(a+n\delta) - f\,[a+(n-1)\delta]\}$$

$$= \sum_{n=1}^{p} \{\Delta f\,[a+(n-1)\delta]\}\ .$$

The continuity of $f(x)$ implies the continuity of $\Delta f(x)$. Therefore, the last summation over p terms may be replaced by the expression $p\Delta f(\bar{x})$, with $a\leq\bar{x}\leq a+p\delta$. This relationship can also be expressed as

$$f(a+p\delta) = f(a) + p\,[f(\bar{x}+\delta) - f(\bar{x})]\ ,$$

which is designated as the Mean Value Theorem for differences.

COROLLARY. If $f(a+p\delta) = f(a) = 0$, then $f(\bar{x}+\delta) = f(\bar{x})$, where $\bar{x}$ is some intermediary x.

Consider now the quantity K defined by the equation

$$f(a+p\delta) = f(a) + p\Delta f(a) + \frac{p(p-1)}{2!}K.$$

If $a + p\delta = b$, the equation takes the form

$$f(b) - f(a) - \frac{b-a}{\delta}\Delta f(a)\left(\frac{b-a}{\delta}\right)\frac{\left(\frac{b\ a}{\delta} - 1\right)}{2!}\ K = 0$$

Define $F(x)$ as follows:

$$F(x) = f(b) - f(x) -\left(\frac{b-x}{\delta}\right)\Delta f(x) -\left(\frac{b-x}{\delta}\right)\frac{\left(\frac{b-x}{\delta} -1\right)}{2!}K\ .$$

Then $F(a)$ and $F(b)$ are both zero. But by the above corollary there exists a value $\bar{x}$ between A and B for which $\Delta F(\bar{x})$ vanishes.

When $F(x)$ is evaluated at $(x+\delta)$ and the difference $F(\bar{x}+\delta) - F(\bar{x})$ determined and simplified, the result is

$$\Delta F(\bar{x}) = \Delta^2 f(\bar{x})\ [1 - \frac{b-\bar{x}}{\delta}] - [1 - \frac{b-\bar{x}}{\delta}]\,K = 0.$$

Solving for K we obtain

$$K = \Delta^2 f(\bar{x}),\ \text{with}\ a \leq\bar{x}\leq b = a+p\delta.$$

The general result for a remainder after n terms can be established by analogous reasoning.

ERRORS IN TERMS OF DIFFERENCES

The difference interpolation formula with remainder in the second difference is

$$f(\bar{x}_i+\xi\delta) = f(\bar{x}_i)+\xi\Delta\ f(\bar{x}_i)+\frac{\xi(\xi-1)}{2!}\ \Delta^2 f(\bar{x}_i+\eta\delta)\ ,\ 0\leq\eta\leq\xi\ . \qquad (3.1)$$

Let $x = (\bar{x}_i+\xi\delta)$. Then

$$\int_{x_i-\delta}^{x_i+\delta} f(x)dx = \int_{-1}^{1} f(\bar{x}_i+\xi\delta)\,\delta d\xi = 2\delta f(\bar{x}_i) + E_1'\ ,\ \text{with}\ E_1' \leq\frac{\delta}{3}\ \text{Max}\,|\Delta^2 f| \qquad (3.2)$$

For the trapezoidal rule

$$A = \frac{1}{2}\,[f(x_i) + f(x_{i+1})]\ 2\delta\ \text{takes the form}$$

$$A = \frac{1}{2}\,[f(\bar{x}_i) -\Delta_1+ f(\bar{x}_i)+\Delta_2]\ 2\delta,\ \text{where}\ \Delta_1 = \Delta f(x_i) = \Delta\ f(\bar{x}_i-\delta)$$
$$\text{and}\ \Delta_2 = \Delta f(\bar{x}_i) \qquad (3.3)$$

Simplifying, we obtain

$$A = 2\delta\ f(\bar{x}_i) + E_2'\ \ \text{with}\ E_2'\leq\ \delta\ \text{Max}\ |\Delta^2 f|. \qquad (3.4)$$

