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NUMERICAL SOLUTION OF IMPROPER INTEGRALS WITH VALID IMPLEMENTATION

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Abstract- In this paper, two theorems are explained which are used in order to find the improper integral $I = \int_a^{\infty} f(x)dx$ numerically. It has been proved in [4], one can use the Trapezoidal and Simpson rules to find the definite integral $I_m = \int_a^m f(x)dx$ numerically using the CESTAC (Control et Estimation Stochastique des Arrondis de Calculs) method which is based on the stochastic arithmetic, [5-8,12]. These theorems are developed on the improper integrals. Then, the CESTAC method and stochastic arithmetic are used to validate the results and implement the numerical examples. By using this method, one can find the optimal integer number $m \geq 1$ such that $I \sim I_m$. In the last section two examples are solved. The programs have been provided with Fortran 90.

Key words- Stochastic Arithmetic, CESTAC method, Trapezoidal rule, and Simpson rule, Improper Integrals.

1.INTRODUCTION

It has been mentioned in [4], the number of common significant digits between two distinct real numbers a and b, denoted by $C_{a,b}$, can be defined by

$$C_{a,b} = \log_{10}\left|\frac{a+b}{2(a-b)}\right| = \log_{10}\left|\frac{a}{a-b} - \frac{1}{2}\right|. \qquad (1)$$

If $a=b$ then, $C_{a,b} = +\infty$. Also, if $|a-b|$ is small enough, one can take $C_{a,b} \sim \log_{10}\left|\frac{a}{a-b}\right|$. It has been proved in [4], if $I_{m,n}$ is the approximate solution of I_m with step size $h = \frac{m-a}{2^n}$ using the Trapezoidal rule then

$$C_{I_{m,n}, I_{m,n+1}} = C_{I_{m,n}, I_m} + \log_{10}\frac{4}{3} + O(\frac{1}{4^n}), \qquad (2)$$

and using the Simpson rule,

$$C_{I_{m,n}, I_{m,n+1}} = C_{I_{m,n}, I_m} + \log_{10}\frac{16}{15} + O(\frac{1}{16^n}). \qquad (3)$$

The relations (2) and (3) can be developed on the improper integral I, according to the theorems in the next section. In these theorems an integer number $m \geq 1$ is considered so that

$$I = I_m + O(\frac{1}{2^m}). \qquad (4)$$

2.THEORY

2.1- Numerical Solution with the Trapezoidal rule

Let f be a real function and $f \in C^k[a,m]$ for $k \geq 4$.

Theorem 1: Let $I_{m,n}$ be the approximate value of $I_m = \int_a^m f(x)dx$ computed using the Trapezoidal rule with step size $h = \frac{m-a}{2^n}$ where, $m > 2n$ and $I = \int_a^\infty f(x)dx$ has a finite value then

$$C_{I_{m,n},I_{m,n+1}} = C_{I,I_{m,n}} + \log_{10}\frac{4}{3} + O(\frac{1}{2^{m-2n}}) + O(\frac{1}{4^n}). \qquad (5)$$

Proof: According to (4), $I - I_{m,n} = I_m - I_{m,n} + O(\frac{1}{2^m})$ also

$$I_{m,n} - I_m = \frac{h^2}{12}[f'(m) - f'(a)] + O(h^4).$$

Because $h = \frac{m-a}{2^n}$,

$$I_{m,n} - I_m = \frac{1}{4^n}k + O(\frac{1}{16^n}),$$

where, $k = [f'(m) - f'(a)]\frac{(m-a)^2}{12}$, hence

$$\frac{I_{m,n}}{I_{m,n}-I} = \frac{I_{m,n}}{I_{m,n} - I_m + O(\frac{1}{2^m})} = \frac{I_{m,n}}{I_{m,n} - I_m}\left(\frac{1}{1 + \frac{1}{\frac{1}{4^n}k + O(\frac{1}{16^n})}O(\frac{1}{2^m})}\right),$$

