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SOME NEW AND EFFICIENT DERIVATIVE-BASED SCHEMES FOR NUMERICAL CUBATURE

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Abstract

In this research work, some new derivative-based numerical cubature schemes have been proposed for the accurate evaluation of double integrals under finite range. The proposed modifications are based on the Trapezoidal-type quadrature and cubature rules. The proposed schemes are important to numerically evaluate the complex double integrals, where the exact value is not available but the approximate values can only be obtained. The proposed derivative-based double integral schemes provide efficient results with regards to higher precision and order of accuracy. The proposed schemes, in basic and composite forms, with local and global error terms are presented with necessary proofs with their performance evaluation against conventional Trapezoid rule through some numerical experiments. The consequent 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, Derivative-based schemes, Precision, Order of accuracy, Trapezoid

I. Introduction

The word *quadrature* is usually used for the numerical computation of single integrals, whereas for the multiple integrals and their numerical computation, the word *cubature* is used. Numerical computation of areas and volumes for irregular regions has remained a topic of interest for engineers and scientists, as highlighted by Burden and Faires in [V], as most often such problems are modeled in terms of integrals. When the functions are complicated, so that analytical evaluation of integrals is not possible or is very difficult, then we use numerical integration. Mathematicians have proposed different quadrature rules for approximating areas, which focus on single integral problems. However, the problem of evaluating volumes using double integrals is also important [XIII].

A novel family of numerical integration of closed Newton-Cotes quadrature rules was presented by [XIX], these kinds of quadrature rules obtain an increase of two orders of precision over the classical closed Newton-Cotes formulas. Authors in [IV] modified a numerical scheme and proposed a new numerical integration algorithm for reducing the errors in a combined hybrid way. Memon et al. in 2020 [XI] developed a new efficient midpoint derivative-based quadrature scheme of trapezoid-type for the Riemann-Stieltjes integrals which is an efficient modification of [XXI]. Shaikh [XVII] in 2019, attempted to compare the polynomial collocation method with uniformly-spaced quadrature rules for the solution of integral equations.

Ramachandran et al. in 2016 [XV] worked for the computation of numerical integration using arithmetic, geometric and harmonic means derivative-based closed Newton-Cotes rules and compared the results with the existing closed Newton-Cotes quadrature (CNC) rules. Shaikh et al. in 2016 [XVIII] proposed a modified four-point quadrature rule for numerical integration by using 2^{nd} order derivative instead of 4^{th} order derivative and achieved efficient modification of a method in Zhao et al. [XX]**.**

There are numerous ancient methods and their modifications to approximate integrals, for example [VI], [III] and [II] by Burg in 2012, Bailey and Borwein in 2011 and Babolian et al. in 2005, respectively. Zafar et al in 2013 [XIX] presented some new families of open Newton-Cotes rules which also involve derivatives with higher accuracy than that of the classical formulas. Other related work is due to Dehghan and colleagues [VII], [VIII], [IX] in 2005-06, Jain in 2007 [X], Pal in 2007 [XIII], Sastry in 1997 [XVI] and Petrovskaya in 2011 [XIV].

A lot of contributions in literature have been devoted to the improvements of existing rules of numerical integration for single integrals, whereas not much work is done on multiple integrals. The only classical and basic rules the closed Newton-Cotes cubature schemes for double integrals, as discussed in [XIII].

In this study, we propose some new and efficient modifications of conventional closed Newton-Cotes Trapezoidal cubature rule (CNCT) by incorporating partial derivatives besides the usual functional evaluations. The proposed rules are higher-order accurate and exhibit higher precision while the errors are smaller than the existing CNCT schemes.

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

In this section, we describe the mathematical formulation of the double integrals over finite rectangles, the basic form of the Trapezoidal rule extension for cubature in two dimensions with the help of [XIII]. This material will help understand the proposed schemes and the main contributions through this research work.

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

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

where V is the volume of the surface defined by the integrand over the area element Here, we consider the 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 is (CNCT double integral Scheme) was discussed in [XIII] to approximate volume in (1) in the form:

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

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

III. Present Work and Proposed Derivative-based Numerical Cubature Schemes

First, we mark 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 done in the present work, and was not discussed in [XIII].

