Testing stochastic arithmetic and CESTAC method via polynomial computation

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Abstract. The CESTAC method and its implementation known as CADNA software have been created to estimate the accuracy of the solution of real life problems when these solutions are obtained from numerical methods implemented on a computer. The method takes into account uncertainties on data and round-off errors. On another hand a theoretical model for this method in which operands are gaussian variables called stochastic numbers has been developed. In this paper numerical examples based on the Lagrange polynomial interpolation and polynomial computation have been constructed in order to demonstrate the consistency between the CESTAC method and the theory of stochastic numbers. Comparisons with the interval approach are visualized.

1 Introduction

The CESTAC method is an approach to deal with numerical problems involving uncertainties. It has been created to estimate the accuracy of the solution of real life problems when these solutions are obtained from numerical methods implemented on a computer. Such applications to real life problems can be found in [4], [6], [10] and [11]. This method is of Monte-Carlo-type and consists in performing each arithmetic operation several times using an arithmetic with a random rounding mode, see [2], [12], [13]. In other words, real numbers are considered as random values with some prescribed probabilities. In the simplest case one considers gaussian distributed random values, so-called stochastic numbers. Stochastic numbers possess only two probability parameters: mean value and standard deviation, and allow for simple arithmetic operations over them. Working with them can be considered as a particular case of granular computing in the same way as it has been done for intervals [9]. The difference is that here, intervals are confidence intervals and the operations on them are also different. The classical operations on gaussian continuous functions is called *Stochastic* Arithmetic or more precisely Continuous Stochastic Arithmetic (CSA).

In the CESTAC method a stochastic number is represented by several, say k, samples x_j , j = 1, ..., k, representing a given number x. The operations on these samples are those of the computer in use followed by a random rounding. The samples are randomly generated in a known confidence interval. The mean value

 \overline{x} is the best approximation of the exact value x and the number of significant digits on \overline{x} is computed by:

$$C_{\overline{x}} = \log_{10} \left(\frac{\sqrt{k} |\overline{x}|}{\sigma \tau_{\eta}} \right), \tag{1}$$

wherein

$$\overline{x} = \frac{1}{k} \sum_{j=1}^{k} x_j, \quad \sigma^2 = \frac{1}{k-1} \sum_{j=1}^{k} (x_j - \overline{x})^2$$

and τ_{η} is the value of the Student distribution for k-1 degrees of freedom and a probability level 0.95. This type of computation on samples approximating the same value is called *Discrete Stochastic Arithmetic (DSA)*.

Operations on stochastic numbers are used as a model for operations on imprecise numbers, i. e. real numbers containing an unknown error, which is supposed to be centered gaussian with a known standard deviation. Some fundamental properties of stochastic numbers are considered in [3], [14].

This work is part of a more general one, which consists in studying the algebraic structures induced by the operations on stochastic numbers in order to provide a good algebraic understanding of the performance of the CESTAC method [1], [7], [8].

The operations addition and multiplication by scalars are well-defined for stochastic numbers and their properties have been studied in some detail. More specifically, it has been shown that the set of stochastic numbers is a commutative monoid with cancelation law in relation to addition. The operator multiplication by -1 (negation) is an automorphism and involution. These properties imply a number of interesting consequences, see, e. g. [7], [8].

In the sequel we first briefly present some algebraic properties of the system of stochastic numbers with respect to the arithmetic operations addition, negation, multiplication by scalars, multiplication between two stochastic numbers and the relation inclusion. This theoretical results are the bases for the numerical experiments presented in the second part of the paper.

2 Stochastic Arithmetic Theory (SAT) approach

A stochastic number a is written in the form a = (a'; a''). The first component a' is interpreted as mean value, and the second component a'' is the standard deviation. A stochastic number of the form (a'; 0) has zero standard deviation and represents a (pure) mean value, whereas a stochastic number of the form (0; a'') has zero mean value and represents a (pure) standard deviation. In this work we shall always assume $a'' \ge 0$; however, in some cases it is convenient to consider negative standard deviations. Denote by \mathbb{S} the set of all stochastic numbers, $\mathbb{S} = \{(a'; a'') \mid a' \in \mathbb{R}, a'' \in \mathbb{R}^+\}$.