$$= \frac{I_{m,n}}{I_{m,n} - I_m}\left(\frac{1}{1 + O\left(\frac{1}{2^{m-2n}}\right)}\right) = \frac{I_{m,n}}{I_{m,n} - I_m}\left(1 - O\left(\frac{1}{2^{m-2n}}\right)\right),$$

and consequently

$$C_{I,I_{m,n}} = \log_{10}\left|\frac{I_{m,n}}{I_{m,n}-I} - \frac{1}{2}\right| \approx \log_{10}\left|\frac{I_{m,n}}{I_{m,n}-I_m}\right| - O(\frac{1}{2^{m-2n}}) = C_{I_{m,n},I_m} - O(\frac{1}{2^{m-2n}}).$$

According to (2)

$$C_{I_{m,n},I_{m,n+1}} = C_{I,I_{m,n}} + \log_{10}\frac{4}{3} + O(\frac{1}{2^{m-2n}}) + O(\frac{1}{4^n}).$$

□

The relation (5) shows that an optimal m where, $m>2n$ exists such that $C_{I_{m,n},I_{m,n+1}} \approx C_{I,I_{m,n}}$.

Therefore for m large enough, the number of common significant digits between $I_{m,n}$ and $I_{m,n+1}$ are almost equal to the number of common significant digits between $I_{m,n}$ and exact value I in company with the term $log_{10}\frac{3}{4} + O(\frac{1}{4^n})$ which is negligible when n increases and the term $O(\frac{1}{2^{m-2n}})$ which is small because $m>2n$. Hence one can find an optimal m so that the number of the significant digits in the error term $|I_{m,n} - I_{m,n+1}|$ becomes zero when n increases from 1 to $\frac{m}{2}-1$. In this case $I_{m,n}$ is an approximate value for I.

2.2- Numerical Solution with the Simpson rule

Let f be a real function and $f \in C^k[a,m]$ for $k \geq 6$.

Theorem2: Let $I_{m,n}$ be the approximate value of $I_m = \int_a^m f(x)dx$ computed using the Simpson rule with step size $h = \frac{m-a}{2^n}$ where, $m > 4n$ and $I = \int_a^\infty f(x)dx$ has a finite value then

$$C_{I_{m,n},I_{m,n+1}} = C_{I,I_{m,n}} + \log_{10}\frac{16}{15} + O(\frac{1}{2^{m-4n}}) + O(\frac{1}{16^n}). \qquad (6)$$

Proof: We know $I_{m,n} - I_m = \frac{h^4}{180}\left[f^{(3)}(m) - f^{(3)}(a)\right] + O(h^6)$. Therefore, we conclude

$$I_{m,n} - I_m = \frac{1}{16^n}k' + O(\frac{1}{64^n}),$$

where, $k' = \left[f^{(3)}(m) - f^{(3)}(a)\right]\frac{(m-a)^4}{180}$, hence

$$\frac{I_{m,n}}{I_{m,n}-I}=\frac{I_{m,n}}{I_{m,n}-I_m+O(\frac{1}{2^m})}=\frac{I_{m,n}}{I_{m,n}-I_m}\left(\frac{1}{1+\frac{1}{\frac{1}{16^n}k'+O(\frac{1}{64^n})}O(\frac{1}{2^m})}\right)$$

$$=\frac{I_{m,n}}{I_{m,n}-I_m}\left(\frac{1}{1+O(\frac{1}{2^{m-4n}})}\right)=\frac{I_{m,n}}{I_{m,n}-I_m}\left(1-O\left(\frac{1}{2^{m-4n}}\right)\right),$$

and consequently

$$C_{I,I_{m,n}}=\log_{10}\left|\frac{I_{m,n}}{I_{m,n}-I}-\frac{1}{2}\right|\approx\log_{10}\left|\frac{I_{m,n}}{I_{m,n}-I_m}\right|-O(\frac{1}{2^{m-4n}})=C_{I_{m,n},I_m}-O(\frac{1}{2^{m-4n}}).$$

