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Some New Time and Cost-Efficient Quadrature Formulas to Compute Integrals Using Derivatives with Error Analysis

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Abstract: Computational mathematics relies heavily on numerical integration, which has many scientific and engineering-related applications. For functions with complicated derivatives in particular, traditional quadrature formulae, while effective, may need substantial processing resources. An innovative method for efficient quadrature formulae that use derivatives for better accuracy and less computing work is presented in this study. Rigid derivation guarantees mathematical correctness and practical usability of the presented approaches. To test how well these formulae hold up under different circumstances, we run them through a thorough error analysis. Research shows that new approaches are more efficient and accurate than traditional ones, making them a good fit for high-precision real-world applications. We go over some of the possible uses and constraints of these approaches, as well as some suggestions for where the field may go from here in terms of improving their use in various computational contexts.

Keywords: Numerical Integration, Quadrature Formulas, Error Analysis, Computational Efficiency, Derivative-Based Methods

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1. INTRODUCTION

Due to the inherent difficulty or impossibility of analytically evaluating integrals, numerical integration is an essential tool in scientific and engineering calculations. For this, quadrature formulas—which use weighted sums of function values to approximatively find definite integrals—are necessary (Wang, Z., & Li, X. 2021). While traditional approaches like Five is the level of accuracy of the mixed quadrature rule Q2,3(f) and Gaussian quadrature are efficient and accurate, they have different degrees of each. But as real-world issues have become more complicated, there has been a greater demand for approaches that are efficient with both time and money (Kumar, S., & Singh, V. 2020).

The possibility for derivative-based quadrature formulae to increase accuracy while decreasing computing cost has led to their increased interest in recent years (Zhang, J., & Liu, W. 2019). The use of derivatives in these approaches allows for a more accurate approximation of the integral with a reduced number of integrand evaluations. Applications like machine learning algorithms, financial modeling, and physics simulations that need great accuracy will find this invention extremely helpful (Zhang, W., & Li, Y. 2019).

2. LITERATURE REVIEW

Rogers, J. A. (2019) It is possible to trace the origins of numerical integration all the way back to historical techniques such as the trapezoidal rule, which served as the foundation for contemporary quadrature procedures. Isaac Newton and James Stirling developed these methods further in order to generate polynomial interpolation formulae, such as the Newton-Cotes rules. Adaptive algorithms have been used in recent advancements to improve these approaches, which has resulted in increased accuracy for applications that include complicated functions. drew attention to the transition from manual approximations to computer-based quadrature techniques, highlighting the robustness of these approaches in terms of computing definite integrals across finite intervals.

Chen, X., & Liu, J. (2018) As a result of its effectiveness in approximating integrals with defined weight functions, Gaussian quadrature continues to be an essential component of numerical integration. The theoretical underpinning of Gaussian quadrature was described by. He explained how the nodes and weights of the quadrature are formed from orthogonal polynomials, such as Legendre or Chebyshev polynomials. Gaussian quadrature, in contrast to Newton-Cotes techniques, is able to reduce error for polynomials with a degree of $2n-1$ or less, provided that n points are provided.

Li, X., & Zhang, H. (2018) To improve efficiency and accuracy for functions with fluctuating smoothness, adaptive quadrature techniques dynamically alter the number of evaluation points dependent on the behavior of the integrand. This allows for the functions to be evaluated more accurately. presented adaptive quadrature as a solution for addressing the inefficiencies of fixed-step approaches. This was accomplished by refining the grid in areas where the integrand exhibited increased complexity.

Sebarchievici, C. (2018) Simpson's rule is a method for numerical integration that is extensively used. It approximates integrals by fitting quadratic polynomials to subintervals of the domain with the use of the approach. It is derived from the Newton-Cotes family of algorithms, which offers a satisfactory equilibrium between the amount of computing work required and the level of precision achieved. This is because Simpson's rule is inaccurate proportional to the fourth power of the interval length, it is very accurate when applied to smooth and continuous functions. On the other hand, its performance is diminished when applied to integrands that have discontinuities or sudden switches.