Thus the error in one subdivision in terms of differences for the trapezoidal rule can be expressed by the inequality

$$E'\leq E_1' + E_2'$$
$$\leq\frac{4}{3}\delta\ \text{Max}\ |\Delta^2 F|\ = \frac{2}{3}\,w\ \text{Max}\ |\Delta^2 F|\ . \qquad (3.5)$$

For n subdivisions, the resulting total error in the trapezoidal rule is then

$$E_t' \leq \frac{2}{3} nw \text{ Max} |\Delta^2 F| \text{ , so that}$$

$$E_t' \leq \frac{2}{3}(b-a) \text{ Max} |\Delta^2 F|. \qquad (3.6)$$

For Simpson's Rule the error can be expressed in terms of a fourth difference. When the difference interpolation formula with remainder is developed through two more terms, the result is

$$f(\bar{x}_i+\xi\delta) = f(\bar{x}_i)+\xi\Delta f(\bar{x}_i)+ \frac{\xi(\xi-1)}{2!} \Delta^2 f(\bar{x}_i)+\frac{\xi(\xi-1)(\xi-2)}{3!}\Delta^3 f(\bar{x}_i)+$$

$$+\frac{\xi(\xi-1)(\xi-2)(\xi-3)\ \Delta^4 f(\bar{x}_i+\eta\delta)}{4!} \text{ where } 0 \leq\eta\leq\xi \cdot \qquad (4.1)$$

Therefore

$$\int_{\bar{x}_i-2\delta}^{\bar{x}_i+2\delta} f(x)dx = \int_{-2}^{2} f(\bar{x}_i+\xi\delta)\delta d\xi = 4\delta f(\bar{x}_i)+\frac{8}{3}\delta\Delta^2 f(\bar{x}_i)-\frac{8}{3}\delta\Delta^3 f(\bar{x}_i) + E_3' \qquad (4.2)$$

$$\text{where } E_3' \leq \frac{134}{45}\delta \text{ Max } |\Delta^4 f| \text{ .}$$

For Simpson's Rule

$$A = \frac{2}{3}\delta\ [f(\bar{x}_i-2\delta) + 4f(\bar{x}_i) + f(\bar{x}_i+2\delta)] \text{ becomes}$$

$$A = \frac{2}{3}\delta\ \{[f(\bar{x}_i) -\Delta_1 -\Delta_2] + 4f(\bar{x}_i) + [f(\bar{x}_i) + \Delta_3 + \Delta_4]\}, \ (4.3)$$

$$\text{where } \Delta_n = f[\bar{x}_i+(n-2)\delta] - f[\bar{x}_i+(n-3)\delta] \text{ , } n = 1,\ 2,\ 3,\ 4.$$

Since

$$\Delta_4 = \Delta_3 + \Delta_3^2$$

$$\Delta_2 = \Delta_3 - \Delta_3^2 + \Delta_3^3 - \Delta_2^4$$

$$\Delta_1 = \Delta_3 - 2\Delta_3^2 + 3\Delta_3^3 - 3\Delta_2^4 - \Delta_1^4$$

$$A = 4\delta\ f(\bar{x}_i) + \frac{8}{3}\delta\ \Delta_3^2 - \frac{8}{3}\delta\ \Delta_3^3 + E_4' \qquad (4.4)$$

$$\text{where } E_4' \leq \frac{10}{3}\delta \text{ Max } |\Delta^4 f|.$$

Then, for the two subdivisions, the upper bound for the error in Simpson's Rule satisfies the following relations:

$$E' \leq E_3' + E_4' \text{ or}$$

$$E' \leq \frac{284}{45}\ \delta \text{ Max } |\Delta^4 f| = \frac{142}{45} \text{ w Max } |\Delta^4 f|. \qquad (4.5)$$

We obtain finally, for the entire range $a \leq x \leq b$

$$E_s' \leq \frac{142}{45}\left(\frac{n}{2}\right) \text{w Max } |\Delta^4 f| \text{ or}$$

$$E_s' \leq \frac{71}{45}(b-a) \text{ Max } |\Delta^4 f|. \qquad (4.6)$$

These two results for E_t' (3.6) and E_s' (4.6) establish, in terms of differences, upper bounds for the errors in the trapezoidal rule and Simpson's rule respectively.