

Modified Results in Adaptive Quadrature Method for the Approximations of Integrals

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Abstract

This paper investigates the role of higher order Newton - Cotes closed quadrature formula in the adaptive quadrature method for approximating integrals. Boole's rule was specifically adopted as a result of its exceptional accuracy, and this was brought to bear in the numerical experiments that followed the derivation of error estimation scheme. The error estimation scheme facilitates the suitability of the method reported in this paper for situations where the exact solution is extremely difficult to arrive at.

Key Words: Error Estimate, Newton - Cotes, Quadrature, Interpolation. Boole

1.0 Introduction

The concept of error estimation is an important concept in numerical analysis, as it avails the opportunity of knowing the error embedded in any particular numerical scheme of interest. The concept is very important as it is useful when the exact solution is known as well as when it is unknown. All other error techniques require the knowledge of the exact solution, since they will involve taking the difference between the analytic solution and numerical (otherwise called approximate) solution. Many researchers at different points in time have developed error estimation schemes for numerical methods they invented or the numerical method they worked on. Very good examples in this regard are those of Lanczos (1956), Ortiz (1969), Adeniyi et al.(1990), Adeniyi

(1991) and El-Daou and Ortiz (1994) that all worked on the derivation of the error estimate for Lanczos' tau method for the solution of initial and boundary value problems. The generalization of their error estimation procedure for the general nonoverdetermined ordinary differential equations was reported by Yisa and Adeniyi (2015). Faires and Burden (2011) and Dukkipati (2010) derived the error estimation scheme for both trapezoidal and Simpson's rules. In fact, the former implemented the error estimate derived for Simpson's

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Statement of Problem

The problem studied in this work is the general integral of the form

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

where a and b are real constants, and $f(x)$ is the function to be approximated in the interval $[a, b]$.

Derivation of Boole's Rule

In this section, the Boole's rule is derived for the sake of completeness. The general Newton - Cotes closed quadrature formula for approximating the integral $\int_a^b f(x)dx$ is given as (see Faires and Burden (2011))

$$\begin{aligned} \int_a^b f(x)dx = nh \left[f_0 + \frac{n}{2} \Delta f_0 + \frac{2n^2 - 3n}{12} \Delta^2 f_0 \right] \\ + nh \left[\frac{n^3 - 4n^2 + 4n}{24} \Delta^3 f_0 + \frac{6n^4 - 45n^3 + 110n^2 - 90n}{720} \Delta^4 f_0 \right] \\ + nh \left[\frac{2n^5 - 24n^4 + 105n^3 - 200n^2 + 144n}{1440} \Delta^5 f_0 + \dots \right], \end{aligned} \quad (1)$$

where h is the stepsize, $f(x)$ is the function to be approximated, Δ is the forward difference operator, and $x \in [a, b]$.

Boole's rule is now derived by taking the curve $f(x)$ through five consecutive points x_0, x_1, x_2, x_3 and x_4 , which is equivalent to taking $n=4$ in (1). In addition to fixing $n=4$ in (1), we equally stop at the fourth difference to arrive at

$$I_1 = \int_{x_0}^{x_4} f(x)dx = \frac{2h}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \quad (2)$$

Also, taking the curve through x_4 to x_8 gives

$$I_2 = \int_{x_4}^{x_8} f(x)dx = \frac{2h}{45} (7f_4 + 32f_5 + 12f_6 + 32f_7 + 7f_8) \quad (3)$$

And so on, until

$$I_n = \int_{x_{n-4}}^{x_n} f(x)dx = \frac{2h}{45} (7f_{n-4} + 32f_{n-3} + 12f_{n-2} + 32f_{n-1} + 7f_n) \quad (4)$$

Now the entire area under the curve $f(x)$ is given by

$$I = \int_a^b f(x)dx = I_1 + I_2 + I_3 + \dots + I_n, \quad (5)$$

which is equivalent to

$$\begin{aligned} I = \int_a^b f(x)dx = \frac{2h}{45} [7f_0 + 32(f_1 + f_3 + f_5 + \dots + f_{n-1})] \\ + \frac{2h}{45} [12(f_2 + f_6 + f_{10} + \dots + f_{n-2})] \\ + \frac{2h}{45} [4(f_4 + f_8 + f_{12} + \dots + f_{n-4}) + 7f_n] \end{aligned} \quad (6)$$

