

A Note on Clamped Simpson's Rule

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Abstract

In this paper we are writing a note on A Clamped Simpson's Rule. In this Method we are using the nodes of Quadrature Method of uniform points. Also we develop the composite formula and we estimated errors.

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1.INTRODUCTION

With the advent of the modern high speed electronic digital computer, the Numerical Integration has been successfully applied to study problems in Mathematics, Engineering, Computer Science and Physical Science. Numerical integration is the study of, how the approximate numerical value of a definite integral can be found. It is helpful for the following cases:

- Many integrals can't be evaluated analytically or don't possess a closed form solution.
- Closed form solution exists, but numerical evaluation of the answer can be bothersome.
- The integrand $f(x)$ is not known explicitly, but a set of data points is given for this integrand.
- The integrand $f(x)$ may be known only at certain points, which are obtained by sampling.

Numerical integration of a function of a single variable is called Quadrature, which represents the area under the curve $f(x)$ bounded by the ordinates x_0 , x_n and x-axis. The numerical integration of a multiple integral is sometimes described as

Cubature. Numerical integration problems go back at least to Greek antiquity when e.g. the area of a circle was obtained by successively increasing the number of sides of an inscribed polygon. In the seventeenth century, the invention of calculus originated a new development of the subject leading to the basic numerical integration rules. In the following centuries, the field became more sophisticated and, with the introduction of computers in the recent past, many classical and new algorithms have been implemented leading to very fast and accurate results. An extensive research work has already been done by many researchers in the field of numerical integration. M. Concepcion Ausin[1] compared different numerical integration procedures and discussed about more advanced numerical integration procedures. Gordon K. Smith[2] gave an analytic analysis on numerical integration and provided a reference list of 33 articles and books dealing with that topic. Rajesh Kumar Sinha[3] worked to evaluate an integrable polynomial discarding Taylor Series. Gerry Sozio[4] analyzed a detailed summary of various techniques of numerical integration. J. Oliver[5] discussed the various processes of evaluation of definite integrals using higher-order formulae. Moreover, every numerical analysis book contains a chapter on numerical integration. The formulae of numerical integrations are described in the books of S.S. Sastry[6], R.L. Burden[7], J.H. Mathews[8] and many other authors.

The purpose of this paper is to apply quadrature methods for approximate calculation of definite integrals

$$I = \int_a^b f(x)dx \quad (1)$$

where $f(x)$ is integrable, in the Riemann sense on $[a, b]$. The limit of the integration may be finite. Numerical integration is always carried out by mechanical quadrature and its basic scheme is as follows:

$$I = \int_a^b f(x)dx = \sum_{i=0}^{n-1} A_i f_i \quad (2)$$

where $f_i = f(x_i)$, $A_i > 0$, $i = 0, 1, 2, \dots, n-1$ and $x_i \in [a, b]$ $i = 0, 1, 2, \dots, n-1$. are called **Coefficients(Weights)** and **Nodes** for Numerical Quadrature, respectively. Once the coefficients and nodes are set down, the scheme (1) can be determined.

2. PRELIMINARIES

2.1 Order of Numerical Integration

Order of accuracy, or precision of a Quadrature formula is the largest positive integer n such that the formula is exact for x^k , for each $k = 0, 1, \dots, n$.

2.2 Definitions

The Integration (1) is approximated by a finite linear combination of value of $f(x)$ in the form (2). The error of approximation of (2) is given as

$$R_n = \frac{C}{(m+1)!} f^{(m+1)}(\xi), \tag{3}$$

where $\xi \in (a, b)$, $m \geq n$ is order of (2) and error constant of (2) is

$$C = \int_0^1 x^{m+1} dx - \sum_{i=0}^{n-1} A_i x_i^{m+1} \tag{4}$$

2.3 Open or Closed type Integration Method

The Quadrature method (2) of (1) is called Open Type method if the nodes $x_i \in (a, b)$, $\forall i = 0, 1, \dots, n - 1$. and is called Closed Type method if the nodes $x_0 = a$, and $x_{n-1} = b$.

