



A Modified Four-point Closed Mid-point Derivative Based Quadrature Rule for Numerical Integration

M. M. SHAIKH⁺⁺, M. S. CHANDIO*, A. S. SOOMRO*

Department of Basic Sciences and Related Studies, Mehran University of Engineering and Technology, Jamshoro.

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Abstract: In this work, a new four-point closed quadrature rule is proposed for numerical integration. The proposed quadrature rule appears to be an efficient modification of Zhao and Li's mid-point derivative based Simpson's 3/8 rule (MDS38) which used fourth order mid-point derivative in each strip of integration. While the proposed Simpson's 3/8 rule uses only the second order mid-point derivative in each strip of integration, we show through numerical experiments that it results in smallest error bounds as compared to the Zhao and Li's MDS38 rule and the original Newton-Cote's Simpson's 3/8 rule (Original S38).

Keywords: Quadrature rule, Numerical integration, Simpson's 3/8 rule.

1. INTRODUCTION

The primary goal of numerical integration lies in providing handy alternatives to approximate definite integrals with finite limits of integration. The main idea is to sum the integrand evaluations at specified nodes by partitioning the interval of integration. This approach appears to be very useful and in some cases the only way-out when the integrand is so complex that its analytical determination is time consuming or not possible. Besides, numerical integration is helpful in approximating the integrals when only the discrete behavior of the integrand is known in a bounded range instead of the closed form integrand itself. The existing and modified numerical integration rules also appear to be a basis for the development of new schemes for solving differential, integral and integro-differential equations (Atkinson, 1978; Smyth, 1998).

Newton and Cote proposed closed numerical integration rules which use "N+1" uniformly spaced nodes dividing the original interval into N sub-intervals (Atkinson, 1978). The concept of end-point derivatives to improve accuracy of original Newton-Cote's rules was first introduced in (Atkinson, 1978) by formulating corrected Trapezoidal rule. Meanwhile, the concept of using derivatives to improve accuracy was also used on other original closed Newton-Cote's rules. The corrected Newton-Cote's rules were further analyzed and used by many researchers (Ujevic and Roberts, 2004; Acuet et al., 2008).

Dehghan et al. (2005, 2006) proposed improvements to open and closed Newton-Cote's quadrature rules by considering the width of interval as an additional parameter.

Zhao and Li (2013) proposed new variants of the Newton-Cote's methods which used even order higher

derivative (like: second, fourth, etc.) at the mid-point of each integration strip. Similar works are also due to (Burg, 2012; Burg and Degny, 2013). These rules also exhibit improved order of accuracy, particularly by two more units, than the original quadrature rules.

Recent works on proposing modified closed and open methods for numerical integration by incorporating derivatives are due (Zafar and Mir, 2010; Burg, 2012; Burg and Degny, 2013; Zafaret al., 2014).

In this work, we propose a new variant of Simpson's 3/8 rule which uses four function evaluations and a mid-point second order derivative in each strip of integration. We show in next sections that the proposed Simpson's 3/8 rule (Proposed S38) is an efficient modification of Zhao and Li's MDS38 rule (Zhao and Li, 2013).

2. MATERIALS AND METHODS

2.1 Basic Numerical Integration

The basic idea of numerical integration is to approximate the definite integral by a weighed sum of integrand evaluations at some nodes from the finite interval of integration. This may be described as:

Integral from a to b of f(x) dx approx equal to sum from i=0 to N of c_i f(x_i) (1)

Where f(x) is the integrand, a and b are finite limits of integration; and c_i's are real constants. It should be noted that if the nodes x_i's include both integration limits, then the corresponding scheme is referred as closed - otherwise open - numerical integration rule. Moreover, in the context of closed Newton-Cote's quadrature rules, the nodes x_i's are uniformly spaced and can be obtained by dividing the original interval of integration into

++ Corresponding Author: Muhammad Mujtaba Shaikh, Email: mujtaba.shaikh@faculty.muett.edu.pk

* Institute of Mathematics and Computer Science, University of Sindh, Jamshoro

desired number of sub-intervals. The underlying definition for the nodes is:

$$x_i = a + i \left(\frac{b - a}{N} \right) \quad (2)$$

where $i = 0, 1, 2, \dots, N$ and N is the number of sub-intervals. Equation (1) with nodes defined from (2) appears as the general form of an $(N+1)$ -point closed Newton-Cote's quadrature rule. The constants c_i 's can be found using different derivation approaches, like: Taylor's series approximation, precision concept, etc.