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]×[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:*

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

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

$$-\frac{h^2(b-a)(d-c)}{12}f_{xx}\left(\underline{\xi},\underline{\eta}\right)-\frac{k^2(b-a)(d-c)}{12}f_{yy}\left(\underline{\xi},\underline{\eta}\right) \quad (3)$$

$$where\ \underline{\xi}\in(a,b)\ and\ \underline{\eta}\in(c,d)$$

In basic form, we attempt to suggest modifications of CNCT rule by using derivatives in the following form:

$$PT(a{:}b,c{:}d) = \int_c^d \int_a^b f(x,y)\,dx\,dy = CNCT + \sum_{i=1}^{i=3} C_i\phi_i \quad (4)$$

Where $C_i = g_i(b-a,d-c)$are coefficients depending on the limits, and the derivative terms are:

$$\phi_1 = \sum_{\forall y} f_{xx}(\mu_x,y),\ \phi_2 = \sum_{\forall x} f_{yy}(x,\mu_y)\ and\ \phi_3 = f_{xxyy}(\mu_x,\mu_y).$$

The notation PT stands for the proposed derivative-based cubature schemes of Trapezoidal-type. In (4), by using arithmetic, geometric and harmonic means, respectively, AM, GM and HaM, we get three new derivative-based schemes, namely AMT, GMT, HaMT for efficient evaluation of numerical cubature. The coefficients C_i's in the basic forms, and the averages with respect to x and y in the proposed PT cubature schemes are summarized in Table 1.

Table 1: Coefficients and means used in the PT cubature schemes

PT schemes	C_1	C_2	C_3	μ_x	μ_y
AMT	$-\frac{(b-a)(d-c)^3}{24}$	$-\frac{(b-a)^3(d-c)}{24}$	$\frac{(b-a)^3\,(d-c)^3}{144}$	$\frac{a+b}{2}$	$\frac{c+d}{2}$
GMT	$-\frac{(b-a)(d-c)^3}{24}$	$-\frac{(b-a)^3(d-c)}{24}$	$\frac{(b-a)^3\,(d-c)^3}{144}$	$\sqrt{ab}$	$\sqrt{cd}$
HaMT	$-\frac{(b-a)(d-c)^3}{24}$	$-\frac{(b-a)^3(d-c)}{24}$	$\frac{(b-a)^3\,(d-c)^3}{144}$	$\frac{2ab}{a+b}$	$\frac{2cd}{c+d}$

The local error terms in the proposed AMT, GMT and HaMT schemes along with the precision are summarized in Table 2.

Table 2: Local error terms and degrees of precision of PT cubature rules

PT schemes	Local Error terms	Precision
AMT	$-\frac{(b-a)^5(d-c)}{480}f_{xxxx}(\xi,\eta)-\frac{(b-a)(d-c)^5}{480}f_{yyyy}(\xi,\eta)$	3
GMT	$-\frac{(b-a)^3(d-c)}{24}\left(\sqrt{b}-\sqrt{a}\right)^2 f_{xxx}(\xi,\eta) -\frac{(b-a)(d-c)^3}{24}\left(\sqrt{d}-\sqrt{c}\right)^2 f_{yyy}(\xi,\eta)$	2
HaMT	$-\frac{(b-a)^5(d-c)}{24(a+b)}f_{xxx}(\xi,\eta)-\frac{(b-a)(d-c)^5}{24(c+d)}f_{yyy}(\xi,\eta)$	2

For example verification and understanding, we prove the precision degree and derive the local error term of the proposed AMT cubature scheme in Theorems 2-3, respectively.

Definition 1. The highest positive integer value of n for which a cubature schemes exactly integrate $f(x,y)=(xy)^n$ 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 fourth-order partial derivatives exist and are continuous in [a, b]×[c, d], then the AMT* *scheme in basic form defined in (4) with coefficients in Table 1 has a degree of precision equal to three.*

Proof of Theorem 2.