3. MODIFYING SIMPSON'S RULE

Simpson's rule is treated in almost any text on numerical analysis. To approximate the area under a given curve $f(x)$ in a subinterval $[x_0, x_2]$ (composed of the two "panels" $[x_0, x_1]$ and $[x_1, x_2]$, each of width h), one constructs a quadratic polynomial $p(x)$ which fits three constraints:

These three constraints define a unique parabola $p(x)$, and $\int_{x_0}^{x_2} p(x) dx$ approximates $\int_{x_0}^{x_2} f(x) dx$. For a wide interval of integration, several parabolas may be placed end-to-end in continuous subintervals, resulting in the composite Simpson's rule with error term (see, for example, [5], p. 253). For $f(x)$ having a continuous fourth derivative $f^{(4)}(x)$ over $[x_0, x_{2m}]$:

$$\int_{x_0}^{x_{2m}} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + \dots + 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m})] - \frac{1}{180} (x_{2m} - x_0) h^4 f^{(4)}(\mu)$$

for some $\mu \in (x_0, x_{2m})$. As the number of subintervals increases the size of h decreases; this decrease in h , the error dramatically since the error is proportional to h^4 .

We now proceed to modify Simpson's rule; the coefficients are altered, derivative terms are added, and-most importantly-the error term is improved. Our method is analogous to the trapezoidal rule with endpoint correction ([6], page no.321). Note, however, that the modified Simpson's method cannot be viewed correction of Simpson's rule based on its error term, whereas the trapezoidal with endpoint correction stems naturally from an estimate of the error trapezoidal rule. Suppose we construct a polynomial $q(x)$ by imposing the three constraints Simpson's rule plus two additional constraints:

$$q(x_0) = f(x_0), \quad q(x_1) = f(x_1), \quad q(x_2) = f(x_2), \quad q^{(1)}(x_0) = f^{(1)}(x_0),$$

$$q^{(1)}(x_2) = f^{(1)}(x_2).$$

The two derivative constraints "clamp" the approximating polynomial $q(x)$ to $f(x)$ at the endpoints x_0 and x_2 . As we shall see below, these five constraints can be used to define a quartic polynomial which, expanded about the midpoint of the subinterval, has the form

$$q(x) = a_4(x - x_1 + 1)^4 + a_3(x - x_1 + 1)^3 + a_2(x - x_1 + 1)^2 + a_1(x - x_1 + 1) + a_0$$

using $x_1 + 0 - x_0 = h = x_2 - x_1$ and

$$\int_{x_0}^{x_2} q(x) dx = \frac{2a_4h^4}{5} + \frac{2a_2h^3}{3} + 2a_0h$$

Note that a_1 and a_3 do not enter into this formula; $(x - x_1)$ and $(x - x_1)^3$ integrate to 0 because they have odd symmetry in the interval of integration. To determine $a_0, a_2,$ and $a_4,$ first differentiate $q(x)$ to get

$$q^{(1)}(x) = 4a_4(x - x_1 + 1)^3 + 3a_3(x - x_1 + 1)^2 + 2a_2(x - x_1 + 1) + a_1,$$

and then invoke the five constraints

$$f(x_0) = q(x_0) = h^4a_4 - h^3a_3 + h^2a_2 - ha_1 + a_0$$

$$f(x_1) = q(x_1) = a_0$$

$$f(x_2) = q(x_2) = h^4a_4 + h^3a_3 + h^2a_2 + ha_1 + a_0$$

$$f^{(1)}(x_0) = q^{(1)}(x_0) = -4h^3a_4 + 3h^2a_3 - 2ha_2 + a_1$$

$$f^{(1)}(x_2) = q^{(1)}(x_2) = 4h^3a_4 + 3h^2a_3 + 2ha_2 + a_1$$

Solving these five equations for $a_0, a_2,$ and a_4 gives

$$a_0 = f(x_1)$$

$$a_2 = \frac{f^{(1)}(x_0) - f^{(1)}(x_2)}{4h} + \frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2}$$

$$a_4 = \frac{f^{(1)}(x_0) - f^{(1)}(x_2)}{4h^3} - \frac{f(x_0) - 2f(x_1) + f(x_2)}{2h^2}$$

Substituting these expressions of a_0, a_2 and a_4 yields

$$\int_{x_0}^{x_2} q(x) dx = \frac{h}{15} [7f(x_0) + 16f(x_1) + 7f(x_2) + h[f^{(1)}(x_0) - f^{(1)}(x_2)]]$$

To compute the composite rule for m continuous subintervals containing m panels we find $q_i(x)$ as above for $q(x)$ but over each subinterval $[x_{2i-2}, x_{2i}]$ for $i = 0, 1, \dots, m$. When the integrals of the $q_i(x)$ over the subintervals are summed, the derivative terms in the subintervals nicely cancel out pairwise except for the first and last, and we obtain

$$\int_{x_0}^{x_{2m}} f(x)dx = \int_{x_0}^{x_2} q_1(x)dx + \int_{x_2}^{x_4} q_2(x)dx + \dots + \int_{x_{2m-2}}^{x_{2m}} q_m(x)dx$$

Note the similarity of this composite rule and Simpson's rule. The only differences are in the coefficients and in the two new derivative terms.