In what follows, we describe formulation of original Simpson's 3/8 rule and its Zhao-Li's version. Finally, we introduce the proposed four-point closed mid-point derivative based Simpson's 3/8 rule for numerical integration.

2.2 Original Simpson's 3/8 (Original S38) Rule

The original Simpson's 3/8 rule was proposed by Newton and Cote (Atkinson, 1978). It is a closed quadrature rule which uses four function evaluations in single strip by dividing the range of integration into three sub-intervals.

The single strip Original S38 rule approximates the integrand with a cubic polynomial and thus the approximation to the integral of $f(x)$ in the range $[a, b]$ is defined as:

$$S_{38} = \frac{b-a}{8} \left[\begin{aligned} & f(a) + 3f\left(\frac{2a+b}{3}\right) \\ & + 3f\left(\frac{a+2b}{3}\right) + f(b) \end{aligned} \right] \quad (3)$$

(Fig. 1) shows that in single strip, say $n = 1$, with three sub-intervals, i.e. $N = 3$, the Original S38 rule uses four uniformly spaced function evaluations to approximate the integral i.e. area under $f(x)$ bounded by the lines $x = a$ and $x = b$.

It is imperative to extend the number of strips if one wants to lower the local error in each strip approximation. Consequently, the composite version of Original S38 with n strips, i.e. with $N = 3n$ sub-intervals (N has to be a multiple of three) is defined as:

$$S_{38}^c = \frac{3h}{8} \left[\begin{aligned} & y_0 + 3 \sum_{i=1}^{N-2} (y_i + y_{i+1}) \\ & + 2 \sum_{i=3}^{N-3} y_i + y_N \end{aligned} \right] \quad (4)$$

where $h = \frac{b-a}{N}$; and $y_i = f(x_i)$ with nodes x_i

defined from (2). (Fig. 2) shows graphical view of the composite version of Original S38 rule. It is also known that the Original S38 rule is fourth order accurate with degree of precision 3.

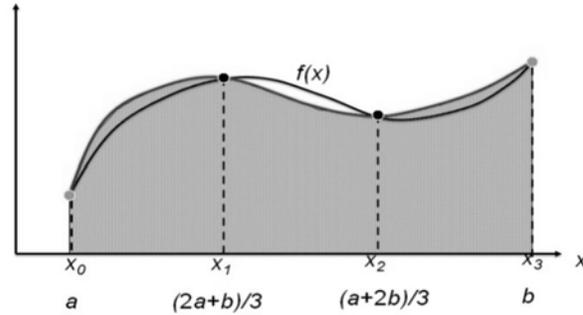


Fig. 1: Simpson's 3/8 rule in one strip ($n=1$) with three sub-intervals ($N=3$).

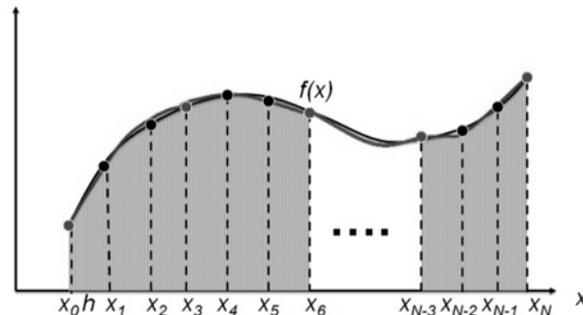


Fig. 2: Composite Simpson's 3/8 rule for "n" strips and $N=3n$ sub-intervals.

