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Approximate Numerical Solution of Singular Integrals and Singular Initial Value Problems

Md. Habibur Rahaman[1, *], M. Kamrul Hasan[2], Md. Ayub Ali[1], Md. Shamsul Alam[2]

[1]Department of Mathematics, Jagannath University, Dhaka, Bangladesh

[2]Department of Mathematics, Rajshahi University of Engineering & Technology, Rajshahi, Bangladesh

Email address:
habiburhpr@gmail.com (M .H. Rahaman), mkh2502@yahoo.com (M. K. Hasan), ayub_ju@yahoo.com (M. A. Ali), msalam1964@yahoo.com (M. S. Alam)

[*]Corresponding author

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Abstract: Numerical integration is one of the important branch of mathematics. Singular integrals arises in different applications in applied and engineering mathematics. The evaluation of singular integrals is one of the most challenging jobs. Earlier different techniques were developed for evaluating such integrals, but these were not straightforward. Recently various order straightforward formulae have been developed for evaluating such integrals but; all these integral formulae depend on Romberg technique for more accurate results. Based on these integral formulae, different order (up to fifth) implicit methods have been developed for solving singular initial value problems. These implicit methods give better results than those obtained by implicit Runge-Kutta methods but; the derivation of such higher order formulae are not so easy. In this article, a new third order straightforward integral formula has been proposed for evaluating singular integrals. This new formula is able to evaluate more efficiently than others existing formulae, moreover it has the independent ability to calculate very near accurate result to the exact value of the numerical integrals. Based on this new integral formula a new third order implicit method has been proposed for solving singular initial value problems. The new method provides significantly better results than other existing methods.

Keywords: Singular Integrals, Romberg Scheme, Singular Initial Value Problems, Implicit Runge-Kutta Methods

1. Introduction

Newton-Cotes formulae are worldwide used tools for evaluating numerical integrals; but cannot be used directly for singular cases [1]. Gauss's quadrature formulae and its extended formulae are used to evaluate such singular integrals [2]. Earlier, Fox used extrapolation technique for evaluating these integrals by Trapezoidal and Simpson's rules [3]. Fox also established a formula (called U formula) for evaluating these integrals [3]. Later than, Huq et al. [4], Hasan et al. [5] and Rahaman et al. [6, 7] derive different order straightforward formulae for evaluating such type of singular integrals; but most of the formulae used Romberg scheme for better accuracy.

The studies of singular initial value problems have concerned the interest of many mathematicians and physicists in the recent years. First order singular initial value problems are encountered in ecology in the computation of avalanche run-up [8]. For the numerical solution of first order singular initial value problems, various schemes have been applied. Auzinger et al. [9] and Koch et al. [10, 11] applied well-known acceleration technique Iterated Defect Correction (IDeC) based on implicit Euler method to obtain high accuracy. Recently, Hasan et al. [12-16] derived second and third order implicit formulae based on the integral formulae for solving initial value problems having an initial singularity. Most Recently, Rahaman et al. [17] derived the third, fourth and fifth order implicit methods for solving initial value problems having initial singular point based on integral formulae. These implicit formulae give more accurate results than those obtained by the implicit Euler and implicit Runge-Kutta (RK2, RK3 and RK4) methods for first order singular initial value problems. In this article, a new third order integral formula has been proposed for evaluating singular integrals by introducing a small parameter ε . Based on the integral formula a third order implicit formula has been derived for solving initial value problems.

2. Methodology

In this section, first we discuss some recent existing formulae related to this topic and then the proposed formula has been derived.

2.1. Recent Existing Formulae

Earlier Huq et al. [4] derived a numerical integral formula for evaluating definite integral having an initial singular point at $x = x_0$ by choosing x_0, x_1, x_2 and using the Lagrange's interpolation formula as

$$f(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f_1 + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f_2 \tag{1}$$

Considering $x_1 = x_0 + h/3$ and $x_2 = x_0 + h$ and integrating Eq. (1) within limits x_0 to x_2, obtained the integral formula as

$$\int_{x_0}^{x_2} f(x)dx = h\left(3f_1 + f_2\right)/4 . \tag{2}$$

Based on formula (2), Hasan et al. [13] derived second order implicit formula as

$$y_{i+1} = y_i + h\left[3f(x_i + h/3, (y_i + (y_{i+1} - y_i)/3)) + f(x_i + h, y_{i+1})\right]/4 , \tag{3}$$

where $i = 0, 1, 2,..$ for solving initial value problems

$$y'(x) = f(x, y), \quad y(x_0) = y_0 \tag{4}$$

having an initial singular point of $f(x, y)$ at $x = x_0$.