Koeffler, H. P. (2018) By recursively applying the trapezoidal rule to successively smaller subintervals and then extrapolating the findings, Romberg integration, which is an extension of the trapezoidal rule, is able to obtain high-order convergence while simultaneously achieving high-order convergence. The approach was created by who proved that large gains in accuracy could be gained by combining trapezoidal estimations with Richardson extrapolation. Romberg's method was named after him. The method proposed by Romberg has the ability to speed up the convergence of numerical integration techniques, especially in situations when the integrand is smooth.

3. METHODOLOGY

A researcher's approach to study design is outlined in a research methodology. This strategy for solving the learning challenge is logical and well-organized. The methodology of a study explains the steps taken by researchers to ensure that the data they collect are valid and reliable, in line with their aims. Everything from the data we gather to its origins, methods of collection, and evaluation is part of this. The reliability of research and the quality of scientific findings are both enhanced by a well-defined research strategy. It also allows for a straightforward, efficient, and controllable method by providing a comprehensive plan to keep researchers on track. Readers may grasp the tactics and procedures employed to get the findings by delving into the researchers' techniques.

4. RESULTS

4.1 Approximate evaluation of real definite integrals: a set of rules from mixed quadrature

The following categories best describe quadrature rules used for approximating the evaluation of the real definite integral:

$$I(f) = \int_{-1}^{1} f(x)\,dx \qquad \text{...} \quad (4.1.1)$$

a. Newton-Cotes-type rules

b. Gauss-type rules.

In n-point Newton-Cotes-type rules the nodes are a set of equidistant points

$$x_k = -1 + \frac{2k}{n-1};\ k = 0, 1, \cdots, n-1$$

As opposed to n-point Gauss-type rules, where the Bodes are the irrational numbers lying on the open interval (-1, 1) that make up the nth degree Legendre polynomial. Because it is commonly known that an n-point Gaussian rule is of precision 2n - 1, and an n-point Newton-Cotes rule is at most n - 1, a Gauss-type rule is more precise than a Newton-Cotes-type rule involving the same number of nodes. Newton-Cotes rules, on the other hand, are best calculated by hand since the rules' associated nodes and weights are simply rational values. The work of Simpson the method in its composite version is often used for integrals with an appreciably broad range of integration, however the one-dimensional real definite integral is known to be approximatively evaluated using this rule, which is one of the Newton-Cotes-type rules.

4.2 Method of construction of mixed quadrature rules

Suppose Q1(f) and Q2(t) are two quadrature rules of different kinds and each of equal precision d in order to get a rough estimate of the actual definite integral. A truncation error E1(f) and a truncation error Q2(f) are connected with rules Q1(f) and Q2(f), therefore

$$I(f) = Q_1(f) + E_1(f) \qquad \text{..} \quad (4.2.1)$$

$$I(f) = Q_2(f) + E_2(f), \qquad \text{..} \quad (4.2.2)$$

ignoring the round-off errors in such approximations. Assuming of to possess derivatives of all order in the interval -1 < x < 1, the function f can be expressed as

$$f(x) = \sum_{k=0}^{\infty} a_k x^k$$
.... (4.2.3)

Where

$$a_k = \frac{f^{(k)}(0)}{k!};\ k = 0, 1, 2, \cdots,$$

which is the Taylor series off about the point x = 0.

Therefore, for i = 1, 2

$$E_i(f) = \sum_{k=0}^{\infty} a_k E_i(x^k).$$
.... (4.2.4)

Since each of the quadrature rules Q1 (f) and Q2(f) is of precision d,

$$E_i(x^k) = 0;\ k = 0, 1, \cdots, d$$

And

$$E_i(x^{d+1}) \neq 0$$
.... (4.2.5)

for i = 1,2.

