Termination Criterion and error analysis of a mixed rule using an anti-Lobatto rule in whole interval and adaptive algorithm

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Abstract: A mixed quadrature rule of higher precision for approximate evaluation of real definite integrals have been constructed using an anti-Lobatto rule. The analytical convergence of the rule has been studied. The error bounds have been determined asymptotically. In adaptive quadrature routines not before mixed quadrature rules basing on anti-Lobatto quadrature rule have been used for fixing termination criterion. Adaptive quadrature routines being recursive by nature, a termination criterion is formed taking in to account a mixed quadrature rule. The algorithm presented in this paper and successfully tested on different integrals by C program. The relative efficiency of the mixed quadrature rule is reflected in the table at the end.

Keywords: Anti-Lobatto rule, Lobatto rule, Fejer’s rule, mixed rule, adaptive algorithm, error analysis, termination criterion.

2000 Mathematics Subject Classification: 65D30, 65D32

1. Introduction:
The Concept of mixed quadrature was first coined by R.N Das and G.pradhan [15].The method of mixing quadrature rules is based on forming a mixed quadrature rule of higher precision by taking linear/convex combination of two quadrature rules of lower precision. Though in literature we find precision enhancement through Richardson Extrapolation and Kronrod extension [11,17,18] taking respectively trapezoidal rule and Gaussian quadrature as base rules, these methods are quite cumbersome. On the other hand, the precision enhancement through mixed quadrature method is very simple and easy to handle. Authors [14-16] have also developed mixed quadrature rules for approximate evaluation of the integrals of analytic functions following F.Lether [10].

So far in this paper in which an anti-Lobatto quadrature rule has been used to construct a mixed quadrature rule by using the concept of anti-Gaussian quadrature formula.

Dirk P. Laurie [1-3,5] is first to coin the idea of anti-Gaussian quadrature formula. An anti-Gaussian quadrature formula is an (n+1) point formula of degree (2n-1) which integrates all polynomials of degree upto (2n+1) with an error equal in magnitude but opposite in sign to that of n-point Gaussian formula. If $H^{(n+1)}(p)$ = $\sum_{i=1}^{n+1} \lambda_i f (\xi_i)$ be (n+1) point anti-Gaussian formula and $G^{(n)}(p)$ be n point Gaussian formula then by hypothesis, $I(p) - H^{(n+1)}(p) = - (I(p) - G^{(n)}(p))$, $p \in P_{2n+1}$ where $p$ is a polynomial of degree $\leq 2n + 1$.

In this paper we design a five point anti-Lobatto rule following LAURIE. We mix this anti-Lobatto five point rule with Fejer’s five point second rule to form a mixed quadrature rule. The relative efficiency of the mixed rule has been shown by numerically evaluating some test integrals.

2. Construction of anti-Lobatto five point rule from Lobatto four point rule.
We choose the Lobatto three point rule:
$Lob_n^4(f) = \frac{1}{6} [f(1) + f(-1) + 5\{f(\frac{1}{\sqrt{5}}) + f(-\frac{1}{\sqrt{5}})\}]$ ................................ (1)

We develop a four point anti-Lobatto rule $RH_n^4(f)$ from three point Lobatto rule $Lob_n^4(f)$. 

ISSN: 2231-5373 http://www.ijmttjournal.org
Using the principle $I(p) - H^{(n+1)}(p) = -\left[I(p) - G^{(n)}(p)\right]$ as adopted in Laurie [1], after simplification we get

$$RH_w^5(f) = 2\int_1^0 f(x)dx - \left(Lob^5_w(f)\right)$$

(2)

$$\Rightarrow w_1f(-1) + w_2f(\xi) + w_3f(\xi_2) + w_4f(\xi_3) + w_5f(1) = 2\int_1^0 f(x)dx - \left(Lob^5_w(f)\right)$$

(3)

Therefore anti-Lobatto five point rule due to Lobatto four point rule is

$$RH_w^5(f) = w_1f(-1) + w_2f(\xi) + w_3f(\xi_2) + w_4f(\xi_3) + w_5f(1)$$

(4)

In order to obtain the unknown weights and nodes, we assume that

(i) The rule is exact for all polynomial of degree $\leq 4$.