Later Hasan et al. [5] derived another integral formula as

$$\int_{x_0}^{x_3} f(x)dx = h\left(4f_1 + 5f_2 + f_3\right)/10 , \tag{5}$$

by choosing $x_1 = x_0 + h/6$, $x_2 = x_0 + 4h/6$ and $x_3 = x_0 + h$. Based on formula (5), Hasan et al. [16] derived the third order implicit formula for solving singular initial value problems having singularity at $x = x_0$ as

$$y_{i+1} = y_i + h\left[4f(x_i + h/6, (y_i + (y_{i+1} - y_i)/6)) + 5f(x_i + 4h/6, (y_i + 4(y_{i+1} - y_i)/6)) + f(x_i + h, y_{i+1})\right]/10 , \tag{6}$$

where $i = 0, 1, 2,...$

In the very recent time, by choosing $x_1 = x_0 + ph$, $x_2 = x_0 + qh$, $x_3 = x_0 + h$; $p = (4 - \sqrt{6})/10$, $q = (4 + \sqrt{6})/10$, $w_1 = (16 - \sqrt{6})$, $w_2 = (16 + \sqrt{6})$, $w_3 = 4$ and using fourth order Lagrange's interpolation formula, Rahaman et al. [17] has been derive an integral formula as

$$\int_{x_0}^{x_3} y(x)\, dx = h\left[w_1 f_1 + w_2 f_2 + w_3 f_3\right]/36 , \tag{7}$$

where f_1, f_2 and f_3 are functional values of $f(x)$ respectively for $x_1 = x_0 + ph$, $x_2 = x_0 + qh$ and $x_3 = x_0 + h$. Based on formula (7) he presented a third order implicit formula for solving initial value problems as

$$y_{i+1} = y_i + h\left[w_1 f(x_i + ph, y_i + p(y_{i+1} - y_i)) + w_2 f(x_i + qh, y_i + q(y_{i+1} - y_i)) + w_3 f(x_i + h, y_{i+1})\right]/36 , \tag{8}$$

where $i = 0, 1, 2,...$

Also utilizing the fifth order Lagrange's interpolation formula, Rahaman et al. [17] derived the fourth order integral formula as

$$\int_{x_0}^{x_4} y(x)\, dx = h\left[w_1 f_1 + w_2 f_2 + w_3 f_3 + w_4 f_4\right], \tag{9}$$

choosing $x_1 = x_0 + ph$, $x_2 = x_0 + qh$, $x_3 = x_0 + rh$, $x_4 = x_0 + h$; $p = 0.08858795951270394$, $q = 0.4094668644407347$, $r = 0.787659461760847$, $w_1 = 0.220462211176768$, $w_2 = 0.3881934688317074$, $w_3 = 0.32884431998006125$ and $w_4 = 0.06250000000000022$.

Based on formula (9), Rahaman et al. [17] derived the fourth order implicit formula as

$$\begin{aligned} y_{i+1} = y_i + h\big[&w_1\ f(x_i + ph, y_i + p(y_{i+1} - y_i)) + w_2\ f(x_i + qh, y_i + q(y_{i+1} - y_i)) \\ &+ w_3\ f(x_i + rh, y_i + r(y_{i+1} - y_i)) + w_4\ f(x_i + h, y_{i+1})\big] \end{aligned} \quad (10)$$

where, $i = 0, 1, 2, ..$.

And, by using sixth order Lagrange's interpolation formula Rahaman et al. [17] derived fifth order integral formula as

$$\int_{x_0}^{x_5} f(x)\, dx = h\big[w_1 f_1 + w_2 f_2 + w_3 f_3 + w_4 f_4 + w_5 f_5\big], \quad (11)$$

where, $x_1 = x_0 + ph$, $x_2 = x_0 + qh$, $x_3 = x_0 + rh$, $x_4 = x_0 + sh$, $x_5 = x_0 + h$, $p = 0.05710419612460134$, $q = 0.27684301367379077$, $r = 0.5835904324091858$, $s = 0.8602401356748276$, $w_1 = 0.14371356081477416$, $w_2 = 0.28135601516952136$, $w_3 = 0.3118265229640613$, $w_4 = 0.2231039010576481$ and $w_5 = 0.03999999999402437$. Based on formula (11), Rahaman et al. [17] derived the fifth order implicit formula as

