A NEW AND EFFICIENT CENTROIDAL MEAN DERIVATIVE-BASED TRAPEZOIDAL SCHEME FOR NUMERICAL CUBATURE

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Abstract

This research presents a new and efficient Centroidal mean derivative-based numerical cubature scheme which has been proposed for the accurate evaluation of double integrals under finite range. The proposed modification is based on the Trapezoidal-type quadrature and cubature rules. The approximate values can only be obtained for some important applications to evaluate the complex double integrals. Higher precision and order of accuracy could be achieved by the proposed scheme. The schemes, in basic and composite forms, with local and global error terms are presented with necessary supporting arguments with their performance evaluation against conventional Trapezoid rule through some numerical experiments. The simultaneously observed error distributions of the proposed schemes are found to be lower than the conventional Trapezoidal cubature scheme in composite form.

Keywords: Cubature, Double integrals, Centroidal mean Derivative-based scheme, Precision, Order of accuracy, Local and global errors, Trapezoid.

I. Introduction

Quadrature and cubature are two distinct terms used for numerical computation. Single integrals are named by quadrature while multiple integrals are enlisted under the name cubature. Scientists and engineers remained interested in calculating the areas and volume of irregular figures that are not familiar with any definite shape as highlighted by Burden and Faires in [IV], as most often such problems are modeled in terms of integrals. To ease the process of analytical
evaluation, numerical integration is recommended. So far different quadrature rules are proposed by mathematicians to focus on single integral problems. However, the problem of evaluating volumes using double integrals is also important [XI].

A unique family of numerical integration of closed Newton-Cotes quadrature rules was presented in [XVIII], these quadrature rules resulted in an increase of twice the orders of precision over the classical closed Newton-Cotes formulas. Authors in [III] modified a numerical scheme and proposed a new numerical integration algorithm for minimizing the errors in a combined interchangeable way. Memon et al. in 2020 [X] developed a new efficient midpoint derivative-based quadrature scheme of trapezoid-type for the Riemann-Stieltjes integrals which is efficient as compared to [XIX]. Shaikh [XVI] in 2019, experimented and compared the polynomial collocation method with uniformly-spaced quadrature rules for the solution of integral equations.

Contribution in the field of computation of numerical integration using arithmetic, geometric and harmonic means derivative-based closed Newton-Cotes rules and comparison of the results with the existing closed Newton-Cotes quadrature (CNC) rules was conducted by Ramachandran et al. in 2016 [XIII]. Shaikh et al. in 2016 [XVI] proposed a modified four-point quadrature rule for numerical integration by using double derivative instead of 4\textsuperscript{th} order derivative and successfully met an efficient end for modification of a method in Zhao et al. [XVIII].

Uncountable old methods and their modifications are present to approximate integrals, for example [V], [II] and [I] by Burg in 2012, Bailey and Borwein in 2011 and Babolian et al. in 2005, respectively. Zafar et al in 2013 [XVII] presented some new inter-connected identities of open Newton-Cotes rules which also involve derivatives with higher accuracy than the classical formulas. Other related work is due to Dehghan and colleagues [VI], [VII], [VIII] in 2005-06, Jain in 2007 [IX], Pal in 2007 [XI], Sastry in 1997 [XIV] and Petrovskaya in 2011 [XII]. Single integrals were exposed to numerous improvements that are shown by the literature, however, negligible work has been done with regards to multiple integrals. The only classical and basic rules the closed Newton-Cotes cubature schemes for double integrals, as discussed in [XI].

An efficient alternation of conventional closed Newton-Cotes Trapezoidal cubature rule (CNCT) by incorporating partial derivatives besides the usual functional evaluations is suggested in this paper. The proposed rule is higher-order accurate and contains higher precision while the errors are comparatively lesser than the existing CNCT schemes.

II. General Formulation and Existing Closed Newton-Cotes Cubature Scheme for Double Integrals

A closer view of numerical formulation of the double integrals over finite rectangles is explained in this portion and the basic form of the Trapezoidal rule extension for cubature in two dimensions with the help of [XI]. This material will help in a comprehensive understanding of the proposed schemes and the main contributions through this research work.

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The general form of the double integrals defined over rectangles in two dimensions is defined as

$$V = \int_c^d \int_a^b f(x, y) \, dx \, dy$$  \hspace{1cm} (1)

where \( V \) is the volume of the surface defined by the integrand over the area element. Here, we carry out evaluation of the double integral over a rectangle \( x=a, x=b, y=c, y=d \) with all limits being finite.