(ii) The rule integrates all polynomials of degree up to seven with an error equal in magnitude and opposite in sign to that of Lobatto rule. Thus we obtain following system of eight equations having eight unknowns namely $w_i, i = 1,2,3,4,5$ and $\xi_i, i = 1,2,3$

For $f(x) = x^i, i = 0,1,2,3,4,5,6,7$

Solving the system of equation we get

$$w_1 = -\frac{1}{18}, w_5, w_3 = \frac{64}{69}, w_2 = \frac{245}{414}, w_4, \xi_1 = -\xi_3, \xi_2 = 0$$

$$\xi_1 = \sqrt{\frac{23}{35}}, \xi_2 = 0, \xi_3 = -\sqrt{\frac{23}{35}}$$

Putting the above value in equation (4),we have

$$RH_w^5(f) = w_1f(-1) + w_2f(\xi) + w_3f(\xi_2) + w_4f(\xi_3) + w_5f(0)$$

$$RH_w^5(f) = -\frac{1}{18}\left(f(-1) + f(1)\right) + \frac{245}{414}\left(f(\xi) + f(-\xi)\right) + \frac{64}{69}f(0)$$

(5)

Therefore anti-Lobatto five point rule due to Lobatto four point rule is

$$RH_w^5(f) = -\frac{1}{18}\left(f(-1) + f(1)\right) + \frac{245}{414}\left(f\left(\sqrt{\frac{23}{35}}\right) + f\left(-\sqrt{\frac{23}{35}}\right)\right) + \frac{64}{69}f(0)$$

But the anti-Lobatto five point rule is

$$RH_w^5(f) = w_1f(-1) + w_2f(\xi) + w_3f(\xi_2) + w_5f(0)$$

Hence, by taylors series expansion, we have

$$RH_w^5(f) = 2(\alpha_1 + \alpha_2)f(0) + 2(\alpha_1 \xi_1^2 + \alpha_2 \xi_2^2)f''(0) + 2(\alpha_1 \xi_1^4 + \alpha_2 \xi_2^4)f^{iv}(0)$$

$$+ 2(\alpha_1 \xi_1^6 + \alpha_2 \xi_2^6)f^{vi}(0) + 2(\alpha_1 \xi_1^8 + \alpha_2 \xi_2^8)f^{viii}(0) + ...$$

By putting the values of $\alpha_1, \alpha_2 and \xi_1, \xi_2$ in the above equation, we have

$$RH_w^5(f) = 2f(0) + \frac{2f''(0)}{3!} + \frac{2f^{iv}(0)}{5!} + \frac{118 \times f^{iv}(0)}{75 \times 7 \times 6!} + \frac{122 \times f^{viii}(0)}{125 \times 9 \times 8!} + ...$$

We have,
\[ I(f) = \int_{-1}^{1} f(x)dx = 2f(0) + 2 \frac{f''(0)}{3!} + 2 \frac{f''(0)}{5!} + 2 \frac{f''(0)}{7!} + 2 \frac{f^v(0)}{9!} + ... \]

The error associated with the method is computed as

\[ EH^5_w(f) = I(f) - RH^5_w(f) = \frac{32}{7 \times 75} f^v(0) + \frac{128}{9 \times 125} f^v(0) \]..........................(6)

3. Construction of mixed Quadrature rule by using anti-Lobatto five point rule with Fejers five point second rule.

\[ Fj_5(f) = \frac{2}{45} [7\{f(-\frac{\sqrt{3}}{2}) + f(\frac{\sqrt{3}}{2})\} + 9\{f(-\frac{1}{2}) + f(\frac{1}{2})\} + 13f(0)] \]..........................(7)

Hence, by taylor’s series expansion, we have

\[ Fj_5(f) = 2f(0) + 2 \frac{f''(0)}{3!} + 2 \frac{f''(0)}{5!} + \frac{11 \times f^v(0)}{40 \times 6!} + \frac{1 \times f^v(0)}{5 \times 8!} + ... \]..........................(8)