According to (3)

$$C_{I_{m,n},I_{m,n+1}}=C_{I,I_{m,n}}+\log_{10}\frac{16}{15}+O(\frac{1}{2^{m-4n}})+O(\frac{1}{16^n}).$$

□

The relation (6) shows that an optimal m with $m>4n$ exists such that $I_{m,n}\sim I$. Similar to the pervious theorem there is an integer number $m>1$ which the significant digits in the error term $\left|I_{m,n}-I_{m,n+1}\right|$ becomes zero when n increases from 1 to $\frac{m}{4}-1$. In the two following sections the CESTAC method and stochastic arithmetic have been explained briefly.

3.CESTAC METHOD

Let F be the set of all the values representable in the computer. Thus any real value r is represented in the form of $R\in F$ in the computer. It has been mentioned in [12], in a binary floating-point arithmetic with P mantissa bits, the rounding error stems from assignment operator is

$$R=r-\varepsilon\,2^{E-P}\alpha. \quad (7)$$

In relation (7), ε is the sign of r and $2^{-P}\alpha$ is the lost part of the mantissa due to round-off error and E is the binary exponent of the result. In single precision case, $P=24$ and in double precision case, $P=53$. Also if the floating-point arithmetic is as rounding to $+\infty$ or $-\infty$ then $-1\leq\alpha\leq1$.

According to (7), if one wants to perturb the last mantissa bit of the value r, it is sufficient that α is changed in the interval [-1,1]. In the CESTAC method if the arithmetic is considered as rounding to $+\infty$ or $-\infty$, α can he considered as a random variable uniformly distributed on [-1,1]. Thus R, the calculated result, is a random variable and its precision depends on its mean (μ) and its standard deviation (σ).

The idea of CESTAC method is to consider that every result $R \in F$ of a floating-point operation corresponds to two informatical results, one rounded off from below (R^-), the second rounded off from above (R^+), each of them representing the exact arithmetical result r, with equal validity. If one runs a computer program N times, the distribution of the results $R_i, i=1,...,N$ is quasi- Gaussian which their mean is equal to the exact value r, that is $E(R)= r$, [5,7]. This N samples are used for estimating the values μ and σ.

In practice, the samples R_i, are obtained by perturbation of the last mantissa bit of every result R, then the mean of random samples R_i, that is $\overline{R} = \frac{\sum_{i=1}^{N} R_i}{N}$, is considered as the result of an arithmetic operation. If $N=3$, it has been proved in [10,12] that the number of decimal significant digits common to $\overline{R}$ and to the exact value r can be estimated by

$$C_{\overline{R},r} = \log_{10} \frac{|\overline{R}|}{\sigma} - 0.39. \qquad (8)$$

In this formula σ, the standard deviation of the samples R_i, is given by

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N} (R_i - \overline{R})^2}{N-1}}. \qquad (9)$$

In CESTAC method if $C_{\overline{R},r} \le 0$, the informatical result R is insignificant and it means a numerical instability exists in its related line.

4.STOCHASTIC ARITHMETIC

In order to simultaneous implementation of the CESTAC method one should substitute a stochastic arithmetic in place of the floating – point arithmetic. In this way one can run every arithmetic operation N times synchronously before running the next operation. Usually $N=2$ or $N=3$. If $N=3$, (8) can be used to estimate the number of decimal significant digits of any result of any arithmetical operation. By using the stochastic arithmetic, sudden losses of accuracy, numerical instabilities, and the appearance of an insignificant result (stochastic zero) are detected. The term set of stochastic numbers, denoted S, is applied to the set of Gaussian random variables. An element $R \in S$ is denoted $R = (\mu, \sigma^2)$ where μ is the mean value of R and σ its standard deviation. The definitions of stochastic zero and arithmetical operations and comparative operators are as follows [8,11,12].