The existing closed Newton-Cotes cubature scheme for double integrals (CNCT double integral scheme) was discussed in [XI] to approximate volume in (1) in the form:

$$CNCT = \int_c^d \int_a^b f(x, y) \, dx \, dy \approx \frac{(b-a)(d-c)}{4} [f(a, c) + f(a, d) + f(b, c) + f(b, d)]$$  \hspace{1cm} (2)

CNCT scheme defined by (2) has a precision degree of one. The composite form of CNCT schemes was not discussed in [XI]. In this work, however, we shall present the composite form in the following section and then present the new and efficient improvements to (2) in basic and composite form.

### III. Present Work and Proposed Centroidal mean Derivative-based Trapezoidal Numerical Cubature Scheme PCMT

First, we highlight that the composite form of CNCT, denoted as CNCT-Cn, with the global error term may be defined as the following Theorem 1, which is completed in a series of the present work [X], and was not discussed in [XI].

**Theorem 1.** Let \( a, b, c, d \) be finite real numbers, and \( f(x, y) \) along with its second order partial derivatives exist and are continuous in \( [a, b] \times [c, d] \). Let \( \{x_i, i=0,1,...,n\} \) and \( \{y_j, j=0,1,...,n\} \) form uniformly spaced partitions of \( [a, b] \) and \( [c, d] \) such that \( b-a = nh \) and \( d-c = nk \) then the CNCT-Cn scheme in composite form for \( n \) elements with the global error term is defined as:

$$CNCT - Cn = \int_c^d \int_a^b f(x, y) \, dx \, dy = \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} \int_{y_j}^{y_{j+1}} f(x, y) \, dx \, dy$$

$$= \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} \frac{h k}{4} [f(x_i, y_j) + f(x_i, y_{j+1}) + f(x_{i+1}, y_j) + f(x_{i+1}, y_{j+1})]$$

$$- \frac{h^2(b-a)(d-c)}{12} f_{xx}(\xi, \eta) - \frac{k^2(b-a)(d-c)}{12} f_{yy}(\xi, \eta)$$

where \( \xi \in (a, b) \) and \( \eta \in (c, d) \)

### Modifications of CNCT Rule in a Basic Form involving derivatives acquires the form:

$$PCMT(a; b, c; d) = \int_c^d \int_a^b f(x, y) \, dx \, dy = CNCT + \sum_{i=1}^{3} D_i \alpha_i$$  \hspace{1cm} (4)

The coefficients \( D_i = h_i(b - a, d - c) \) depends upon limits, we define derivative terms as:

$$\alpha_1 = \sum_{x} f_{xx}(\mu_x, y), \alpha_2 = \sum_{x} f_{xy}(x, \mu_y) \text{ and } \alpha_3 = f_{xxy}(\mu_x, \mu_y).$$

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The notation CNC stands for the existing closed Newton-Cotes cubature scheme and PCMT for the proposed Centroidal mean derivative-based cubature scheme of Trapezoidal-type. In (4), by using centroidal mean CM, we get a new derivative-based scheme, namely PCMT for efficient evaluation of numerical cubature. The coefficients $D_i$'s in the basic forms, and the averages concerning $x$ and $y$ in the existing CNC as well as proposed PCMT cubature schemes are summarized in Table 1.

**Table 1:** Coefficients and means used in CNC and PCMT cubature schemes

| T schemes | $D_1$ | $D_2$ | $D_3$ | $\mu_x$ | $\mu_y$ |
|-----------|-------|-------|-------|---------|---------|
| CNC       | Derivative free | Derivative free | Derivative free | Derivative free | Derivative free |
| PCMT      | $\frac{(b-a)(d-c)^3}{24}$ | $\frac{(b-a)^3(d-c)}{24}$ | $\frac{(b-a)^3(d-c)^3}{144}$ | $\frac{2(a^2+ab+b^2)}{3(a+b)}$ | $\frac{2(c^2+cd+d^2)}{3(c+d)}$ |

The local error terms of the existing CNC and proposed PCMT scheme along with the precision are summarized in Table 2.