Using the equation, we obtain

$$E_1(f) = a_{d+1} E_1(x^{d+1}) + \sum_{k>d+1} a_k E_1(x^k)$$
.... (4.2.6)

And

$$E_2(f) = a_{d+1} E_2(x^{d+1}) + \sum_{k>d+1} a_k E_2(x^k)$$
.... (4.2.7)

Writing the expression for E1(f) (given in equation) (4.2.6) and E2(f) (given in equation (4.2.7)) in equation (4.2.1) and (4.2.2) respectively we obtain

$$I(f) = Q_1(f) + a_{d+1} E_1(x^{d+1}) + \sum_{k>d+1} a_k E_1(x^k)$$
.... (4.2.8)

And

$$I(f) = Q_2(f) + a_{d+1}E_2(x^{d+1}) + \sum_{k>d+1} a_k E_2(x^k)$$

.... (4.2.9)

Now multiplying equations (4.2.8) and (4.2.9) by $E_2(x^{d+1})$ and $E_1(x^{d+1})$ respectively we have

$$E_2(x^{d+1})I(f) = E_2(x^{d+1})Q_1(f) + a_{d+1}E_1(x^{d+1})E_2(x^{d+1}) + E_2(x^{d+1}) \sum_{k>d+1} a_k E_1(x^k)$$

... (4.2.10)

And

$$E_1(x^{d+1})I(f) = E_1(x^{d+1})Q_2(f) + a_{d+1}E_1(x^{d+1})E_2(x^{d+1}) + E_1(x^{d+1}) \sum_{k>d+1} a_k E_2(x^k) .$$

.... (4.2.11)

Equation (4.2.10) is now subtracted from equation (4.2.11), and further simplification yields

$$I(f) = \frac{1}{E_1(x^{d+1})-E_2(x^{d+1})}\left[E_1(x^{d+1})Q_2(f) - E_2(x^{d+1})Q_1(f)\right] + \frac{1}{E_1(x^{d+1})-E_2(x^{d+1})}\left[E_1(x^{d+1}) \sum_{k>d+1} a_k E_2(x^k) - E_2(x^{d+1}) \sum_{k>d+1} a_k E_1(x^k)\right] .$$

.... (4.2.12)

Writing

$$Q_{1;2}(f) = \frac{1}{E_1(x^{d+1})-E_2(x^{d+1})}\left[E_1(x^{d+1})Q_2(f) - E_2(x^{d+1})Q_1(f)\right]$$

... (4.2.13)

And

$$E_{1;2}(f) = \frac{1}{E_1(x^{d+1})-E_2(x^{d+1})}\left[E_1(x^{d+1}) \sum_{k>d+1} a_k E_2(x^k) - E_2(x^{d+1}) \sum_{k>d+1} a_k E_1(x^k)\right]$$

... (4.2.14)

Che equation (4.2.12) can be rewritten as

$$I(f) = Q_{1;2}(f) + E_{1;2}(f)$$

.... (4.2.15)

The first term on the right hand side of the equation ie. Q12(f) is the desired mixed quadrature rule, obtained from the rules Q1(f) and Q2(f) of equal precision but of different kinds and the second term $E_{1,2}(f)$ on the right hand side of equation is the truncation error associated with such approximation.

4.3 Construction of some mixed quadrature rules of precision five

For the construction of the mixed quadrature rule of precision five to approximate the real definite integral, the following symmetric quadrature rules each of precision three have been chosen.

(a) Simpson's 1/3 rule

$$\int_{-1}^{1} f(x)\,dx \approx Q_1(f) = \frac{1}{3}[f(-1) + 4f(0) + f(1)],$$

.... (4.3.1)

(b) Simpson's 3/8 rule

$$\int_{-1}^{1} f(x)\,dx \approx Q_2(f) = \frac{1}{4}[f(-1) + 3\{f(-\tfrac{1}{3}) + f(\tfrac{1}{3})\} + f(1)]$$

... (4.3.2)

(c) Gauss-Legendre 2.point rule

$$\int_{-1}^{1} f(x)\,dx \approx Q_3(f) = f(-\tfrac{1}{\sqrt{3}}) + f(\tfrac{1}{\sqrt{3}})$$

.... (4.3.3)

The rules (a) and (b) are of Newton-Cotes-type while the rule (c) is of Gauss-type. It may be noted here that all the weights of the quadrature rules (a) to (c) are positive. Here onwards these rules from (a) to (c) will be referred to as basic rules.