The error associated with Fejer’s five point rule is computed as

\[ EFj_5(f) = I(f) - Fj_5(f) = \frac{1}{67200} f^v(0) + \frac{1}{9 \times 5} f^v(0) \]..........................(9)

The error associated with the anti-Lobatto five point rule is computed as

\[ EH^5_w(f) = I - RH^5_w(f) = \frac{2}{23625} f^v(0) + \frac{128}{9 \times 125} f^v(0) \]..........................(10)

Eliminating \( f^v(0) \) from the equation (9) and (10), we have

\[ \left( \frac{I(f)}{67200} \right) - \frac{2I(f)}{15750} = \frac{1}{67200} RH^5_w(f) - \frac{2}{23625} Fj_5(f) + \left( \frac{128}{9 \times 125 \times 67200} - \frac{2}{9 \times 5 \times 23625} \right) f^v(0) + ... \]..........................(11)

\[ I(f) = \frac{RH^5_w(f) \times 134400}{110775} - \frac{RH^5_w(f) \times 23625}{110775} + \]..........................(12)

\[ 2 \times \frac{67200 \times 23625}{9 \times 5 \times 23625 \times 110775} \frac{128 \times 67200 \times 23625}{9 \times 125 \times 67200 \times 110775} f^v(0) + ... \]..........................(13)

\[ I(f) = \frac{1}{110775} [134400Fj_5(f) - 23625RH^5_w(f)] + \frac{2688}{22155 \times 9!} f^v(0) + ... \]..........................(14)

\[ I(f) = RH^5_wFj_5(f) + EH^5_wFj_5(f) \]..........................(15)

\[ RH^5_wFj_5(f) = \frac{1}{110775} [134400Fj_5(f) - 23625RH^5_w(f)] \]..........................(16)

\[ EH^5_wFj_5(f) = \frac{1}{110775} [134400EFj_5(f) - 23625EHR^5_w(f)] \]..........................(17)
\[ RH_w^5 F_j^5 f(f) = \frac{1}{110775} \left[ \frac{134400 \times 14}{45} \left( f\left(\frac{\sqrt{3}}{2}\right) + f\left(-\frac{\sqrt{3}}{2}\right) \right) + 9\left( f\left(\frac{1}{2}\right) + f\left(-\frac{1}{2}\right) \right) + 13f(0) \right] + \frac{23625}{18} \left( f(1) + f(-1) \right) - \frac{23625 \times 245}{414} \left( f\left(\frac{\sqrt{35}}{3}\right) + f\left(-\frac{\sqrt{35}}{3}\right) \right) - \frac{23625 \times 64}{69} f(0) \]

This is the desired mixed quadrature rule of precision seven for the approximate evaluation of \( I(f) \). The truncation error generated in this approximation is given by

\[ EH_w^5 F_j^5 f(f) = \frac{1}{110775} \left[ 134400E F_j^5 f(f) - 23625EH_w^5 f(f) \right] \]

or

\[ EH_w^5 F_j^5 f(f) = \frac{2688}{22155 \times 9!} f^{vii}(0) + \ldots \] (14)

\[ \left| EH_w^5 F_j^5 f(f) \right| \approx \frac{2688}{22155 \times 9!} \left| f^{vii}(\eta) \right|_{-1 \leq \eta \leq 1} \]

The rule \( RH_w^5 F_j^5 f(f) \) is called a mixed type rule of precision seven as it is constructed from two different types of the rules of the same precision.

4. **Error analysis:**
   An asymptotic error estimate and an error bound of the rule (11) and (14) are given by.

**Theorem - 4.1**
Let \( f(x) \) be sufficiently differentiable function in the closed interval \([-1,1]\). Then the error

\[ EH_w^5 F_j^5 f(f) \] associated with the rule \( RH_w^5 F_j^5 f(f) \) is given by

\[ \left| EH_w^5 F_j^5 f(f) \right| \approx \frac{2688}{22155 \times 9!} \left| f^{vii}(\eta) \right|_{-1 \leq \eta \leq 1} \]

**Proof**: The theorem follows from (11) and (12) we have,

\[ RH_w^5 F_j^5 f(f) = \frac{1}{110775} \left[ 134400F_j^5 f(f) - 23625RH_w^5 f(f) \right] \]