Definition 1. The $R \in S$ is a "stochastic zero", denoted by $\underline{O}$, if and only if

$$C_{\overline{R},r} \le O \quad OR \quad \overline{R} = O. \quad (10)$$

Definition 2. If $R \in S$ is a " stochastic zero" then, the notation $@0$ is used to show the detection of this case in implementation of the CESTAC method. Hence, if $C_{\overline{R},r} \leq 0$ or $\overline{R} = 0$ then we write $R = @0$.

Definition 3. Let $R_1 = (\mu_1, \sigma_1^2)$ and $R_2 = (\mu_2, \sigma_2^2)$ be elements of S. The four elementary operations, denoted $S^+, S^-, S*$ and $S^/$ are defined as follows:

$$R_1 S^+ R_2 = (\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2),$$

$$R_1 S^- R_2 = (\mu_1 - \mu_2, \sigma_1^2 + \sigma_2^2),$$

$$R_1 S^* R_2 = (\mu_1 . \mu_2, \mu_2^2 \sigma_1^2 + \mu_1^2 \sigma_2^2),$$

$$R_1 S^/ R_2 = (\frac{\mu_1}{\mu_2}, \left(\frac{\sigma_1}{\mu_2}\right)^2 + \left(\frac{\mu_1 \sigma_2}{\mu_2^2}\right)^2); \quad \mu_2 \neq 0.$$

Definition 4. Let $R_1 = (\mu_1, \sigma_1^2)$ and $R_2 = (\mu_2, \sigma_2^2)$ be elements of S. The comparative operators are defined as follows:

$$R_1 S^= R_2 \Leftrightarrow R_1 S^- R_2 = \underline{O},$$

$$R_1 S^> R_2 \Leftrightarrow \mu_1 - \mu_2 > 1.96\sqrt{\sigma_1^2 + \sigma_2^2},$$

$$R_1 S^< R_2 \Leftrightarrow \mu_2 - \mu_1 > 1.96\sqrt{\sigma_1^2 + \sigma_2^2},$$

$$R_1 S^\geq R_2 \Leftrightarrow R_1 S^= R_2 \ or \ \mu_1 \geq \mu_2,$$

$$R_1 S^\leq R_2 \Leftrightarrow R_1 S^= R_2 or \ \mu_1 \leq \mu_2.$$

It has been proved in [6], if $\mu_1 = \mu_2$ then $R_1 S^= R_2$.

Let $a, b, c \in F$, in order to implement the arithmetical operator $c = a \, \omega \, b$, first for any of the values a and b, we obtain $N=3$ random samples as mentioned. The operation ω is in the form of $c_i = a_i \, \omega \, b_i ; i = 1,2,3$, in this new arithmetic. Let μ_a, μ_b and μ_c be the variances of the random samples a_i, b_i and c_i respectively. The result c from implementation the stochastic operation S^ω between two random variables $a, b \in S$ is an element of S. Its mean and variance can be obtained directly using the samples a_i

and b_i so that the relations in definition **3** be established exactly or approximately. At last μ_c is considered as the result of the stochastic operation S^{ω}. The σ_c is used for estimating the number of decimal significant digits of this result [1,2].

5. NUMERICAL EXAMPLES

In this section, two examples are solved. The solutions are obtained by using the Trapezoidal (Th) and Simpson (Sh) rules in the stochastic arithmetic. It has not been used the CADNA library [12] in order to implement the CESTAC method. The results are shown in double precision and the programs have been provided with Fortran 90. At first m=4 in Trapezoidal and m=8 in Simpson rule. Then m increases with step 2. According to the relations (5) and (6) in the previous theorems the conditions $n < \frac{m}{2}$ for Trapezoidal and $n < \frac{m}{4}$ for Simpson rule are considered. For each m, the n increases until the number of significant digits in the difference between two approximate values $I_{m,n}$ and $I_{m,n+1}$ becomes zero. In other word, if $I_{m,n+1} - I_{m,n} = @0$ then, m is an optimal value which yields the approximate of I.