$$\begin{aligned} y_{i+1} = y_i + h\big[&w_1\ f(x_i + ph, y_i + p(y_{i+1} - y_i)) + w_2\ f(x_i + qh, y_i + q(y_{i+1} - y_i)) \\ &+ w_3\ f(x_i + rh, y_i + r(y_{i+1} - y_i)) + w_4\ f(x_i + sh, y_i + s(y_{i+1} - y_i)) + w_5\ f(x_i + h, y_{i+1})\big] \end{aligned} \quad (12)$$

where, $i = 0, 1, 2, ...$

2.2. Derivation of the Proposed Formula

In [17] (formulae (Eq. (7), (9) and (11))), we observe that the existing higher order formula is giving better result than the lower order because the starting point of the higher order formula is nearer to the singular point than lower order formula. In this respect obtaining the first point nearer to the singular point in a lower order formula, we are trying to obtaining better results as the higher order.

Now by considering four points x_0, x_1, x_2 and x_3 where $x_1 = x_0 + p\,h$, $x_2 = x_0 + qh$, $x_3 = x_0 + h$ and using Lagrange's fourth order interpolation formula

$$\begin{aligned} f(x) = &\frac{(x - x_1)(x - x_2)(x - x_3) f_0}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} + \frac{(x - x_0)(x - x_2)(x - x_3) f_1}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} + \\ &\frac{(x - x_0)(x - x_1)(x - x_3) f_2}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} + \frac{(x - x_0)(x - x_1)(x - x_2) f_3}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)}. \end{aligned} \quad (13)$$

The integration of the first term of Lagrange's formula (13) is obtain as

$$\int_{x_0}^{x_3} f(x) dx = \frac{h(1 - 2q + p(-2 + 6q)) f_0}{12pq}. \quad (14)$$

For excludes f_0 from our new formula, equating the coefficient of f_0 to zero and solving for q, we obtain

$$q = (-1 + 2p)/(-2 + 6p) \quad (15)$$

Now choosing $p = \varepsilon$ where $\varepsilon << 1$ but positive and expanding Eq. (15) for ε in the limit 0 to 1, we obtain

$$q = \frac{1}{2} + \frac{\varepsilon}{2} + O(\varepsilon^2) \quad (16)$$

Then substituting the values of p and q and integrating the Lagrange's formula (*i.e* Eq. (13)) from x_0 to x_3 we obtain our proposed third order formula as

$$\int_{x_0}^{x_3} f(x)\, dx = h[(f_1 + 4f_2 + f_3) + \varepsilon(5f_1 - 4f_2 - f_3)]/6 \quad (17)$$

where the higher order terms of ε has been neglected. It is interesting that, if $\varepsilon = 0$, the formula Eq. (17) reduces to Simpson's 1/3 rule with half spacing.

Based on formula (17), a new third order implicit method has been proposed for solving initial value problem having initial singularity at $x = x_0$ as

$$\begin{aligned} &y_{i+1} = y_i + h\,[f(x_i + ph, y_i + p(y_{i+1} - y_i)) + 4\ f(x_i + qh, y_i + q(y_{i+1} - y_i)) + f(x_i + h, y_{i+1}) \\ &+\varepsilon\,(5f(x_i + ph, y_i + p(y_{i+1} - y_i)) - 4\ f(x_i + qh, y_i + q(y_{i+1} - y_i)) - f(x_i + h, y_{i+1}))]/6, \end{aligned} \quad (18)$$

where, $i = 0, 1, 2, ..$. Generally for both Numerical integrations and Initial value problems, the parameter ε has been chosen as $\varepsilon = 0.05$ and the Romberg scheme has been applied in singular integrals. Moreover displacing the parameter ε to different small values depending on the nature of functions it gives very near accurate results to the exact solutions of numerical integrals.

Table 1. *Approximate values and absolute errors of the integral (19) by existing methods and proposed third order formula (17) for* $\varepsilon = 0.05$.

Formulas	Used ordinates	Approx. Value	Abs. Error	Exact
Huq_2nd	16	1.8396167933	0.1603832067	
Hasan_3rd	12	1.8460350986	0.1539649014	
Rahaman_3rd	12	1.8525557599	0.1474442401	
Rahaman_4th	12	1.8732054149	0.1267945850	2
Rahaman_5th	10	1.8761623901	0.1238376098	
Gauss-Legender	10	1.9170639420	0.0829360580	
Prroposed_3rd	3	1.9641113658	0.0358886342	