And the truncation error generated in this approximation is given by

\[ EH_w^5 F_j^5 f(f) = \frac{1}{110775} \left[ 134400EF_j^5 f(f) - 23625EH_w^5 f(f) \right] \]

Hence we have,

\[ \left| EH_w^5 F_j^5 f(f) \right| \approx \frac{2688}{22155 \times 9!} \left| f^{vii}(\eta) \right|_{-1 \leq \eta \leq 1} \]

**Theorem - 4.2**
The bound of the truncation error
\[ \text{If } n \geq 1 \text{, then } R_n f(x) \text{ is given by} \]

\[ R_n f(x) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} F_n(s) e^{sx} ds \]

\[ F_n(s) = \frac{1}{2\pi i} \int_{C} \frac{1}{s^2 + 1} \prod_{j=1}^{n} \left( x - \alpha_j \right)^{-1} \left( x - \beta_j \right)^{-1} \left( x - \gamma_j \right)^{-1} \left( x - \delta_j \right)^{-1} \left( x - \varepsilon_j \right)^{-1} ds \]

\[ \text{where } \alpha_j, \beta_j, \gamma_j, \delta_j, \varepsilon_j \text{ are the roots of } f(t) \text{ and } C \text{ is any contour in the upper half-plane containing the points } \alpha_j, \beta_j, \gamma_j, \delta_j, \varepsilon_j. \]

\[ \text{The error bound for the truncation error } E_n f(x) \text{ is given by} \]

\[ |E_n f(x)| \leq \frac{M}{110775} |x| |x - 1| |x + 1|, \quad -1 < x < 1 \]

\[ \text{where } M = \max_{|x| \leq 1} f^{(n)}(x) \]

\[ \text{Proof:} \quad \text{The proof follows from theorem (4.2)}. \]

\[ \text{Corollary} - 1 \]

The error bound for the truncation error \( E_n f(x) \) is given by

\[ |E_n f(x)| \leq \frac{4M}{110775} \]

\[ \text{Proof:} \quad \text{The proof follows from theorem (4.2)}. \]
5 Numerical verification by table and graphs

Using the results of the table and the notations for the errors of different methods given above the table, four bar graphs for the errors of the mixed quadrature rule and its constituent rules have been constructed in figures A, B, C and D correspond to

\[ I_1 = \int_{-1}^{1} e^x \, dx \]
\[ I_2 = \int_{0}^{1} e^{-x^2} \, dx \]
\[ I_3 = \int_{0}^{1} e^{x^2} \, dx \]
\[ I_4 = \int_{1}^{3} \left( \frac{\sin^2 x}{x} \right) \, dx \]

respectively.

In the four graphs, the error names of the mixed quadrature rule and its constituent rules have been embedded along X-axis and the respective values of the errors depicting heights of the bars are given along Y-axis. The graphical representation of these errors is given above in figures A, B, C, D. From the above four graphs the unit in Y-axis is:

<table>
<thead>
<tr>
<th>Sl No</th>
<th>Integrals</th>
<th>Exact Value</th>
<th>( \text{Lob}_w^4(f)/E_1 )</th>
<th>( \text{RH}_w^5(f)/E_2 )</th>
<th>( \text{Fj}_5(f)/E_3 )</th>
<th>( \text{RH}_w^5\text{Fj}_5(f)/E_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( I_1 = \int_{-1}^{1} e^x , dx )</td>
<td>2.350402387</td>
<td>2.3504899/0.000087</td>
<td>2.350314882/0.000068</td>
<td>2.3504709/0.0000</td>
<td>2.3504023148/0.00000072</td>
</tr>
<tr>
<td>2</td>
<td>( I_2 = \int_{0}^{1} e^{-x^2} , dx )</td>
<td>0.746825</td>
<td>0.74683659/0.00011</td>
<td>0.746811633/0.000013</td>
<td>0.746822002/0.000029</td>
<td>0.7468242/0.000008</td>
</tr>
<tr>
<td>3</td>
<td>( I_3 = \int_{0}^{1} e^{x^2} , dx )</td>
<td>1.4627</td>
<td>1.46297858/0.00027</td>
<td>1.4623254/0.00037</td>
<td>1.4625933/0.000106</td>
<td>1.46265043/0.000049</td>
</tr>
<tr>
<td>4</td>
<td>( I_4 = \int_{1}^{3} \left( \frac{\sin^2 x}{x} \right) , dx )</td>
<td>0.7948251</td>
<td>0.79505264/0.00022</td>
<td>0.7945974/0.000227</td>
<td>0.7947857/0.000039</td>
<td>0.7948259/0.0000008</td>
</tr>
<tr>
<td>5</td>
<td>( I_5 = \int_{0}^{1} \sqrt{x} , dx )</td>
<td>0.666666</td>
<td>0.6568258/0.00984</td>
<td>0.67273993/0.00607</td>
<td>0.667996/0.00133</td>
<td>0.66698455/0.000318</td>
</tr>
</tbody>
</table>