Example 1- In this example, the numerical solution of the improper integral $\int_0^{\infty} e^{-x^2} dx$ is considered. The exact solution is $\frac{\sqrt{\pi}}{2} = 0.8862269254527579$, [3]. The results are obtained using Trapezoidal (Th) and Simpson (Sh) rules in stochastic arithmetic. At first $\int_0^{m} e^{-x^2} dx$ has been solved with a determine m. Then m increases and this integral is solved again. This calculation is continued until a stochastic zero is detected in the difference between two sequential results.

The last values m in tables 1 and 2 are the optimal values.

Table 1
Trapezoidal rule

m	n_{max}	Th
4	1	8.863185461318505E-001
6	2	8.862269679596997E-001
8	3	8.862269254527581E-001
10	4	8.862269254527577E-001
12	5	8.862269254527581E-001

Table 2
Simpson rule

m	n_{max}	Sh
8	1	7.155085204168580E-001
10	2	7.676289922918276E-001
12	2	7.109218621382717E-001
14	3	8.626895370294552E-001
16	3	8.362143022684955E-001
18	4	8.859844119802730E-001
20	4	8.851598079412636E-001
22	5	8.862269249482280E-001
24	5	8.862269112837772E-001
26	6	8.862269254527581E-001
28	6	8.862269254527578E-001
30	7	8.862269254527581E-001

Example 2- In this example, the improper integral $\int_0^{\infty} \frac{\cos x}{(1+x^2)^2} dx$ is evaluated. The exact solution is $\frac{\pi}{2e} = 0.577863674895460$, [9]. This integral is computed like previous example. The results are determined in tables 3 and 4.The last values m in these tables are the optimal values.

Table 3
Trapezoidal rule

m	n_{max}	Th
4	1	6.073989067227689E-001
6	2	5.822252574845663E-001
8	3	5.781670757805998E-001
10	4	5.778449272437490E-001
12	5	5.778297353499192E-001
14	6	5.778861289578933E-001
16	7	5.778628731824415E-001
18	8	5.778556797692490E-001
20	9	5.778686221848727E-001
22	10	5.778643671400727E-001
24	11	5.778608409337444E-001
26	12	5.778650844201345E-001
28	13	5.778643188001559E-001
30	14	5.778624591113437E-001
32	15	5.778640935095384E-001
34	16	5.778641362094003E-001
36	17	5.778631023887175E-001
38	18	5.778634677709927E-001
40	16	5.778639875869761E-001

Table 4
Simpson rule

m	n_{max}	Sh
8	1	6.211093651259351E-001
10	2	4.791966356984850E-001
12	2	5.032810782059101E-001
14	3	5.060642694218668E-001
16	3	4.888465119135796E-001
18	4	5.605837668411248E-001
20	4	5.510278958691134E-001
22	5	5.770513360182029E-001
24	5	5.762621516184915E-001
26	6	5.778626495100095E-001
28	6	5.778574861539080E-001
30	7	5.778624590603949E-001
32	7	5.778640932613278E-001
34	8	5.778641362094233E-001
36	8	5.778631023886115E-001
38	9	5.778637677709814E-001
40	9	5.778639875869904E-001
42	10	5.778633959637324E-001
44	10	5.778636557167814E-001
46	11	5.778638825139500E-001
48	11	5.778635414376049E-001
50	10	5.778636210867866E-001

6.CONCLUSION

The numerical solution of an improper integral in the form of $I = \int_a^{\infty} f(x)dx$ is an important matter in integration discussions. If this integral is convergent, the analytic methods for solving it are complicated. By using the CESTAC method based on the stochastic arithmetic, one can use the Trapezoidal and Simpson rules to approximate it with a definite integral such as $I_m = \int_a^m f(x)dx$ where $m \in N$. One can find an optimal value m so that $I \approx I_{m,n}$. Therefore, the stochastic arithmetic and the CESTAC method are able to approximate a convergent improper integral with a valid implementation and obtain the optimal step.

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