Error Estimation in the Boole's Rule

It is always desirable in numerical analysis to have a reliable way of estimating the error embedded in any numerical method of interest. Here, the derivation of the error estimate in Boole's rule is carried out. This is done by first expanding the function $f(x)$ using Taylor's series between x_0 and x_4 as shown below. Let

$$\int_{x_0}^{x_4} f(x) dx = \int_{x_0}^{x_4} \left[f_0 + \frac{(x-x_0)}{1!} f'_0 + \dots + \frac{(x-x_0)^6}{6!} f_0^{(vi)} + \dots \right] dx \quad (7)$$

Also, let $x-x_0 = p$ which implies that $dx = dp$, so that (7) now becomes

$$I_1 = \int_{x_0}^{x_4} \left[f_0 + pf'_0 + \frac{p^2}{2} f''_0 + \dots + \frac{p^5}{120} f_0^{(v)} + \frac{p^6}{720} f_0^{(vi)} + \dots \right] dp \quad (8)$$

and

$$I_1 = \left[pf_0 + \frac{p^2}{2} f'_0 + \frac{p^3}{6} f''_0 + \dots + \frac{p^6}{720} f_0^{(v)} + \frac{p^7}{5040} f_0^{(vi)} + \dots \right]_0^{4h} \quad (9)$$

Thus

$$I_1 = 4hf_0 + 8h^2 f'_0 + \frac{32h^3}{3} f''_0 + \dots + \frac{256h^6}{45} f_0^{(v)} + \frac{1024h^7}{315} f_0^{(vi)} + \dots \quad (10)$$

The next thing is to apply Taylor's series expansion on the terms in the Boole's rule. The Boole's rule for the first five points is written as

$$I_2 = \frac{2h}{45} [7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4] \quad (11)$$

which can as well be written as

$$I_2 = \frac{2h}{45} [7f_0 + 32f(x_0+h) + 12f(x_0+2h) + 32f(x_0+3h) + 7f(x_0+4h)] \quad (12)$$

On expansion, (12) gives

$$\begin{aligned} I_2 = \frac{2h}{45} & \left[7f_0 + 32\left(f_0 + hf'_0 + \frac{h^2}{2!} f''_0 + \dots + \frac{h^5}{120} f_0^{(v)} + \frac{h^6}{720} f_0^{(vi)} + \dots\right) \right. \\ & + \frac{2h}{45} \left[12\left(f_0 + 2hf'_0 + 2h^2 f''_0 + \dots + \frac{4}{15} h^5 f_0^{(v)} + \frac{4}{45} h^6 f_0^{(vi)} + \dots\right) \right. \\ & + \frac{2h}{45} \left[32\left(f_0 + 3hf'_0 + \frac{9}{2} h^2 f''_0 + \dots + \frac{81}{40} h^5 f_0^{(v)} + \frac{81}{80} h^6 f_0^{(vi)} + \dots\right) \right. \\ & \left. \left. + \frac{2h}{45} \left[7\left(f_0 + 4hf'_0 + 8h^2 f''_0 + \dots + \frac{128}{15} h^5 f_0^{(v)} + \frac{256}{45} h^6 f_0^{(vi)} + \dots\right) \right] \right] \right] \quad (13) \end{aligned}$$

When fully simplified, we have

$$I_2 = 4hf_0 + 8h^2 f'_0 + \frac{32}{3} h^3 f''_0 + \frac{32}{3} h^4 f'''_0 + \frac{128}{15} h^5 f_0^{(iv)} + \frac{256}{45} h^6 f_0^{(v)} + \frac{88}{27} h^7 f_0^{(vi)} + \dots \quad (14)$$

Let the error in $[x_0, x_4]$ be denoted by e_1 , which is

$$e_1 = I_1 - I_2 \quad (15)$$

$$e_1 = -\frac{8}{945} h^7 f_0^{(vi)} + \dots \quad (16)$$

Following the same procedure, we have $e_2, e_3, \dots, e_n$ as

$$e_2 = -\frac{8}{945} h^7 f_4^{(vi)} + \dots \quad (17)$$

$$e_3 = -\frac{8}{945} h^7 f_8^{(vi)} + \dots \quad (18)$$

$$e_n = -\frac{8}{945} h^7 f_{n-4}^{(vi)} + \dots \quad (19)$$

respectively.