Where \( E_1 = \left| I(f) - \text{Lob}_w^4(f) \right| \), \( E_2 = \left| I(f) - \text{RH}_w^5(f) \right| \), \( E_3 = \left| I(f) - \text{Fj}_5(f) \right| \), \( E_4 = \left| I(f) - \text{RH}_w^5\text{Fj}_5(f) \right| \) are errors of various rules.

The graphical representation of these errors is given below in figures A, B, C, D.
Using the results of the table and the notations for the errors of different methods given above the table, four bar graphs for the errors of the mixed quadrature rule and its constituent rules have been constructed in figures

A, B, C and D correspond to \( I_1 = \int_{-1}^{1} e^x \, dx \), \( I_2 = \int_{0}^{1} e^{-x^2} \, dx \), \( I_3 = \int_{0}^{1} e^{x^2} \, dx \) and \( I_4 = \int_{1}^{3} (\sin^2 \frac{x}{x}) \, dx \)

respectively.

In the four graphs, the error names of the mixed quadrature rule and its constituent rules have been embedded along X-axis and the respective values of the errors depicting heights of the bars are given along Y-axis. The graphical representation of these errors is given above in figures: A, B, C, D. From the above four graphs the unit in Y-axis is:

\[ 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6} \]

Thus from the graphs, we conclude that larger the height of the bar the smaller is the error. Here we derived most significant result that our mixed rule is more accurate than its constituent rules.

6 Adaptive quadrature algorithm

A simple Adaptive Strategy

Given a real integrable function \( f \) an interval \([a, b]\) and a prescribed tolerance \( \varepsilon \), it is desired to compute an approximation \( P \) to the integral \( I = \int_{a}^{b} f(x) \, dx \). So that \( |P - I| \leq \varepsilon \). This can be done following adaptive integration schemes developed in papers [4-7,9,12,13]. In adaptive integration, the points at which the integrand is evaluated are chosen in a way that depends on the nature of the integrand. The basic principle of adaptive quadrature routines is discussed in the following manner.

The idea is that if we can approximate each of the two integrals on the right to within a specified tolerance, then the sum gives us the desired result. If not we can recursively apply the adaptive property to each of the intervals \([a, c]\) and \([c, b]\). Adaptive subdivision of course has geometrical appeal. It seems intuitive that points should be concentrated in regions where the integrand is badly behaved. The whole interval rules can take no direct account of this.

In this paper we design an algorithm for numerical computation of integrals in the adaptive quadrature routines involving mixed rules. The literature of the mixed quadrature rule [9,14-16] involves construction of a symmetric quadrature rule of higher precision as a linear/convex combination of two other rules of equal lower precision.

Algorithm for adaptive quadrature routines:

The input to this schemes is \( a, b, \varepsilon, n, f \), the output \( I \approx \int_{a}^{b} f(x) \, dx \) with the error hopefully less than \( \varepsilon \). \( n \) is the number of intervals initially chosen. A Simple adaptive strategy is outlined in the following step algorithm.

**Step - 1**: An approximation \( I_1 \) to \( I \approx \int_{a}^{b} f(x) \, dx \) is computed.

**Step - 2**: The interval is divided into pieces \([a, c]\) and \([c, b]\).
Where \( c = \frac{a+b}{2} \) and then \( I_2 = \int_a^c f(x)dx \) and

\[
I_3 = \int_c^b f(x)dx
\]

are computed.