Let

$$E_i(f) = I(f) - Q_i(f)$$

.... (4.3.4)

Notes the truncation error associated with the rule Q ;(f); i = 1, 2, 3. This article consists of two parts: Part - A1, and Part - Ay In Part - A,, a mixed The fifth rule of quadrature has been derived from the basic rules Q1(f) and Q2(f) and in Part - A^ another mixed quadrature rule of same precision has been constructed from the basic, rules Q1(f) and Q2(f). For further discussion we use the following notations.

The mixed quadrature rule constructed from the basic rules Qr(f) and Qs (f) is denoted as Q1,2 (f) and die corresponding truncation error is denoted as Sr.s (i)- Thus It is assumed that the function f(x) is infinitely differentiable in (-1,1)

$$I(f) = Q_{r,s}(f) + E_{r,s}(f).$$

.... (4.3.5)

Part – A_1 The Mixed Quadrature Rule $Q_{1,2}$(F)

The Taylor series expansion of the function f(x) about x = 0 is given by are the Taylor coefficients.

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

.... (4.3.6)

Where

$$a_n = \frac{f^{(n)}(0)}{n!}; n = 0, 1, 2, \cdots$$

The series given in equation (4.3.6) is uniformly convergent in the interval t (-1,1). Therefore, integrating it term by term from -1 to 1 we have

$$I(f) = 2a_0 + \frac{2}{3}a_2 + \frac{2}{5}a_4 + \cdots$$

.... (4.3.7)

Further substituting x = -1, 0 and 1 successively in equation we get

$$f(-1) = a_0 - a_1 + a_2 - \cdots + (-1)^n a_n + \cdots,$$

$$f(0) = 0$$

$$f(1) = a_0 + a_1 + a_2 + \cdots + a_n + \cdots.$$

Now substituting the respective expansion of f(-l), f(0) and f(l) in Q1(f) and then simplifying we obtain

$$Q_1(f) = 2a_0 + \frac{2}{3}a_2 + \frac{2}{3}a_4 + \cdots$$

.... (4.3.8)

Again proceeding in the same way, we have

$$Q_3(f) = 2a_0 + \frac{2}{3}a_2 + \frac{2}{9}a_4 + \cdots$$

.... (4.3.9)

Thus from equations (4.3.4) for i = 1, (4.3.7) and (4.3.8) we have

$$E_1(f) = \left(2a_0 + \frac{2}{3}a_2 + \frac{2}{5}a_4 + \cdots\right) - \left(2a_0 + \frac{2}{3}a_2 + \frac{2}{3}a_4 + \cdots\right)$$

.... (4.3.10)

Similarly, from equations (4.3.4) for i = 3, (4.3.7) and (4.3.9) we obtain

$$E_3(f) = \left(2a_0 + \tfrac{2}{3}a_2 + \tfrac{2}{5}a_4 + \cdots\right)$$

$$- \left(2a_0 + \tfrac{2}{3}a_2 + \tfrac{2}{9}a_4 + \cdots\right). \qquad \text{.......................} (4.3.11)$$

On simplification we finally have

$$E_1(f) = -\tfrac{4}{15}a_4 - \tfrac{8}{21}a_6 - \cdots \qquad \text{....................................} (4.3.12)$$

$$E_3(f) = \tfrac{8}{45}a_4 + \tfrac{40}{189}a_6 + \cdots . \qquad \text{....................................} (4.3.13)$$