4.EMPIRICAL TESTING

These seemingly minor differences in the formulas lead to fairly major differences in performance. Extensive empirical testing of the "clamped Simpson's rule" and Simpson's rule, a small portion of which is listed here, highlights the advantages of each method. In the examples below, the "Exact Clamped Rule" uses an explicit expression for derivative evaluations, whereas the "Approximate Clamped Rule" uses $[f(x + h) - f(x - h)]/2h$ with $h = 10^{-6}$ to approximate the derivatives. Times, shown in sixtieths of seconds, were calculated by running the integration procedure one hundred times (using Macintosh? Pascal) and dividing the elapsed time on the system clock by one hundred. Errors are the exact integral minus the approximation; m is the number of subintervals used to approximate the integral ($2m$ is the number of panels).

Example 1. Evaluate $\int_2^4 \frac{1}{x} dx$

m	Exact Clamped Rule	Simpson's Rule
2	2.34e-6	-1.07e-4
4	4.41e-8	-7.35e-6
8	7.30e-10	-4.72e-7
16	1.16e-11	-2.97e-8

Example 2. Evaluate $\int_1^5 \ln(x)$

m	Exact Clamped Rule	Simpsons Rule
2	-6.57e-4	5.71e-3
4	-2.24e-5	5.35e-4
8	-5.10e-7	3.98e-5
16	-9.16e-9	2.63e-6

Example 3. Evaluate $\int_0^1 e^{-x^2} dx$

m	Exact Clamped Rule	Simpson's Rule
2	1.17e-7	-3.12e-5
4	1.33e-9	-1.99e-6
8	1.91e-11	-1.25e-7
16	2.92e-11	-7.79e-9

The above data give a rough feel for where Simpson's rule is advantageous to the clamped rule (and vice versa) with respect to the time required to achieve a certain accuracy. For example, for $f(x) = 1/x$, the "Approximate Clamped Rule" with $m = 2$ has absolute error and evaluation times roughly equal to Simpson's rule with $m = 4$. The "Approximate Clamped Rule" is more time-efficient at decreasing error beyond this magnitude (if higher accuracy is needed) because the clamped rule converges faster than Simpson's rule; however, Simpson's rule is more time-efficient for computing integrals with an error greater than this magnitude (if only low accuracy is needed) because there is no need for the derivative computations.

5.ERROR ESTIMATE

Let us now examine the error of $\int q(x)dx$ in approximating $\int f(x)dx$. This examination, making use of many key results of calculus, will establish the following:

Theorem:- If $f^{(6)}(x)$ is continuous on $[x_0, x_{2m}]$, then for some $v \in (x_0, x_{2m})$

$$\int_{x_0}^{x_{2m}} f(x)dx = \frac{h}{15} [7f(x_0) + 16f(x_1) + 14f(x_2) + 16f(x_3) + \dots + 16f(x_{2m-1}) + 7f(x_{2m}) + h[f^{(1)}(x_0) - f^{(1)}(x_{2m})] - \frac{1}{9450} (x_{2m} - x_0)h^6 f^{(6)}(v)]$$

To determine the error, we first take a slight detour by constructing a fifth degree polynomial

$$t(x) = q(x) + k(x - x_0)^2(x - x_1)(x - x_2)^2$$

which has the same integral as our previously defined quartic $q(x)$ but which permits us to calculate much sharper error estimates. Since $(x - x_0)^2(x - x_2)^2$ is an even function expanded about x_1 and $(x - x_1)$ is an odd function expanded about x_1 the product of these functions is odd with respect to the midpoint of the subinterval, and so its integral over $[x_0, x_2]$ is zero. Thus, an estimate of the error $\int f(x)dx - \int t(x)dx$ will also be an estimate of the error $\int f(x)dx - \int q(x)dx$.