If the total error is represented by E , then it is given by

$$E = \sum_{i=1}^n e_i = -\frac{8h^7}{945} [f_0^{(vi)} + f_4^{(vi)} + f_8^{(vi)} + \dots + f_{n-4}^{(vi)}] \quad (20)$$

and when simplified gives

$$E = -\frac{8nh^7}{945} f^{(vi)}(\bar{x}) \quad (21)$$

where $f^{(vi)}(\bar{x})$ is the largest value of the sixth order derivatives, with $h = \frac{b-a}{n}$, but

$n = 4$ for Boole's method, hence $h = \frac{b-a}{4}$.

The error estimation in Boole's rule is therefore written as

$$e = \frac{-8h^7}{945} f^{(vi)}(\xi) \quad (22)$$

where $a = x_0 < \xi < x_n = b$ (for n sub-intervals of length h).

Implementation of Boole's Rule in Adaptive Quadrature

In this section, Boole's rule shall be implemented in the adaptive quadrature to see its superiority over some earlier results, especially those implementations that used trapezoidal and Simpson's $\frac{1}{3}$ rules. The curve $f(x)$ is again taken

through five points to conform with requirement of Boole's rule, that is $h = \frac{b-a}{4}$, for x in $[a, b]$.

$$B(a,b) = \frac{2h}{45} [7f(a) + 32f(a+h) + 12f(a+2h) + 32f(a+3h) + 7f(b)] \quad (23)$$

Now, with the interval $[a,b]$ partitioned so that $n=8$, which implies that $\frac{b-a}{8} = \frac{h}{2}$, we have

$$B(a, \frac{a+b}{2}) = \frac{h}{45} \left[7f(a) + 32f(a+\frac{h}{2}) + 12f(a+h) + 32f(a+\frac{3h}{2}) + 7f(a+2h) \right] \quad (24)$$

and

$$B(\frac{a+b}{2}, b) = \frac{h}{45} \left[7f(a+2h) + 32f(a+\frac{5h}{2}) + 12f(a+3h) + 32f(a+\frac{7h}{2}) + 7f(b) \right] \quad (25)$$

But $B(a, \frac{a+b}{2}) + B(\frac{a+b}{2}, b) = B(a,b)$. Thus

$$\begin{aligned} \int_a^b f(x)dx &= \frac{h}{45} \left[7f(a) + 32f(a+\frac{h}{2}) + 12f(a+h) + 32f(a+\frac{3h}{2}) \right] \\ &+ \frac{h}{45} \left[14f(a+2h) + 32f(a+\frac{5h}{2}) + 12f(a+3h) + 32f(a+\frac{7h}{2}) + 7f(b) \right] \end{aligned} \quad (26)$$

Also

$$\int_a^b f(x)dx = B(a,b) - \frac{8h^7}{945} f^{(vi)}(\xi) \quad (27)$$

for some number ξ in (a,b) where Boole's rule approximation denoted $B(a,b)$ is given as stated in (23) above.

Now, we derive as estimate for the accuracy of the approximation in (27), especially the one that does not involve the determination of $f^{(vi)}(\xi)$. To achieve this, we use composite Boole's rule with $n=8$ and stepsize $\frac{b-a}{8} = \frac{h}{2}$. Thus,

$$\begin{aligned} \int_a^b f(x)dx &= \frac{h}{45} \left[7f(a) + 32f(a+\frac{h}{2}) + 12f(a+h) + 32f(a+\frac{3h}{2}) \right] \\ &+ \frac{h}{45} \left[14f(a+2h) + 32f(a+\frac{5h}{2}) + 12f(a+3h) + 32f(a+\frac{7h}{2}) + 7f(b) \right] \\ &- \frac{1}{64} \left(\frac{8h^7}{945} \right) f^{(vi)}(\bar{\xi}) \end{aligned} \quad (28)$$

for some $\bar{\xi}$ in (a,b) . Meanwhile, Boole's rule approximations in $\left(a, \frac{a+b}{2}\right)$ and $\left(\frac{a+b}{2}, b\right)$ are as given in (24) and (25) respectively. Thus, (28) can be written as

$$\int_a^b f(x)dx = \left(a, \frac{a+b}{2}\right) + \left(\frac{a+b}{2}, b\right) - \frac{1}{64} \left(\frac{8h^7}{945} \right) f^{(vi)}(\bar{\xi}) \quad (29)$$