The exact double integrations of the $f(x, y) = (xy)^n$ with n = 0, 1, 2, 3 and 4 are given as, over the rectangle [a, b]×[c, d]:

$$\int_c^d \int_a^b (1)\, dx\, dy = (b-a)(d-c) \tag{5}$$

$$\int_c^d \int_a^b (xy)\, dx\, dy = \frac{(b^2-a^2)(d^2-c^2)}{4} \tag{6}$$

$$\int_c^d \int_a^b (x^2y^2)\, dx\, dy = \frac{(b^3-a^3)(d^3-c^3)}{9} \tag{7}$$

$$\int_c^d \int_a^b (x^3y^3)\, dx\, dy = \frac{(b^4-a^4)(d^4-c^4)}{16} \tag{8}$$

$$\int_c^d \int_a^b (x^4y^4)\, dx\, dy = \frac{(b^5-a^5)(d^5-c^5)}{25} \tag{9}$$

Using the proposed AMT scheme with coefficient in Table 1 and general expression (4), the approximate evaluation of the integral with the same values of n are computed as:

$$AMT(1) = (b-a)(d-c) \tag{10}$$

$$AMT(xy) = \frac{(b^2-a^2)(d^2-c^2)}{4} \tag{11}$$

$$AMT(x^2y^2) = \frac{(b^3-a^3)(d^3-c^3)}{9} \tag{12}$$

$$AMT(x^3y^3) = \frac{(b^4-a^4)(d^4-c^4)}{16} \tag{13}$$

$$AMT(x^4y^4) = \frac{(b-a)(b^4+2b^2a^2+a^4)(d-c)(d^4+2d^2c^2+c^4)}{16} \tag{14}$$

By comparing (5)-(9) with (10)-(14), it appears that:

For

$$n \le 3, \qquad \int_c^d \left(\int_a^b (xy)^n dx\right) dy - AMT(xy)^n = 0. \tag{15}$$

But if

$$n \ge 4, \text{ then } \int_c^d \left(\int_a^b x^4y^4 dx\right) dy - AMT(x^4y^4) \neq 0. \tag{16}$$

Therefore, using Definition 1 and (15)-(16), we conclude that the degree of precision of the *AMT* double integral scheme is three. ■

Definition 2. If the degree of precision of a cubature scheme is M, then the leading local error term is the difference of exact and approximate evaluations of the integral for the (M+1)th order term in the Taylor's series development of $f(x, y)$ defined in the neighborhood of (x_o, y_0).

Theorem 3. *Let a, b, c, d be finite real numbers, and f (x, y) along with its fourth order partial derivatives exist and are continuous in [a, b]×[c, d], then the local* *error term of the proposed AMT scheme in basic form defined in (4) with coefficients in Table 1 is given as:*

$$LE_{AMT} = -\frac{(b-a)^5(d-c)}{480} f_{xxxx}(\xi,\eta) - \frac{(b-a)(d-c)^5}{480} f_{yyyy}(\xi,\eta) \tag{17}$$

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

Proof of Theorem 3.

From equations (15)-(16), is evident that the degree of precision of the proposed AMT cubature scheme is 3. So the leading local error term can be obtained through the exact and AMT integral evaluations of the fourth-order term in Taylor's series expression, which is given as [XVI]:

$$\frac{1}{4!}\begin{bmatrix} (x-x_0)^4 \frac{\partial^4 f}{\partial x^4}(x_0,y_0) + 4(x-x_0)^3(y-y_0)\frac{\partial^4 f}{\partial x^3 \partial y}(x_0,y_0) \\ +6(x-x_0)^2(y-y_0)^2 \frac{\partial^4 f}{\partial x^2 \partial y^2}(x_0,y_0) \\ +4(x-x_0)(y-y_0)^3 \frac{\partial^4 f}{\partial x \partial y^3}(x_0,y_0) + (y-y_0)^4 \frac{\partial^4 f}{\partial y^4}(x_0,y_0) \end{bmatrix} \tag{18}$$