The quintic $t(x)$ has derivative

$$t^{(1)}(x) = q^{(1)}(x) + k[2(x - x_0)(x - x_1)(x - x_2)^2 + (x - x_0)(x - x_2)^2 + 2(x - x_0)^2(x - x_1)(x - x_2)]$$

Observe that $t(x)$ satisfies all the constraints on $q(x)$:

$$t(x_i) = q(x_i) = f(x_i) \text{ for } i=0,1,2$$

$$t^{(1)}(x_i) = q^{(1)}(x_i) = f^{(1)}(x_i) \text{ for } i=0,2$$

In addition, we can choose $k = (f^{(1)}(x_1) - q^{(1)}(x_1))/h^4$ so as to further "clamp" $t(x)$ to satisfy (see figure)

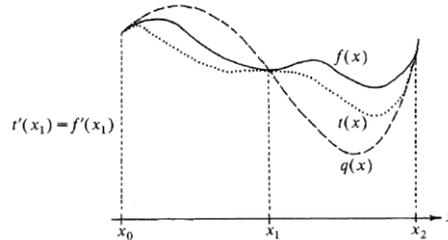


Figure 1: -

We now proceed to determine an estimate of the error $\int f(x)dx - \int t(x)dx$. Suppose α is some fixed value in $[x_0, x_2]$. To estimate the error, we seek to construct a polynomial which will give us the difference between $f(\alpha)$ and $t(\alpha)$ (in a convenient form). Any sixth degree polynomial of the form

$$g(x) = t(x) + c(x - x_0)^2(x - x_1)^2(x - x_2)^2$$

will fit the six constraints on $t(x)$, no matter what the value of the constant c . Moreover, for our $\alpha \in [x_0, x_2]$, it is possible to choose $c = c_\alpha$ so that $g(x)$ satisfies the additional constraint

$$g(\alpha) = f(\alpha)$$

(The subscript on α indicates that c is dependent on the choice of α) Thus, at this particular value α

$$f(\alpha) - t(\alpha) = c_\alpha(\alpha - x_0)^2(\alpha - x_1)^2(\alpha - x_2)^2$$

Now, we must find a suitable expression for c_α . Suppose $f^{(6)}(x)$ is continuous on $[x_0, x_2]$; the sixth degree polynomial $g(x)$ is obviously six times differentiable. Let $h(x) = f(x) - g(x)$. Then the seven constraints on $g(x)$ may be written

$$f(x_i) = g(x_i) \Leftrightarrow h(x_i) = 0$$

$$f(\alpha) = g(\alpha) \Leftrightarrow h(\alpha) = 0$$

$$f^{(1)}(x_i) = g^{(1)}(x_i) \Leftrightarrow h^{(1)}(x_i) = 0$$

for $i = 0, 1, 2$. Suppose, without loss of generality, that $x_0 < \alpha < x_1$. Then remark successively

$$h^{(1)}(\beta_1) = 0 \text{ for some } \beta_1 \in (x_0, \alpha)$$

$$h^{(1)}(\beta_2) = 0 \text{ for some } \beta_2 \in (\alpha, x_1)$$

$$h^{(1)}(\beta_3) = 0 \text{ for some } \beta_3 \in (x_1, x_2)$$

Since $x_0, \beta, \beta_2, \beta_3, x_1$ and x_2 are six distinct points, we can invoke the following theorem ([7], p. 6) to reduce our six constraints to a single more useful constraint.

The Generalized Rolle's Theorem. Suppose $f(x)$ is continuous on $[a, b]$ and n times differentiable on (a, b) , and vanishes at $n + 1$ distinct numbers in $[a, b]$. then $f^{(n)}(c) = 0$ for some $c \in (a, b)$ Applying this theorem to the function $h'(x)$ which vanishes at $x_0, \beta_1, \beta_2, \beta_3, x_1$ and x_2 in $[x_0, x_2]$, we have

$$h^{(6)}(\gamma) = 0$$

for some $\gamma \in (x_0, x_2)$.

$$0 = h^{(6)}(\gamma) = f^{(6)}(\gamma) - g^{(6)}(\gamma),$$

and $g(x)$ is a sixth degree polynomial with leading coefficient c_α , we see that

$$f^{(6)}(\gamma) = 720c_\alpha.$$

Substituting the expression for c_α into equation (6) yields

$$f(\alpha) - t(\alpha) = \frac{f^{(6)}(\gamma)}{720} (\alpha - x_0)^2 (\alpha - x_1)^2 (\alpha - x_2)^2$$