2.3 Zhao and Li's Mid-point Derivative Based Simpson's 3/8 (MDS38) Rule

Zhao and Li (2013) used the fourth order mid-point derivative in each strip in addition to the four function evaluations in the Original S38 rule and hence increased the order of accuracy of the original rule by two. Zhao and Li's MDS38 rule, sixth order accurate and having precision degree of 5, is defined in equation (5) for single strip and its composite version is given in equation (6).

$$MDS_{38} = \frac{b-a}{8} \left[\begin{aligned} & f(a) + 3f\left(\frac{2a+b}{3}\right) + \\ & 3f\left(\frac{a+2b}{3}\right) + f(b) \end{aligned} \right] \quad (5)$$

$$- \frac{(b-a)^5}{3480} f^{(4)}\left(\frac{a+b}{2}\right)$$

$$MDS_{38}^c = \frac{3h}{8} \left[\begin{aligned} & y_0 + 3 \sum_{i=1}^{N-2} (y_i + y_{i+1}) \\ & + 2 \sum_{i=3}^{N-3} y_i + y_N \\ & - \frac{81h^5}{1160} \sum_{i=0}^{N-1} y_{i+1/2}^{(4)} \end{aligned} \right] \quad (6)$$

2.4 Proposed Modified Mid-point Derivative Based Simpson's 3/8 (Proposed S38) Rule

The main contribution of this work lies in proposing a modification to Zhao and Li's MDS38 rule – which uses fourth order mid-point derivative in each strip to

approximate the definite integral – by using a lower order derivative than the fourth, second order in this work, such that the errors in Proposed S38 are also smaller than the Zhao and Li’s MDS38 rule. We define the proposed four-point closed quadrature rule– which is obtained by collocation technique on one segment Zhao and Li’s rule with mid-point derivative (Zhao and Li, 2013) and the Original S38 rule (3) – in the single strip as:

$$PS38 = \frac{b-a}{200} \left[19f(a) + 81f\left(\frac{2a+b}{3}\right) + 81f\left(\frac{a+2b}{3}\right) + 19f(b) \right] + \frac{(b-a)^3}{150} f''\left(\frac{a+b}{2}\right) \quad (7)$$

The composite version of the Proposed S38 rule can be defined as:

$$PS38^C = \frac{3h}{200} \left[19y_0 + 81 \sum_{i=1}^{N-2} (y_i + y_{i+1}) + 2 \sum_{i=3}^{N-3} y_i + 19y_N \right] + \frac{9h^3}{50} \sum_{i=0}^{N-1} y''_{i+1/2} \quad (8)$$

The order of accuracy and the degree of precision for the proposed rule can be derived by approaches stated in relevant literature. However, without loss of generality, in present work we can assume that the order of accuracy and degree of precision of the proposed S38 rule are at least 6 and 5 respectively. This is obvious from the fact that the performance of the proposed rule is better than the Zhao and Li’s MDS38 (sixth order accurate having degree of precision 5). The numerical experiments in the next section also confirm the same.

3. RESULTS AND DISCUSSION

For comparing the performance of Original S38, Zhao and Li’s MDS38 and Proposed S38 rules, the underlying integration schemes were implemented on various problems. Results on three problems are presented here whose examination also appears in other works.

Example-1: $\int_0^1 \cos x dx = 0.841470984807897$ (Smith, 1992)

Example-2: $\int_0^1 \frac{\ln(1+x)}{1+x^2} dx = 0.272198261287950$ (Zhao and Li, 2013), (Zafar et al., 2014)

Example-3: $\int_0^2 e^{-x^2} dx = 0.882081390762422$ (Burg, 2012; Burg and Degny, 2013; Zafar et al., 2014)

Because exact solutions for Examples 2 and 3 were not available, we have used 16 decimal places’ correct approximation to the same using MATLAB. We have used the concept of absolute errors to test the performance of the results by Simpson’s 3/8 rule variants w.r.t. the exact integration results quoted in Examples 1-3.

The integral in Example-1 was approximated by all rules using number of strips ranging from 1 to 35, equivalently, using number of sub-intervals in the range: 3 to 105. Corresponding absolute errors for this range of number of strips by all discussed methods are shown in (Fig. 3).

(Fig. 4) presents the absolute errors comparison versus the number of strips (from 1 to 40, i.e. for $N = 3:120$) in the three methods for Example-2. This comparison also confirms that the proposed S38 rule has lower error bounds as compared to the Original S38 and MDS38 rules.

The absolute errors caused by approximation to the integrals in Example-3 by the three methods are shown in (Fig. 5). In this example, the integration schemes were used in the range of 1 to 35 number of strips, equivalent to dividing the original interval of integration into the sequence of sub-intervals: {3, 6, ..., 105}.