For the derivation of error estimate, $f^{(iv)}(\bar{\xi})$ is taken to be approximately equal to $f^{(iv)}(\xi)$. If this assumption is accurate, then the technique is very successful. Relying on the accuracy of our assumption, the right hand sides of (27) and (29) are equated to have

$$B(a,b) - \frac{8h^7}{945} f^{(iv)}(\xi) = \left(a, \frac{a+b}{2}\right) + \left(\frac{a+b}{2}, b\right) - \frac{1}{64} \left(\frac{8h^7}{945}\right) f^{(iv)}(\bar{\xi}) \quad (30)$$

So

$$\frac{8h^7}{945} f^{(iv)}(\xi) = \frac{64}{63} \left[B(a,b) - \left(a, \frac{a+b}{2}\right) - \left(\frac{a+b}{2}, b\right) \right] \quad (31)$$

Using this estimate in (29) produces the error estimate

$$\left| \int_a^b f(x) dx - B\left(a, \frac{a+b}{2}\right) - B\left(\frac{a+b}{2}, b\right) \right| \approx \frac{1}{63} \left| B(a,b) - B\left(a, \frac{a+b}{2}\right) - B\left(\frac{a+b}{2}, b\right) \right| \quad (32)$$

It can, therefore, be deduced from (31) that $B(a, \frac{a+b}{2}) + B(\frac{a+b}{2}, b)$ approximates $\int_a^b f(x) dx$ 63 times better than $B(a,b)$ does. Thus, $B(a, \frac{a+b}{2}) + B(\frac{a+b}{2}, b)$ approximates $\int_a^b f(x) dx$ to within ξ in as much as the two approximations $B(a, \frac{a+b}{2}) + B(\frac{a+b}{2}, b)$ and $B(a,b)$ differ by less than 63ξ . In conclusion, if $\left| B(a,b) - B\left(a, \frac{a+b}{2}\right) - B\left(\frac{a+b}{2}, b\right) \right| \leq 63\xi$, then

$$\left| \int_a^b f(x) dx - B\left(a, \frac{a+b}{2}\right) - B\left(\frac{a+b}{2}, b\right) \right| \approx \xi \quad (33)$$

Numerical Experiments

In this section, the results obtained in the earlier sections shall be validated by applying them to some selected numerical problems.

Problem 1

Evaluate the integral $\int_0^{0.35} \frac{2}{x^2-4} dx$, also obtain the error estimate of the scheme. The exact solution of the integral is -0.1768200201 .

Solution

The stepsize, $h = \frac{b-a}{4} = \frac{0.35}{4} = 0.0875$.

$$B(a,b) = \frac{2h}{45} [7f(a) + 32f(a+h) + 12f(a+2h) + 32f(a+3h) + 7f(b)]$$

$$B(0,0.35) = \frac{2(0.0875)}{45} [7f(0) + 32f(0.0875) + 12f(0.175) + 32f(0.2625) + 7f(0.35)]$$

$$B(0,0.35) = \frac{0.175}{45} [7(-0.5) + 32(-0.5009588666) + 12(-0.5038576602)] \\ + \frac{0.175}{45} [32(-0.5087642593) + 7(-0.5157962605)]$$

$$B(0,0.35) = -0.1768200225.$$

Also,

$$B(a, \frac{a+b}{2}) = \frac{h}{45} \left[7f(a) + 32f(a + \frac{h}{2}) + 12f(a+h) \right] + \frac{h}{45} \left[32f(a + \frac{3h}{2}) + 7f(a+2h) \right]$$