Linear operations. For two stochastic numbers $(m_1; s_1)$, $(m_2; s_2)$, $s_1, s_2 \ge 0$, we define addition by

$$(m_1; s_1) + (m_2; s_2) \stackrel{def}{=} (m_1 + m_2; \sqrt{s_1^2 + s_2^2}),$$
 (2)

Multiplication by real scalars $\gamma \in \mathbb{R}$ is defined by:

$$\gamma * (m_1; s_1) \stackrel{def}{=} (\gamma m_1; |\gamma| s_1).$$
(3)

In particular multiplication by -1 (*negation*) is

$$-1 * (m_1; s_1) = (-m_1; s_1), \tag{4}$$

and subtraction of $(m_1; s_1)$, $(m_2; s_2)$ is:

$$(m_1; s_1) - (m_2; s_2) \stackrel{def}{=} (m_1; s_1) + (-1) * (m_2; s_2) = (m_1 - m_2; \sqrt{s_1^2 + s_2^2}).$$
 (5)

Symmetric stochastic numbers. A symmetric (centered) stochastic number has the form $(0; s), s \in \mathbb{R}$. The arithmetic operations (2)–(5) show that mean values subordinate to familiar real arithmetic whereas standard deviations induce a special arithmetic structure that deviates from the rules of a linear space. If we denote addition of standard deviations defined by (2) by " \oplus " and multiplication by scalars by "*", that is:

$$s_1 \oplus s_2 = \sqrt{s_1^2 + s_2^2},\tag{6}$$

$$\gamma * s_1 = |\gamma| s_1, \tag{7}$$

then we can say that the space of standard deviations is an abelian additive monoid with cancellation, such that for any two standard deviations $s, t \in \mathbb{R}^+$, and real $\alpha, \beta \in \mathbb{R}$:

$$\begin{aligned} \alpha * (s \oplus t) &= \alpha * s \oplus \alpha * t, \\ \alpha * (\beta * s) &= (\alpha \beta) * s, \\ 1 * s &= s, \\ (-1) * s &= s, \\ \sqrt{\alpha^2 + \beta^2} * s &= \alpha * s \oplus \beta * s. \end{aligned}$$

Examples. Here are some examples for computing with standard deviations:

 $1 \oplus 1 = \sqrt{2}, \quad 1 \oplus 2 = \sqrt{5}, \quad 3 \oplus 4 = 5, \quad 1 \oplus 2 \oplus 3 = \sqrt{14}.$ Note that $s_1 \oplus s_2 \oplus \ldots \oplus s_n = t$ is equivalent to $s_1^2 + \ldots + s_n^2 = t^2$.

Multiplication of two stochastic numbers. The product of two stochastic numbers $(m_1; s_1)$, $(m_2; s_2)$, $s_1, s_2 \ge 0$, is defined as:

$$(m_1; s_1) \ _{s^*} \ (m_2; s_2) \stackrel{def}{=} \left(m_1 m_2; \ \sqrt{m_2^2 s_1^2 + m_1^2 s_2^2 + s_1^2 \ s_2^2} \right).$$
(8)

Some properties of the multiplication of stochastic numbers are the following: It is easy to show that associativity holds. If X, Y, Z are stochastic numbers then the proof that $X_{s*}(Y_{s*}Z) = (X_{s*}Y)_{s*}Z$ is a straightforward calculation. Concerning the distributivity with addition, it can be seen that it is not true in general. More specifically, the difference $X_{s}*(Y+Z) - (X_{s}*Y + X_{s}*Z)$ has the form (0; s), $s \neq 0$, i. e. it is a symmetric stochastic number. Anyhow, if we denote by Ω the set of symmetric stochastic numbers and the relation between two stochastic numbers defined by: $X \sim Y \stackrel{def}{=} X - Y \in \Omega$, then it can be shown that relation " \sim " is an equivalence and that distributivity holds for the corresponding equivalence classes. A ring structure can thus be obtained for these equivalence classes.

Inclusion. Inclusion of stochastic numbers plays important roles in applications. We next discuss two relations for inclusion of stochastic numbers. The socalled *interval inclusion* (briefly: i-inclusion) is defined for $X_1 = (m_1; s_1), X_2 = (m_2; s_2) \in \mathbb{S}$, by:

$$X_1 \subseteq_i X_2 \iff |m_2 - m_1| \le s_2 - s_1. \tag{9}$$

Note that addition is i-inclusion isotone, that is: $X_1 \subseteq X_2$ implies $X_1 + Y \subseteq X_2 + Y$ [1]. However, it is easy to see that inverse inclusion isotonicity does not hold, i. e. $X_1 + Y \subseteq X_2 + Y$ does not imply $X_1 \subseteq X_2$. If we want that

$$X_1 \subseteq X_2 \Longleftrightarrow X_1 + Y \subseteq X_2 + Y$$

holds in S, then the inclusion relation " \subseteq_s " between two stochastic numbers should be defined by

$$X_1 \subseteq_s X_2 \iff (m_2 - m_1)^2 \le s_2^2 - s_1^2.$$
 (10)

Relation (10) will be called *stochastic inclusion*, briefly: s-inclusion.