The local error term in the proposed AMT scheme takes the shape for some $\xi \in (a,b)$ and $\eta \in (c,d)$:

$$\begin{aligned} LE_{AMT} = \frac{1}{4!}\left[\int_c^d \int_a^b x^4 dx\,dy - AMT(x^4)\right] f_{xxxx}(\xi,\eta) \\ + \frac{1}{6}\left[\int_c^d \int_a^b x^3 y dx\,dy - AMT(x^3 y)\right] f_{yxxx}(\xi,\eta) \\ + \frac{1}{4}\left[\int_c^d \int_a^b x^2 y^2 dx\,dy - AMT(x^2 y^2)\right] f_{yyxx}(\xi,\eta) \\ + \frac{1}{6}\left[\int_c^d \int_a^b x y^3 dx\,dy - AMT(x y^3)\right] f_{yyyx}(\xi,\eta) \\ + \frac{1}{4!}\left[\int_c^d \int_a^b y^4 dx\,dy - AMT(y^4)\right] f_{yyyy}(\xi,\eta) \end{aligned} \tag{19}$$

Using the exact and approximate evaluations of the integrals in (19), we observe that the three middle terms vanish since the precision of AMT is 3, and then using the exact and approximate integrals of the first and last terms in (19), we have:

$$LE_{AMT} = \frac{1}{4!}\left[\frac{(b^5-a^5)(d-c)}{5} - \frac{(b-a)(b^2+a^2)^2(d-c)}{4}\right] f_{xxxx}(\xi,\eta)$$

$$+\frac{1}{4!}\left[\frac{(b-a)(d^5-c^5)}{5} - \frac{(b-a)(d-c)(d^2+c^2)^2}{4}\right] f_{yyyy}(\xi,\eta) \tag{20}$$

After simplification in (20), we finally have:

$$LE_{AMT} = -\frac{(b-a)^5(d-c)}{480} f_{xxxx}(\xi,\eta) - \frac{(b-a)(d-c)^5}{480} f_{yyyy}(\xi,\eta)$$

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

The composite form of the proposed PT schemes in general, denoted as *PT-Cn*, may be defined as (21).

$$PT - Cn = \int_c^d \int_a^b f(x,y)\, dx\, dy = \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} PT\left(x_i : x_{i+1}, y_j : y_{j+1}\right) \qquad (21)$$

In n^2 elements, the averages are the means of each sub-square-element with $b - a = n\,h$ and $d - c = n\,k$ partitioning the original square element.

IV. Numerical Experiments, Results and Discussion

We use the following two test problems from the literature [XIII] to test the performance of proposed AMT, GMT and HaMT cubature schemes against the conventional CNCT scheme.

Example 1.

$$\int_2^3 \int_1^{3/2} \frac{x+y}{\sqrt{x^2+y^2}} dx dy$$

Example 2.

$$\int_0^2 \int_0^3 x \sin(xy) dx dy$$

With the help of MATLAB software, the correct decimal places' approximations for Examples 1-2 which have been used to compute absolute errors are, respectively, 0.6700784884724 and 3.139707749099465.

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 various number of elements, n = 1,2,3,…. We present results up to a maximum of 40 elements for brevity and a sufficient understanding of the decreasing trend of absolute errors in different methods.

The absolute errors of proposed AMT, GMT and HaMT schemes and existing CNCT scheme for Examples 1-2 are shown in Figs. 1-2 for n = 1,2,3,…,40. All the proposed schemes show reduced errors in both problems, whereas the GMT or AMT taking the lead in one or another problem. However, generally speaking, the AMT is prone to no disadvantage as for as the limits of integration region are concerned, whereas for GMT and HaMT schemes may not be as good as AMT in all problems. Nevertheless, all proposed schemes are efficient modifications of the CNCT rule in basic and composite forms.

The computational cost in terms of the number of functional and partial derivative evaluations of the CNCT, and the proposed AMT, GMT and HaMT schemes have been compared in Figs. 3-4 for Examples 1-2. The substantial efficiency of the proposed schemes and cost saving is evident through Figs. 3-4.