3. Examples

In this section, firstly, some singular integral have been evaluated by proposed integral formula Eq. (17) and compare the results among Huq's (*i.e* .Eq. (2)), Hasan's (*i.e.* Eq. (5)), Rahaman's third (*i.e.* Eq. (7)), fourth (*i.e.* Eq. (9)), fifth (*i.e.* Eq. (11)) order integral formulae and Gauss quadrature formula. Then Romberg scheme and choosing optimum value of ε , very near accurate results to the exact values of some integrals have been presented. Secondly, some first order singular initial value problems have been solved by the proposed implicit formula (*i.e.* Eq. (18)) and the compared absolute errors among Hasan's third (*i.e.* Eq. (6)) and Rahaman's third (*i.e.* Eq. (8)), Rahaman's fourth (*i.e.* Eq. (10)) and Rahaman's fifth order (*i.e.* Eq. (12)) implicit formulae has been presented in graphs.

Example 3.1: Consider a singular integral in the form as

$$I = \int_0^1 \frac{1}{\sqrt{x}}\,dx \tag{19}$$

Table 2. *The Romberg scheme of the integral (19) by the proposed formula (17) for* $\varepsilon = 0.05$.

$N(h) =$ 1.9641113657918943	
$N\left(\frac{h}{2}\right) =$ 1.9744124023521268	$N\left(h, \frac{h}{2}\right) =$ 1.999281304522341

Example 3.2: Consider another stronger singular integral in the form as

$$I = \int_0^1 \frac{e^{-x}}{x^{\frac{3}{4}}}\,dx \tag{20}$$

Table 3. *Approximate values and absolute errors of the integral (20) by existing methods and proposed formula (17) for* $\varepsilon = 0.05$.

Formulas	Used ordinates	Approx. Value	Error	Exact
Huq_2nd	16	2.1618969054	1.2174574736	
Hasan_3rd	12	2.1837126223	1.1956417567	
Rahaman_3rd	12	2.2089397760	1.1704146029	
Rahaman_4th	12	2.2934285211	1.0859258578	3.379354379028
Rahaman_5th	10	2.3058271615	1.0735272174	
Gauss-Legender	10	2.5007326738	0.8786217052	
Proposed_3rd	3	2.5398969989	0.8394573801	

Table 4. *The Romberg scheme of the integral (20) by the proposed formula (17) for* $\varepsilon = 0.05$.

$N(h) =$ 2.53989699891691	
$N\left(\frac{h}{2}\right) =$ 2.67086388350260	$N\left(h, \frac{h}{2}\right) =$ 3.36305183100028

Table 5. *Approximate values of the different integrals by proposed integral formula (17) for proper chose or optimum values of* ε .

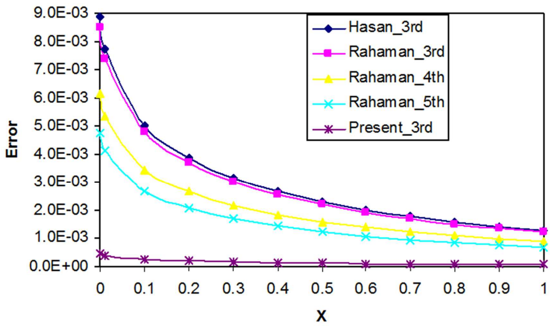
Problems	Optimum values of ε	Exact value	Approx. value	Error
$\int_0^1 \frac{dx}{\sqrt{x}}$	0.045291458012	2	1.9999999999987602	1.2399×10^{-12}
$\int_0^1 \frac{e^{-x}dx}{x^{\frac{3}{4}}}$	0.028278057125	3.3793543790284106	3.3793543790229128	5.49782×10^{-12}
$\int_0^1 \sqrt{x}\,dx$	0.0633974569	$\frac{2}{3}$	0.6666666666665948	7.18314×10^{-14}
$-\int_0^1 x\log x\,dx$	0.07340721	$\frac{1}{4}$	0.2499999999003209	9.96791×10^{-11}
$-\int_0^1 \frac{x\log x\,dx}{1+x}$	0.087639324981	$1-\pi^2/12=$ 0.1775329665758869	0.17753296657884635	2.95938×10^{-12}

Problems	Optimum values of ε	Exact value	Approx. value	Error
$-\int_0^1 \sqrt{x}\log x\,dx$	0.0801627431	$\frac{4}{9}$	0.4444444444468951	2.45071×10^{-12}
$-\int_0^1 \frac{\log x}{\sqrt{x}}dx$	0.036523596871863	4	3.999999999999943	5.68434×10^{-14}
$\int_{0.}^1 e^{-x^2}dx$	0.0498246631	0.746824132812427	0.7468241328126574	2.30371×10^{-13}
$\int_0^\pi x^\pi \operatorname{Sin}\sqrt{x}\,dx$	0.226804165965	27.255515984803424	27.25551598480386	4.36984×10^{-13}