Thus, the error in approximating $\int f(x)dx$ by $\int t(x)dx$ using one subinterval is

$$\begin{aligned} E_{t,1} &= \int_{x_0}^{x_2} [f(\alpha) - t(\alpha)]d\alpha \\ &= \int_{x_0}^{x_2} \frac{f^{(6)}(\gamma)}{720} (\alpha - x_0)^2 (\alpha - x_1)^2 (\alpha - x_2)^2 d\alpha \end{aligned}$$

Since $f^{(6)}(\gamma)$ depends on $\alpha \in [x_0, x_2]$, it cannot be taken outside the integral as a constant. However, $f^{(6)}(x)$ is continuous on $[x_0, x_2]$, and so

$$\min_{[x_0, x_2]} f^{(6)}(x) \leq f^{(6)}(\gamma) \leq \max_{[x_0, x_2]} f^{(6)}(x)$$

therefore,

$$\begin{aligned} &\min_{[x_0, x_2]} \int_{x_0}^{x_2} \frac{f^{(6)}(\gamma)}{720} (\alpha - x_0)^2 (\alpha - x_1)^2 (\alpha - x_2)^2 d\alpha \\ &\leq E_{t,1} \leq \max_{[x_0, x_2]} \int_{x_0}^{x_2} \frac{f^{(6)}(\gamma)}{720} (\alpha - x_0)^2 (\alpha - x_1)^2 (\alpha - x_2)^2 d\alpha \end{aligned}$$

Accordingly, by the intermediate Value theorem

$$E_{t,1} = \frac{f^{(6)}(\delta)}{720} \int_{x_0}^{x_2} (\alpha - x_0)^2 (\alpha - x_1)^2 (\alpha - x_2)^2 d\alpha$$

for some $\delta \in (x_0, x_2)$. Integrating the sixth degree polynomial yields

$$E_{t,1} = \frac{h^7 f^{(6)}(\delta)}{4725}$$

This error estimate, that we computed for the fifth degree polynomial $t(x)$ is , as previously noted, also an error estimate for the fourth degree polynomial $q(x)$ that we are investigating.

The global error arising from replacing $f(x)$ by $q_i(x)$ over m subintervals ($i = 1, 2, \dots, m$) is

$$E_{q,m} = \frac{h^7}{4725} [\sum_{i=1}^m f^{(6)}(\delta_i)],$$

where each $\delta_i \in (x_{2i-2}, x_{2i})$ for $i = 1, 2, 3, \dots, m$. Since $f^{(6)}(x)$ is assumed continuous for $x \in (x_0, x_{2m})$,

$$\min_{[x_0, x_{2m}]} f^{(6)}(x) \leq f^{(6)}(\delta_i) \leq \max_{[x_0, x_{2m}]} f^{(6)}(x).$$

Thus

$$\min_{[x_0, x_{2m}]} f^{(6)}(x) \leq \frac{1}{m} \sum_{i=1}^m f^{(6)}(\delta_i) \leq \max_{[x_0, x_{2m}]} f^{(6)}(x).$$

and by the Intermediate Value Theorem

$$E_{q,m} = \frac{mh^6 f^{(6)}(\eta)}{4725}$$

for some $\eta \in (x_0, x_{2m})$, since $\frac{1}{m} \sum f^{(6)}(\delta_i) = f^{(6)}(\eta)$ and this completes the proof of the theorem.

6 CONCLUSIONS

- 1). The clamped rule is exact for polynomials of degree five or less, whereas Simpson's rule gives the exact value of the integral for polynomials of degree three or less.
- 2). As h decreases, the clamped rule yields more rapid convergence than does Simpson's rule since errors are proportional to h^6 , rather than h^4 as in Simpson's rule.
- 3). Very few extra computations are required to achieve this improvement in convergence rate; the implementation of the clamped rule is identical to that of Simpson's rule except that two additional derivative computations are required (independent of the number of subintervals).
- 4). The necessity for derivative computations may make the clamped rule inaccurate or inconvenient for use with experimental or tabulated data.
- 5). If the function to be integrated must be differentiated by numerical methods, care must be taken to avoid the possibility of relatively large errors which are likely to arise in the "unstable" process of numerical differentiation.

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