V. Conclusion

In this research work, the CNCT scheme from literature for evaluating numerical cubature has been successfully extended to composite form. Three new and efficient numerical cubature schemes i.e. AMT, GMT and HaMT for approximating the double integrals were proposed in basic and generalized composite forms. The theorems concerning the degrees of precision and local error terms have been proved. All proposed schemes were found to be more efficient than the existing CNCT scheme through numerical experiments. The proposed AMT scheme is applicable to all double integral problems in all situations, even for non-trigonometric integrals AMT is very efficient than CNCT when the number of elements is increased for higher digits approximations. The lower absolute error distributions and the reduced computational cost have been the main feature of the proposed cubature schemes.

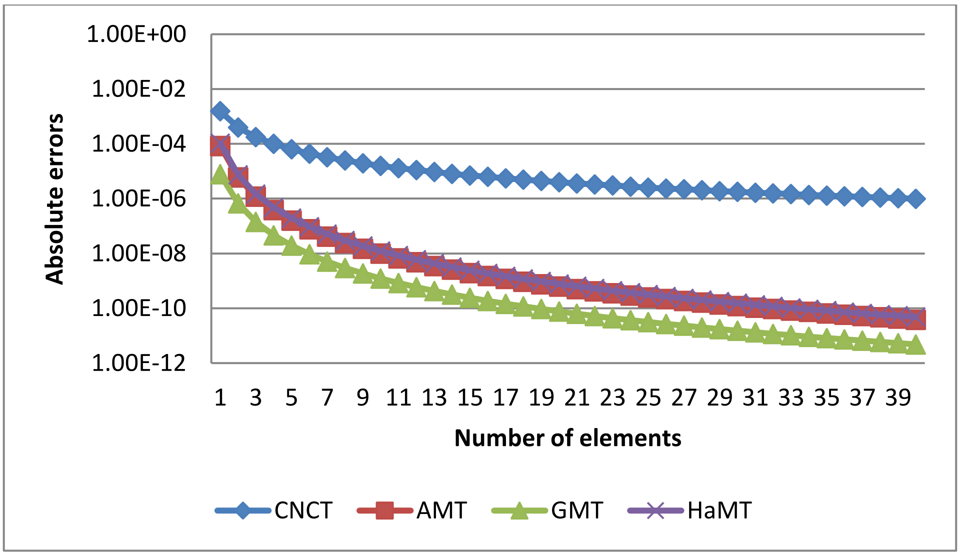

Fig 1. Absolute error distributions versus number of elements for Example 1.

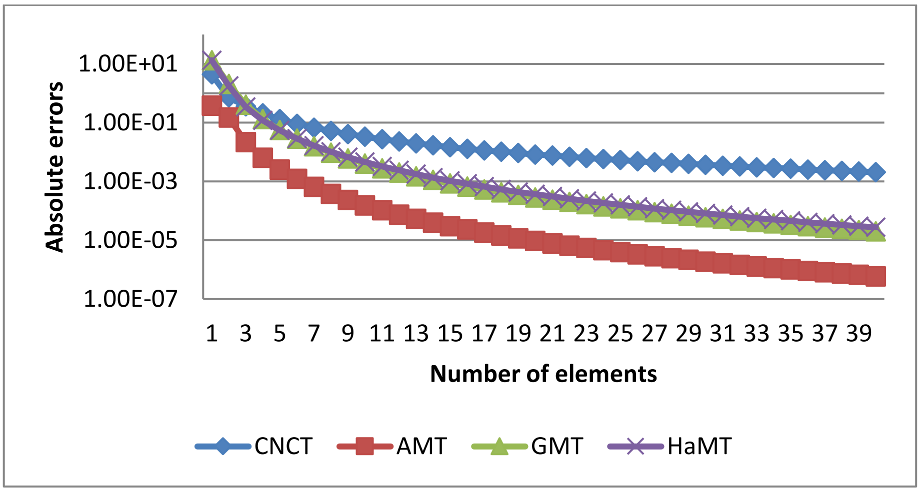

Fig 2. Absolute error distributions versus the number of elements for Example 2.