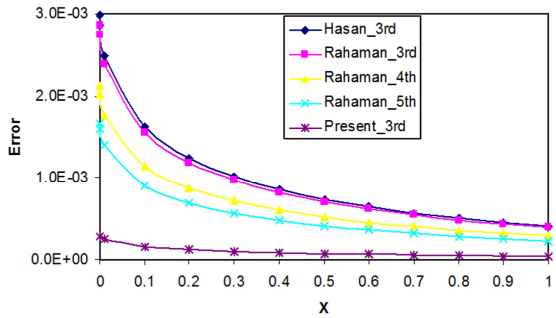
Example 3.4: Consider the first order linear singular initial value problem as

$$y'(x) = -\frac{y(x)}{\sqrt{x}},\quad 0 < x \le 1,\ y(0) = 1 \tag{21}$$

The exact solution of equation (21) is obtained as $e^{-2\sqrt{x}}$. The absolute error of the solution of the equation (21) obtained by the Hasan's [13], Rahaman's [17] and the present method (18) for $\varepsilon = 0.05$ are plotted in *Figure-1 (a)* for $h = 0.001$ and in *Figure-1 (b)* for $h = 0.0001$.



(a)



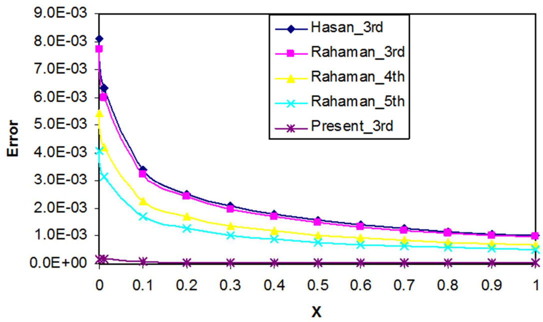
(b)

Figure 1. *The absolute error of the Eq. (21) by different methods for $h = 0.001$ in (a) and for $h = 0.0001$ in (b).*

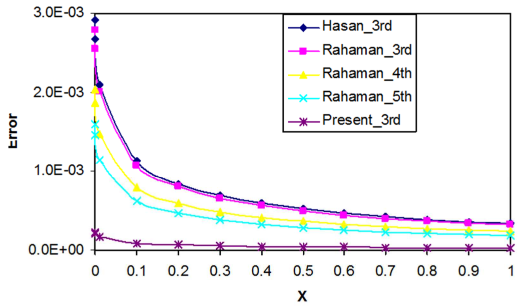
Example 3.5: Considering a first order non-non linear singular initial value problem as

$$y'(x) = -\frac{y^2(x)}{\sqrt{x}},\quad 0 < x \le 1,\ y(0) = 1 \tag{22}$$

The exact solution of equation (22) is obtained as $1/(1+2\sqrt{x})$. The absolute error of the solution of the equation (22) obtained by the Hasan's [13], Rahaman's [17] and the present method (18) for $\varepsilon = 0.05$ are plotted in *Figure-2 (a)* for $h = 0.001$ and in *Figure-2 (b)* for $h = 0.0001$.



(a)



(b)

Figure 2. *The absolute error of the Eq. (22) by different methods for $h = 0.001$ in (a) and for $h = 0.0001$ in (b).*

4. Results and Discussion

The results of singular integrals and singular initial value problems obtained by this proposed method has been compared with others existing methods.

For the singular integral, in Table 1 and Table 3 it is observed that the proposed formula (17) gives significantly better result than existing formulae using fewer ordinates. In Table 2 and Table 4 it is shown that, the Romberg scheme of the proposed formula also converges. In Table 5 it is shown that, without the help of Romberg technique; the proposed formula (17) provides very near accurate results to the exact values of different integrals by proper (optimal) chose of ε depending on the nature of functions.

Also, for first order initial value problems, in Figure 1 (a), Figure 1 (b), Figure 2 (a) and Figure 2 (b), it is observed that, the absolute error of solution of Eqs. (21) and (22) obtained by the proposed formula (18) is smaller than Hasan's [13] and Rahaman's [17] formulae.

5. Conclusion

From the above discussion it is observed that, the proposed third order formula provide significant better results than existing methods both for singular integrals and singular initial value problems. Moreover, the proposed integral formula provide very close results to exact values for optimal choice of parameter ε . So, it may conclude that the proposed third order formula may play an important role in the field of numerical integrations as well as singular initial value problems.

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