Therefore, from equations (4.3.4) for i = 1 and (4.3.12)

$$I(f) = Q_1(f) - \tfrac{4}{15}a_4 - \tfrac{8}{21}a_6 - \cdots \qquad \text{........................} (4.3.14)$$

And from equations (4.3.4) for i = 3 and (4.3.13)

$$I(f) = Q_3(f) + \tfrac{8}{45}a_4 + \tfrac{40}{189}a_6 + \cdots \qquad \text{..........................} (4.3.15)$$

Now multiplying the equation (4.3.14) by -2/3 and then adding it to the equation (4.3.15) we have

$$5I(f) = [2Q_1(f) + 3Q_3(f)]$$

$$-\left[\tfrac{8}{63}a_6 + \tfrac{8}{27}a_8 + \cdots\right] \qquad \text{...} (4.3.16)$$

From this we now obtain

$$I(f) \approx Q_{1;3}(f) = \tfrac{1}{5}[2Q_1(f) + 3Q_3(f)], \qquad \text{.......................................} (4.3.17)$$

The ideal mixed quadrature rule with five degrees of freedom (to be shown later).

You can now find the truncation mistake linked to the rule Qi;J(f) by using

$$E_{1:3}(f) = -\tfrac{8}{315}a_6 - \tfrac{8}{135}a_8 - \cdots \qquad \text{.................................} (4.3.18)$$

Clearly

$$E_{1:3}(f) = \tfrac{1}{5}[2E_1(f) + 3E_3(f)]. \qquad \text{.......................................} (4.3.19)$$

It may be it should be mentioned that the mixed quadrature rule's weights Q1?(f), are all positive, since those of the basic rules Q1(f) and 2(f) are positive and E^x4); i = 1,3 differ in signs

rule's level of accuracy q1;j (f):

Both quadrature rules Q1(f) and 2(f) have an accuracy level of three. Therefore for i = 1, 3

$$E_i(x^r) = 0; \; r = 0(1)3. \quad \text{..} \; (4.3.20)$$

Hence from equations we have

$$E_{1;3}(x^r) = 0; \; r = 0(1)3.$$

Further

$$E_1(x^4) = \int_{-1}^{1} x^4 dx - Q_1(x^4)$$

$$= -\frac{4}{15}$$

And

$$E_3(x^4) = \int_{-1}^{1} x^4 dx - Q_3(x^4)$$

$$= \frac{8}{45}.$$

Thus

$$E_{1;3}(x^4) = \frac{1}{5}[2E_1(x^4) + 3E_3(x^4)]$$

$$= \frac{1}{5}[2(-\frac{4}{15}) + 3(\frac{8}{45})]$$

$$= 0.$$

Moreover, the rule Q1(f) being a symmetric quadrature rule, exactly integrates f(x) = x5. Hence

$$E_{1;3}(x^r) = 0; \; r = 0(1)5.$$

So the degree of precision of the mixed quadrature rule Q1,2(f) is at least five. Further

$$E_{1;3}(x^6) = \frac{1}{5}[2E_1(x^6) + 3E_3(x^6)]$$

$$= \frac{1}{5}\left[2\left(-\frac{8}{21}\right) + 3\left(\frac{40}{189}\right)\right]$$

$$= -\frac{8}{315} \neq 0. \qquad \text{.............................. (4.3.21)}$$

Hence the mixed quadrature rule

$$Q_{1;3}(f) = \frac{1}{5}[2Q_1(f) + 3Q_3(f)]$$

Is of degree of precision five.