$$B(0,0.175) = \frac{0.0875}{45} [7f(0) + 32f(0.04375) + 12f(0.0875)] \\ + \frac{0.0875}{45} [32f(0.13125) + 7f(0.175)]$$

$$B(0,0.175) = \frac{0.0875}{45} [7(-0.5) + 32(-0.5038576602)] \\ + \frac{0.0875}{45} [12(-0.5009588666) + 32(-0.502162634)] \\ + \frac{0.0875}{45} [7(-0.5038576602)]$$

$$B(0,0.175) = -0.08772433877.$$

And

$$B(\frac{a+b}{2}, b) = \frac{h}{45} \left[7f(a+2h) + 32f(a + \frac{5h}{2}) + 12f(a+3h) \right] + \frac{h}{45} \left[32f(a + \frac{7h}{2}) + 7f(b) \right]$$

$$B(0.175,0.35) = \frac{0.0875}{45} [7f(0.175) + 32f(0.21875) + 12f(0.2625)] \\ + \frac{h}{45} [32f(0.30625) + 7f(0.35)]$$

$$B(0.175,0.35) = \frac{0.0875}{45} [7(-0.5038576602) + 32(-0.5060538671)] \\ + \frac{0.0875}{45} [12(-0.5087642593) + 32(-0.5120051201) + 7(0.35)]$$

$$B(0.175,0.35) = -0.0890956814.$$

$$B(0,0.175) + B(0.175,0.35) = -0.1768200202.$$

Actual error is computed as

$$\left| \int_0^{0.35} \frac{2}{x^2-4} dx - B(0,0.175) - B(0.175,0.35) \right| = |-0.1768200201 + 0.1768200202|$$

$$\left| \int_0^{0.35} \frac{2}{x^2 - 4} dx - B(0, 0.175) - B(0.175, 0.35) \right| = 1.0 * 10^{-10}.$$

$$\text{Error estimate} = \frac{1}{63} |B(0, 0.35) - B(0, 0.175) - B(0.175, 0.35)|$$

$$= \frac{1}{63} |-0.1768200225 + 0.1768200202|$$

$$\text{Error estimate} = \frac{1}{63} |B(0, 0.35) - B(0, 0.175) - B(0.175, 0.35)|$$

$$= 3.65079 * 10^{-11}.$$

Problem 2

Evaluate the integral $\int_1^{1.5} x^2 \ln x dx$ and obtain its error estimate.

Solution

$$\text{Here, } h = \frac{1.5-1}{4} = \frac{0.5}{4} = 0.125$$

$$B(1, 1.5) = \frac{2(0.125)}{45} [7f(1) + 32f(1.125) + 12f(1.25)]$$

$$+ \frac{2(0.125)}{45} [32f(1.375) + 7f(1.5)]$$

$$B(1, 1.5) = \frac{0.25}{45} [7(1^2 \ln 1) + 32[(1.125)^2 \ln 1.125] + 12[(1.25)^2 \ln 1.25]]$$

$$+ \frac{2(0.125)}{45} [32[(1.375)^2 \ln 1.375] + 7[(1.5)^2 \ln 1.5]]$$

$$B(1, 1.5) = 0.1922593373.$$

$$B(1, 1.25) = \frac{0.125}{45} [7f(1) + 32f(1.0625) + 12f(1.125)]$$

$$+ \frac{0.125}{45} [32f(1.1875) + 7f(1.25)]$$

$$B(1, 1.25) = \frac{0.25}{45} [7(1^2 \ln 1) + 32[(1.0625)^2 \ln 1.0625] + 12[(1.125)^2 \ln 1.125]]$$

$$+ \frac{0.125}{45} [32[(1.1875)^2 \ln 1.1875] + 7[(1.25)^2 \ln 1.25]]$$

$$B(1, 1.25) = 0.03937297154.$$

$$B(1.25, 1.5) = \frac{0.125}{45} [7f(1.25) + 32f(1.3125) + 12f(1.375)]$$

$$+ \frac{0.125}{45} [32f(1.4375) + 7f(1.5)]$$

$$B(1.25, 1.5) = \frac{0.25}{45} [7(1.25^2 \ln 1.25) + 32[(1.3125)^2 \ln 1.3125]] \\ + \frac{0.125}{45} [21(1.375)^2 \ln 1.375 + 32[(1.4375)^2 \ln 1.4375] + 7[(1.5)^2 \ln 1.5]]$$

$$B(1.25, 1.5) = 0.1528863859$$

$$B(1, 1.25) + B(1.25, 1.5) = 0.1922593574.$$

The actual error:

$$\left| \int_1^{1.5} x^2 \ln x dx - B(1, 1.25) - B(1.25, 1.5) \right| = |0.1922593577 - 0.1922593574| \\ = 3 \times 10^{-10}$$