Proposition 1. Addition and multiplication by scalars are (inverse) inclusion isotone (invariant with respect to s-inclusion).

Proof. Denote $X_1 = (m_1; s_1), X_2 = (m_2; s_2), X = (m; s) \in \mathbb{S}$. We shall prove that

$$X_1 \subseteq_s X_2 \Longleftrightarrow X_1 + X \subseteq_s X_2 + X.$$

According to (2)

$$X_1 + X = (m_1; s_1) + (m; s) = (m_1 + m; \sqrt{s_1^2 + s^2}),$$

$$X_2 + X = (m_2; s_2) + (m; s) = (m_2 + m; \sqrt{s_2^2 + s^2}),$$

and according to (10) $X_1 + X \subseteq_s X_2 + X$ is equivalent to

$$((m_2 + m) - (m_1 + m))^2 \le (s_2^2 + s^2) - (s_1^2 + s^2),$$

that is $(m_2 - m_1)^2 \leq s_2^2 - s_1^2$, which means that $X_1 \subseteq_s X_2$.

The equivalence $X_1 \subseteq_s X_2 \iff \gamma * X_1 \subseteq_s \gamma * X_2$ is proved similarly. \Box

We shall next compare relations (10) and (9). To this end we introduce an end-point presentation.

End-point presentation. We shall next look for an end-point presentation for stochastic inclusion. This presentation may be useful when dealing with confidence intervals. The confidence interval corresponding to the stochastic number (m; s) is $[m - \gamma s, m + \gamma s]$, where $\gamma > 0$ is a chosen number (usually $\gamma \approx 2$). For simplicity in the sequel we assume $\gamma = 1$, which corresponds to usual compact intervals on \mathbb{R} .

Recall that the relation between the end-point presentation of an interval $A = [a^-, a^+] \subseteq \mathbb{R}$ and its mid-point/radius presentation A = (a'; a'') is given by:

$$a^{-} = a' - a'', \qquad a^{+} = a' + a'';$$

 $a' = (a^{-} + a^{+})/2, \quad a'' = (a^{+} - a^{-})/2$

Recall also the relation $a^+a^- = a'^2 - a''^2$.

The i-inclusion (9) admits a simple end-point presentation, namely for $A \subseteq_i B$ condition $|b' - a'| \leq b'' - a''$ is presented in end-point form as $b^- \leq a^-$, $a^+ \leq b^+$. We next look for an end-point presentation for the s-inclusion (10): $A \subseteq_s B \iff (b' - a')^2 \leq b''^2 - a''^2$.

The condition $(b'-a')^2 \le b''^2 - a''^2$ can be written as $b'^2 - b''^2 + a'^2 + a''^2 \le 2a'b'$. Replacing $b'^2 - b''^2 = b^+b^-$, $a' = (a^- + a^+)/2$, $a'' = (a^+ - a^-)/2$, etc. we obtain: $2b^+b^- + a^{+2} + a^{-2} \le (a^+ + a^-)(b^+ + b^-)$. Thus the end-point condition for s-inclusion obtains the form:

$$A \subseteq_s B \iff a^{+2} + a^{-2} + 2b^+b^- \le (a^+ + a^-)(b^+ + b^-),$$

equivalently: $A \subseteq_s B \iff 2(b^+b^- - a^+a^-) \le (a^+ + a^-)(b^+ + b^- - a^+ - a^-).$

Proposition 2. Interval inclusion (9) implies stochastic inclusion (10).

Proof. We sketch the proof for proper stochastic numbers. Assume that A = (a'; a'') is i-included in B = (b'; b''), $A \subseteq_i B$, which according to (9) means $|b' - a'| \leq b'' - a''$. We have to show that (10) holds true. Note first that from (9) we have $0 \leq a'' \leq b''$. Now from $|b' - a'| \leq b'' - a''$ we have $(b' - a')^2 \leq (b'' - a'')(b'' + a'') = b''^2 - a''^2$.

As a consequence from Proposition 2, stochastic addition is i-inclusion isotone.

3 Application: Lagrange interpolation

The goal of this section is to compare the results obtained with the theory developed in this paper, which is named *Continuous Stochastic Arithmetic (CSA)*, with respective results obtained with the CESTAC method and with interval arithmetic [3], [12]–[14].

As said before, in the CESTAC method, each stochastic variable is represented by a k-tuple of gaussian random values with known mean value m and standard deviation σ . The method also uses a special arithmetic called *Discrete Stochastic Arithmetic (DSA)*, which acts on the above mentioned k-tuples.