It is easy to note, in view of (Figs. 3-5), that the absolute errors caused in Examples 1-3 by the Proposed S38 rule are smaller than those by the Original S38 and Zhao and Li’s mid-point derivative based S38 rules throughout the used range of number of strips.

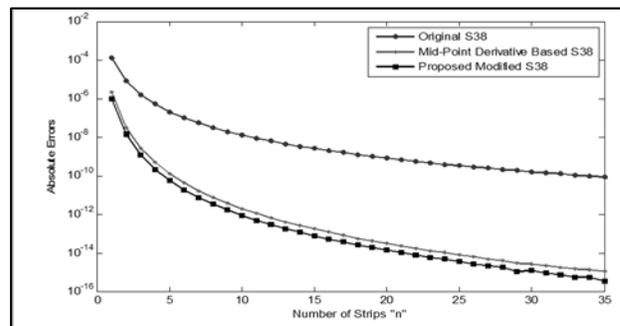


Fig. 3: Absolute errors to approximate integral in Example-1 versus number of strips

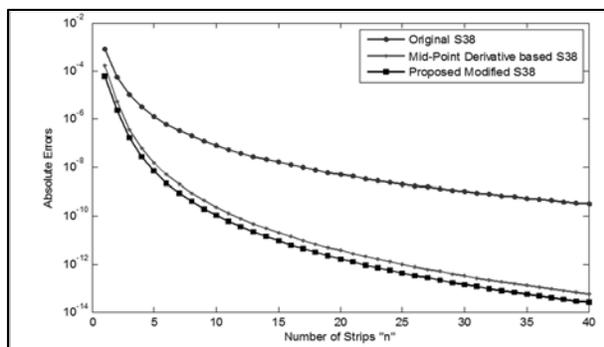


Fig. 4: Absolute errors to approximate integral in Example-2 versus number of strips

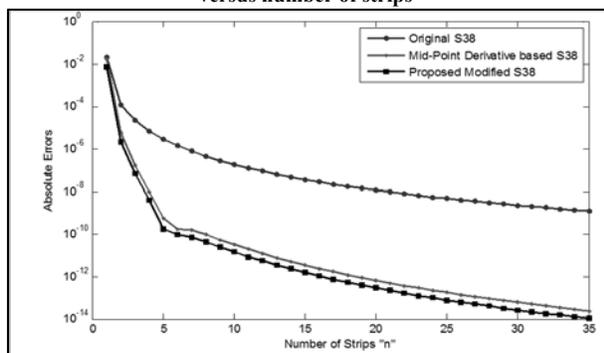


Fig. 5: Absolute errors to approximate integral in Example-3 versus number of strips

It is also worth-mentioning, for a reference we claim in the context of Example-2, that to reach an accuracy of at least 10^{-12} , the Original S38 rule needs 508 evaluations (only functional), the MDS38 rule needs a total of 101 evaluations (76 functional and 25 fourth order derivative); and the Proposed S38 rule needs just 89 evaluations (67 functional and 22 second order derivatives). This shows that the Proposed S38 rule, besides minimizing the computational cost of Zhao and Li's MDS38 rule by using second order mid-point derivative instead of fourth order derivative in each strip, does not compromise on the consequent accuracy (since the errors in presented examples are smaller).

In view of the numerical experiments and the followed discussion, we recommend the Proposed S38 rule as an efficient four-point closed mid-point derivative based quadrature rule for numerical integration in parallel to the Zhao and Li's MDS38 rule which puts more computational burden per strip and has larger magnitude of errors versus proposed rule.

4. CONCLUSION

A new four-point closed mid-point derivative based quadrature rule was proposed for numerical integration. The proposed rule appears to be a modification of the Zhao and Li's mid-point derivative based version of the Simpson's 3/8 rule (Zhao and Li, 2013). The proposed S38 rule minimizes the computational cost of Zhao and Li's MDS38 rule by using the second order derivative –

instead of the fourth order – at mid-point per integration strip without compromising on the accuracy. Infact, the absolute errors contributed by the proposed S38 rule in the three numerical experiments (discussed as Examples 1-3) are smaller than the original and Zhao and Li's mid-point derivative based Simpson's 3/8 rules. The proposed S38 rule, in view of the present analysis, is an efficient four-point variant of the Simpson's 3/8 rule and a good modification of the Zhao and Li's MDS38 rule for numerical integration.

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