The error estimate is given as

$$\text{Error estimate} = \frac{1}{63} |B(1, 1.5) - B(1, 1.25) - B(1.25, 1.5)| \\ = \frac{1}{63} |0.192259337 - 0.1922593574| \\ = 3.19048 \times 10^{-10}$$

This results further established the corrections of the error estimate in (3.6).

Problem 3

Evaluate the integral $\int_0^{\frac{\pi}{2}} \sin x dx$, also obtain the error estimate.

Solution

$$\text{Here, } h = \frac{b-a}{4} = \frac{\frac{\pi}{2} - 0}{4} = \frac{\pi}{8}, \text{ since } a = 0 \text{ and } b = \frac{\pi}{2}.$$

$$B(0, \frac{\pi}{2}) = \frac{\pi}{180} \left[7f(0) + 32f(\frac{\pi}{8}) + 12f(\frac{\pi}{4}) + 32f(\frac{3\pi}{8}) + 7f(\frac{\pi}{2}) \right]$$

$$B(0, \frac{\pi}{2}) = \frac{\pi}{180} \left[7\sin(0) + 32\sin(\frac{\pi}{8}) + 12\sin(\frac{\pi}{4}) + 32\sin(\frac{3\pi}{8}) + 7\sin(\frac{\pi}{2}) \right]$$

$$B(0, \frac{\pi}{2}) = 0.9999915655.$$

Also,

$$B(0, \frac{\pi}{4}) = \frac{\pi}{360} \left[7f(0) + 32f(\frac{\pi}{16}) + 12f(\frac{\pi}{8}) + 32f(\frac{3\pi}{16}) + 7f(\frac{\pi}{4}) \right]$$

$$B(0, \frac{\pi}{4}) = 0.2928931826. \text{ and}$$

$$B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = \frac{\pi}{360} \left[7f\left(\frac{\pi}{4}\right) + 32f\left(\frac{5\pi}{16}\right) + 12f\left(\frac{3\pi}{8}\right) + 32f\left(\frac{7\pi}{16}\right) + 7f\left(\frac{\pi}{2}\right) \right]$$

$$B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = 0.7071066937.$$

Thus,

$$B\left(0, \frac{\pi}{4}\right) + B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = 0.9999998762$$

The actual error involved in approximating $\int_0^{\pi/2} \sin x dx$ by using $B\left(0, \frac{\pi}{4}\right) + B\left(\frac{\pi}{4}, \frac{\pi}{2}\right)$ is given as

$$\left| \int_0^{\pi/2} \sin x dx - B\left(0, \frac{\pi}{4}\right) - B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) \right| = 1 - 0.9999998762$$

$$\left| \int_0^{\pi/2} \sin x dx - B\left(0, \frac{\pi}{4}\right) - B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) \right| = 1.238 * 10^{-7}$$

while the error estimate is given as

$$\begin{aligned} \text{Error estimate} &= \frac{1}{63} \left| B\left(0, \frac{\pi}{2}\right) - B\left(0, \frac{\pi}{4}\right) - B\left(\frac{\pi}{4}, \frac{\pi}{2}\right) \right| \\ &= \frac{1}{63} |0.9999915655 - 0.9999998762| \\ &= 1.31916 * 10^{-7} \end{aligned}$$

Thus, (36) is completely satisfied, hence the accuracy of the error estimation scheme.

Conclusion

The error estimate for Boole's rule, its implementation in the adaptive quadrature and the error estimate for the adaptive quadrature have been presented. The beauty of these results is that their computations are not much involving, and they give very good results.

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