**Step - 3**: \( I_2 + I_3 \) is computed with \( I_1 \) to estimate the error in \( I_2 + I_3 \).

**Step - 4**: If \( | \text{estimated error} | \leq \frac{\varepsilon}{2} \) (termination-criterion), then \( I_2 + I_3 \) is accepted as an approximation to \( I \approx \int_a^b f(x)dx \). Otherwise the same procedure is applied to \([a,c]\) and \([c,b]\) allowing each piece a tolerance of \( \frac{\varepsilon}{2} \).

### TABLE - 2

<table>
<thead>
<tr>
<th>Sl No</th>
<th>Integrals</th>
<th>Exact Value</th>
<th>( Lob^4_w(f) )</th>
<th>( RH^5_h(f) )</th>
<th>( Fj_5(f) )</th>
<th>( RH^5_wFj_5(f) )</th>
<th>Prescribed tolerance</th>
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<td>( I_1 = \int_{-1}^1 e^x ) dx</td>
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<td>03</td>
<td>01</td>
<td>01</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>( I_2 = \int_{0}^1 e^{-x^2} ) dx</td>
<td>0.746825</td>
<td>0.74682413</td>
<td>0.746824128</td>
<td>0.746824124</td>
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<td>03</td>
<td>01</td>
<td>01</td>
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<tr>
<td>3</td>
<td>( I_3 = \int_{0}^1 e^{x^2} ) dx</td>
<td>1.4627</td>
<td>1.46265176</td>
<td>1.46265172</td>
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<td>05</td>
<td>03</td>
<td>01</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>( I_4 = \int_{1}^3 \left( \frac{\sin^2 x}{x} \right) ) dx</td>
<td>0.7948251</td>
<td>0.79482521</td>
<td>0.79482514</td>
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<td>0.794825183</td>
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<td>03</td>
<td>03</td>
<td>01</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>( I_5 = \int_{0}^1 \sqrt{x} ) dx</td>
<td>0.666666</td>
<td>0.6666642</td>
<td>0.6666681</td>
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<td>15</td>
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Adaptive quadrature routines essentially consist of applying the mixed rule \( RH^5_wFj_5(f) \) and its constituents rules \( Lob^4_w(f) \), \( RH^5_h(f) \) and \( Fj_5(f) \) are to each of the sub intervals covering until the termination criterion is satisfied. If the termination criterion is not satisfied on one or more the sub intervals, then those subintervals must be
further sub divided and the entire process repeated. The result obtained by a shorter program in standard CPP which should be more transportable and efficient.

7 Observation

In whole interval routine from the table-1 as well as from the bar graph it is observed that the absolute error corresponding to the mixed rule $RH_w^5 F_{j5}(f)$ is lesser than those corresponding to its constituent rules $Lob_w^5 (f), RH_w^5 (f), F_{j5}(f)$ are compared and mixed rule is better than its constituents rules, when the test integrals are evaluated. However when these rules are used in adaptive mode, table-2 depict that the mixed quadrature rule using anti-Gaussian rule give very good result and less number of steps than its constituent rules when tested on a number of integrals.

8. Conclusion:

After observation one can smartly draw conclusion over the efficiency of the rule formed in this paper as follows:

(1) The mixed $RH_w^5 F_{j5}(f)$ rule is more efficient than its constituent rules $Lob_w^5 (f), RH_w^5 (f), F_{j5}(f)$ and previously developed mixed rules.

(2) In this paper we have concentrated mainly on computation of definite integrals in the adaptive quadrature routines involving mixed quadrature rule. We observed that mixed quadrature rule so formed can be very well used for evaluating real definite integrals than its constituent rules in the adaptive quadrature routines.

Acknowledgement:

The research work has been supported by the Department of Science and Technology, Govt. of India under INSPIRE Fellowship and my code no is IF10203. I also thankful to Director and Professor of Institute of Mathematics and Application, BBSR, Odisha, India (my place of research), who guide me and provide good research facilities.

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