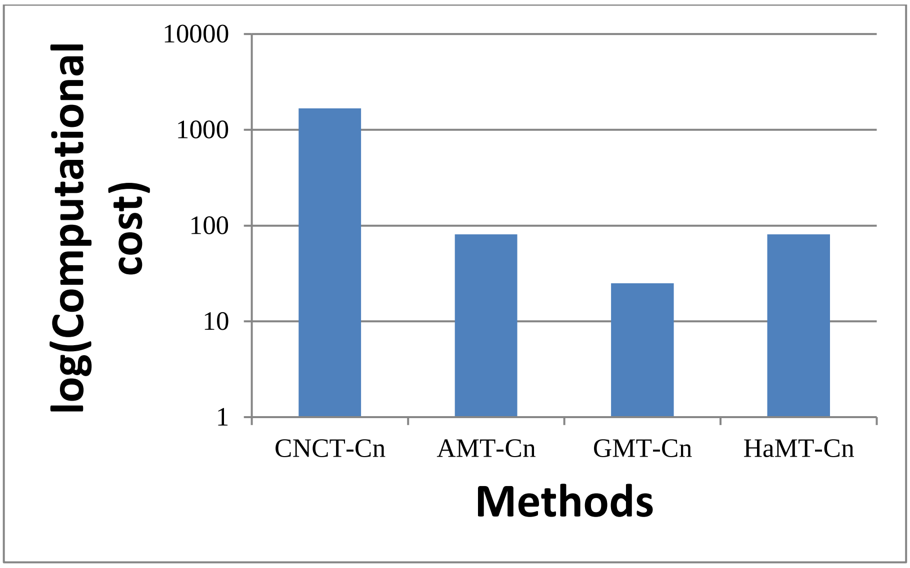

Fig 3. Computational cost (in logarithm scale) to achieve an absolute error of at most 1E-06 from Example 1.

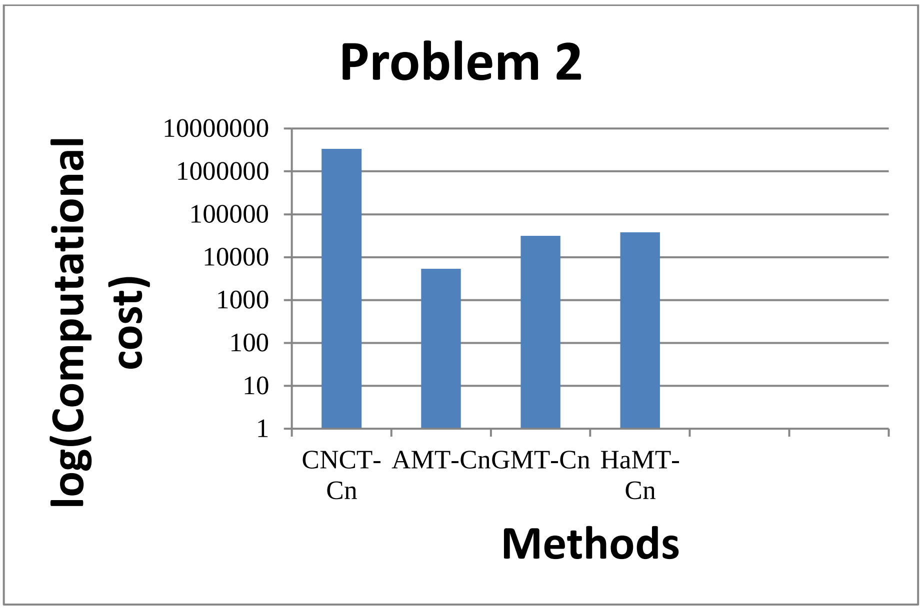

Fig 4. Computational cost (in logarithm scale) to achieve an absolute error of at most 1E-06 from Example 2.

Conflict of Interest :

Authors decleared : There is No conflict of interest regarding this article.

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