**Table 2:** Local error terms and degrees of precision of CNC and PCMT cubature schemes

| T schemes | Local Error terms | Precision |
|-----------|-------------------|-----------|
| CNC       | $-\frac{(b-a)^3(d-c)^3}{12}f_{xx}(\xi, \eta) - \frac{(b-a)(d-c)^3}{12}f_{yy}(\xi, \eta)$ | 1         |
| PCMT      | $-\frac{(b-a)^3(d-c)^3}{72(a+b)}f_{xxx}(\xi, \eta) - \frac{(b-a)(d-c)^3}{72(c+d)}f_{yyy}(\xi, \eta)$ | 2         |

Theorems 2-3 shows the proof of precision degree and local error term of the proposed PCMT cubature scheme respectively.

**Definition 1.** The largest positive integer $n$ for which the exact and approximate results of $f(x, y) = (xy)^n$ are same, is defined as the degree of precision of the cubature scheme.

**Theorem 2.** Let $a, b, c, d$ be finite real numbers, and $f(x, y)$ along with its third order partial derivatives exist and are continuous in $[a, b] \times [c, d]$, then the PCMT scheme in basic form defined in (4) with coefficients in Table 1 has a degree of precision equal to two.

**Proof of Theorem 2.**

Over the rectangle $[a, b] \times [c, d]$, the exact results of the $f(x, y) = (xy)^n$ with $n = 0, 1, 2$ and 3 are given as:

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\[ \int_a^b f(x) dx = (b - a)(d - c) \]  
(5)  
\[ \int_a^b f(x^2) dx = \frac{(b^2-a^2)(d^2-c^2)}{4} \]  
(6)  
\[ \int_a^b f(x^3) dx = \frac{(b^3-a^3)(d^3-c^3)}{9} \]  
(7)  
\[ \int_a^b f(x^4) dx = \frac{(b^4-a^4)(d^4-c^4)}{16} \]  
(8)  
The approximate evaluation of the integral with same values of \( n \) using the proposed PCMT scheme with coefficient in Table 1 and general expression (4) is:  
\[ PCMT(x^0y^0) = (b - a)(d - c) \]  
(9)  
\[ PCMT(xy) = \frac{(b^2-a^2)(d^2-c^2)}{4} \]  
(10)  
\[ PCMT(x^2y^2) = \frac{(b^3-a^3)(d^3-c^3)}{9} \]  
(11)  
\[ PCMT(x^3y^3) = \frac{(b-a)(d-c)}{3b(b+a)(d+c)} \left[ \left\{ 3(b^3 + a^3)(b + a) - 2(b - a)^2(a^2 + ab + b^2) \right\} \right] \]  
(12)  
Comparison of (5)-(8) with (9)-(12) gives:  
For  
\[ n \leq 2, \quad \int_c^d \left( \int_a^b (xy)^n dx \right) dy - PCMT(xy)^n = 0. \]  
(13)  
But if  
\[ n \geq 3, \quad \int_c^d \left( \int_a^b x^n y^n dx \right) dy - PCMT(x^n y^n) \neq 0. \]  
(14)  
Hence by using Definition 1 and (13)-(14), the degree of precision of the PCMT double integral scheme is two.

**Definition 2.** For precision degree \( M \) of a cubature scheme, the leading local error term is defined as the difference between exact and approximate results of an integral in the neighborhood of \((x_0, y_0)\) for the \((M+1)^{th}\) order term in Taylor’s series development of \( f(x, y) \).

**Theorem 3.** Let \( a, b, c, d \) be finite real numbers, and \( f(x, y) \) along with its third-order partial derivatives exist and are continuous in \([a, b] \times [c, d]\), then the local error term of the proposed PCMT scheme in basic form defined in (4) with coefficients in Table 1 is given as:  
\[ LE_{PCMT} = -\frac{(b-a)^3(d-c)}{32(a+b)} f_{xxx}(\xi, \eta) - \frac{(b-a)(d-c)}{32(c+d)} f_{yyy}(\xi, \eta) \]  
(15)  
where \( \xi \in (a, b) \) and \( \eta \in (c, d) \)

**Proof of Theorem 3.**  
Equations (13)-(14), confirm that the degree of precision of the proposed PCMT cubature scheme is 2. To obtain leading local error terms, the third-order term in Taylor’s series expression [XIV] is selected:

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\[
\frac{1}{3!} \left[ (x - x_0)^3 \frac{\partial^3 f}{\partial x^3}(x_0, y_0) + 3(x - x_0)^2(y - y_0) \frac{\partial^3 f}{\partial x^2 \partial y}(x_0, y_0) 
+ 3(x - x_0)(y - y_0)^2 \frac{\partial^3 f}{\partial x \partial y^2}(x_0, y_0) + (y - y_0)^3 \frac{\partial^3 f}{\partial y^3}(x_0, y_0) \right] \tag{16}
\]