Part - A1, The Mixed Quadrature Rule Q1,3,4(f):

Now proceeding as in Part – A1 of this article we here have

$$E_2(f) = -\frac{16}{135}a_4 - \frac{368}{1701}a_6 - \cdots \qquad \text{.................................. (4.3.22)}$$

And

$$E_3(f) = \frac{8}{45}a_4 + \frac{40}{189}a_6 + \cdots \qquad \text{... (4.3.23)}$$

Therefore

$$I(f) = Q_2(f) - \frac{16}{135}a_4 - \frac{368}{1701}a_6 - \cdots \qquad \text{............................... (4.3.24)}$$

And

$$I(f) = Q_3(f) + \frac{8}{45}a_4 + \frac{40}{189}a_6 + \cdots \qquad \text{.................................... (4.3.25)}$$

Now multiplying the equation (4.3.25) by 2/3 and then adding the product to the equation (4.3.24) we obtain after simplification

$$5I(f) = [3Q_2(f) + 2Q_3(f)]$$

$$-\left[\frac{128}{567}a_6 + \frac{320}{729}a_8 + \cdots\right] \qquad \text{... (4.3.26)}$$

Thus

$$I(f) \approx Q_{2;3}(f) = \frac{1}{5}[3Q_2(f) + 2Q_3(f)]$$ .... (4.3.27)

Is the desired mixed quadrature rule constructed from the rules Q2(f) and Q1(f) and the truncation error associated with this quadrature rule is given by

$$E_{2;3}(f) = -\frac{128}{2835}a_6 - \frac{64}{729}a_8 - \cdots.$$ .... (4.3.28)

B^(f) in terms of Ez(f) and E3(f) is given by

$$E_{2;3}(f) = \frac{1}{5}[3E_2(f) + 2E_3(f)].$$ .... (4.3.29)

Degree Of Precision Of The Rule Q(F) «

For i = 2, 3

$$E_i(x^r) = 0; r = 0, 1, 2, 3.$$ .... (4.3.30)

Hence from equations (4.3.29) and (4.3.30)

$$E_{2;3}(x^r) = 0; r = 0, 1, 2, 3.$$

Further

$$E_{2;3}(x^4) = \int_{-1}^{1} x^4 dx - \frac{1}{5}[3Q_2(x^4) + 2Q_3(x^4)]$$

$$= \frac{2}{5} - \frac{1}{5}\left[3\left(\frac{14}{27}\right) + 2\left(\frac{2}{9}\right)\right]$$

$$= 0$$ .... (4.3.31)

And

$$E_{2;3}(x^5) = 0$$ .... (4.3.32)

Since the rule Q1(f) is a symmetric quadrature rule.

However

$$E_{2;3}(x^6) = \int_{-1}^{1} x^6 dx - \tfrac{1}{5}[3Q_2(x^6) + 2Q_3(x^6)]$$

$$= \tfrac{2}{7} - \tfrac{1}{5}\left[3\left(\tfrac{122}{243}\right) + 2\left(\tfrac{2}{27}\right)\right]$$

$$= -\tfrac{128}{2835} \neq 0.$$

.... (4.3.33)

Hence Five is the level of accuracy of the mixed quadrature rule Q2,3(f). A similar type of rule may be constructed by taking the pair of rules Q1(f) and Q2(f). However this is not discussed here, since their respective truncation errors E1(f) and E2(f) arc of the same sign.

5. CONCLUSION

Our research has focused on finding ways to improve numerical integration's accuracy and computing performance via the use of derivatives in novel quadrature formulae that are both cost- and time-efficient. When dealing with complex integrals requiring high accuracy, these approaches overcome the shortcomings of classic quadrature techniques. The suggested formulae are well suited for computationally difficult issues since they use derivatives to decrease the number of necessary function evaluations while keeping or enhancing accuracy. The suggested approaches show broad error boundaries, guaranteeing dependability across varied applications, as shown by a detailed error analysis. Numerical investigations corroborated the theoretical results, demonstrating that the new formulae outperformed older methods like the Trapezoidal and Simpson's rules in terms of accuracy while using much less computing power. Applications in computational mathematics, engineering, and physics that need accurate numerical integration stand to benefit greatly from the suggested approaches. Nevertheless, there are still certain restrictions, such the fact that derivative computations may be somewhat complicated in some cases. Exploring adaptive strategies to further increase their adaptability and efficiency and expanding these methods to multidimensional integrals might be the subject of future effort.

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