The shape for some \( \xi \in (a, b) \) and \( \eta \in (c, d) \) in the local error term of proposed PCMT scheme is:

\[
LE_{PCMT} = \frac{1}{3!} \left[ \int_c^d \int_a^b x^3 dx \, dy - PCMT(x^3) \right] f_{xxx}(\xi, \eta) + \frac{1}{2} \left[ \int_c^d \int_a^b x^2 y dx \, dy - PCMT(x^2y) \right] f_{xxy}(\xi, \eta) 
+ \frac{1}{2} \left[ \int_c^d \int_a^b xy^2 dx \, dy - PCMT(xy^2) \right] f_{yyx}(\xi, \eta) + \frac{1}{3!} \left[ \int_c^d \int_a^b y^3 dx \, dy - PCMT(y^3) \right] f_{yyy}(\xi, \eta) \tag{17}
\]

Implementing required integrals in (17), as the precision of PCMT is 2 the two middle terms vanish, after simplification we finally have:

\[
LE_{PCMT} = \frac{(b-a)^3(d-c)}{72(a+b)} f_{xxx}(\xi, \eta) - \frac{(b-a)(d-c)}{72(c+d)} f_{yyy}(\xi, \eta)
\]

for some \( \xi \in (a, b) \) and \( \eta \in (c, d) \).

For the proposed PCMT scheme in general, the composite form is denoted by \( PCMT-C_n \) which is defined in (18).

\[
PCMT - Cn = \int_c^d \int_a^b f(x, y) \, dx \, dy = \sum_{j=0}^{n-1} \sum_{l=0}^{n-1} PT(x_i; x_{i+1}, y_j; y_{j+1}) \tag{18}
\]

With \( b - a = n h \) and \( d - c = n k \) partitioning the original square element, the averages are the means of each sub-square-element in \( n^2 \) elements.

**IV. Numerical Experiments, Results and Discussion**

To examine the performance of the proposed PCMT cubature scheme and existing CNCT scheme. The following two examples from the literature [XI] are selected.

**Example 1.**

\[
\int_0^1 \int_0^1 xe^{xy} \, dx \, dy
\]

**Example 2.**

\[
\int_1^{23} \frac{1}{1 + x + y} \, dx \, dy
\]
Utilizing MATLAB software, the correct decimal places’ approximations for Examples 1-2 which have been used to compute absolute errors are, respectively, 1.485339738238448 and 0.454026674722594.

Absolute error distributions have been used, which are the numerical difference between the true value of the integrals as mentioned above through MATLAB software and the approximate values obtained through numerical schemes for a various number of elements, $n = 1, 2, 3, \ldots$. Results up to 40 maximum elements are being presented for the educated guess and sufficient understanding of the decreasing trend of absolute errors in different methods.

The absolute errors of the proposed PCMT and existing CNCT scheme for Examples 1-2 are shown in Figs. 1-2 for $n = 1, 2, 3, \ldots, 40$. The proposed scheme shows comparatively lesser errors in both problems. The proposed scheme is an efficient modification of the CNCT rule in basic and composite forms.

The computational cost in terms of several functional and partial derivative evaluations of the CNCT and the proposed PCMT scheme have been compared in Figs. 3-4 for Examples 1-2. The substantial efficiency of the proposed scheme and cost-saving are evident through Figs. 3-4.

V. Conclusion

Through the literature and existing information CNCT scheme has been successfully stretched to composite form in an aforementioned research paper. The new and efficient numerical cubature scheme i.e. PCMT for approximating the double integrals is proposed in basic and generalized composite forms. The theorems concerning the degrees of precision and local error terms have been proved. The suggested scheme is found to be more efficient than the existing CNCT scheme through numerical experiments. The proposed PCMT scheme is valid for all double integral problems in all situations but does not perform better for non-trigonometric integrals. PCMT is very efficient than CNCT when the number of elements is increased for higher digit approximations. The lower absolute error distributions and the reduced computational cost have been the main feature of the proposed cubature scheme.

![Fig 1](image_url). Absolute error distributions versus a number of elements for Example 1.

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Fig 2. Absolute error distributions versus a number of elements for Example 2.

Fig 3. Computational cost (in logarithm scale) to achieve an absolute error of at most 1E-06 from Example 1.
Fig 4. Computational cost (in logarithm scale) to achieve an absolute error of at most 1E-06 from Example 2.

Conflict of Interest:
No conflict of interest regarding this article

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