Within the scope of granular computing [15], as seen above, CSA operates on stochastic numbers and is directly derived from operations on independent gaussian random variables. Hence a stochastic number is a granule and continuous stochastic arithmetic is a tool for computing with these granules.

Within the same point of view, in DSA which is used in the CESTAC method, a granule is composed by a k-tuple representing k samples of the same mathematical result of an arithmetic operator implemented in floating point arithmetic. These samples differ from each other because the data are imprecise and because of different random rounding. The operator acting on these granules is a floating point operator corresponding to the exact arithmetical operator which is performed k times in a synchronous way with random rounding. Thus the result is also a granule. This granule is called a *discrete stochastic number*. It has been shown that DSA operating on discrete stochastic numbers possesses many properties (but not all) of real numbers; in particular the notion of stochastic zero has been defined [12]–[14]. The CADNA library merely implements the DSA [2].

To compare the two models, a specific library has been developed which implements both continuous and discrete stochastic arithmetic. The computations are done separately. The *CSA* implements the mathematical rules defined in Section 2.

The comparison has been first done on the Lagrangian interpolation method. Let (x_i, y_i) , i = 1, ..., n, be a set of n pairs of numbers where all x_i are different. The Lagrangian polynomial p at the point t is:

$$p(t) = y_0 l_0(t) + y_1 l_1(t) + \dots + y_n l_n(t), \quad l_i(t) = \frac{\prod_{i \neq j} (t - x_j)}{\prod_{i \neq j} (x_i - x_j)}.$$

We consider the situation when the values of y_i are imprecise and x_i are considered exact.

For all examples presented below, we take n = 11; the exact x-values are defined as $x_i = i$, i = 1, ..., n, and the imprecise values y_i are close to 1. This means that in the interval case all intervals y_i have a midpoint 1, whereas in the stochastic case they have a mean value 1.

3.1 Interval approach

Assume first that some guaranteed bounds are given for the y_i 's in the form of intervals Y_i , that is $y_i \in Y_i$, i = 1, ..., n. Then it is well-known that at each t

$$p(t) \in P(t) = l_0(t) * Y_0 + l_1(t) * Y_1 + \dots + l_n(t) * Y_n.$$

The computation of the interval polynomial P(t) has been performed with the Intlab implementation [5] of interval arithmetic. The maximum error on the Y_i value is ierr = 0.02. With the case $Y_i = [1 - ierr; 1 + ierr] = constant$ and $x_i = i, i = 1, ..., 11$, the upper and lower bounds of P are shown on Fig. 1. In this example so-called naive interval arithmetic produces exact (sharp) bounds. Normally, naive interval arithmetic produces pessimistic bounds. In most cases, such sharp bounds cannot be obtained by naive interval arithmetic and more sophisticate methods should be used.

3.2 The Continuous Stochastic Arithmetic

Corresponding computations are performed on stochastic numbers with the CSA. As seen in the preceding sections, this approach is based on operations defined on gaussian random variable $(m; \sigma)$. It is well-known that 95% of the samples of a such variable are inside the interval $[m - 2\sigma, m + 2\sigma]$. Thus, to compare the results with the interval approach, the value of σ is taken $\sigma = ierr/2 = 0.01$, so that $(m; \sigma)$ is equal to (1; 0.01).

The computation has been performed with our specific implementation of CSA. The gray lower and upper curves in the Fig. 2 represent the results of the CSA computation. Each point of the lower curve (respectively the upper curve) is equal to $m - 2\sigma$ (respectively $m + 2\sigma$). More specifically, a set of values $(m_{P(t_i)}; \sigma_{P(t_i)})$ is obtained. Each point of the lower curve (respectively the upper curve) on Fig. 2 is equal to $m_{P(t_i)} - 2\sigma_{P(t_i)}$ (respectively $m_{P(t_i)} + 2\sigma_{P(t_i)}$).

3.3 The Discrete Stochastic Arithmetic

The last goal is to compare the results obtained with CSA and those obtained with the CESTAC method with k samples, i.e. with DSA, k taking successively the values 3, 5, 10, 30. The results obtained for each value of k are reported in figures 3–6 in which the lower and upper curves obtained with the CSA are shown. All figures are composed of two sub-figures. The left sub-figure shows the curves obtained as result of the k samples. The right part compares the computed mean value and standard deviation obtained from the k-samples to the theoretical mean value and standard deviation obtained with CSA.

As observed from the figures, if $\overline{P(t_i)}$ is the mean value of the samples obtained at point t_i with the *DSA* for the computation of $P(t_i)$, then we always have: $m_{P(t_i)} - 2\sigma_{P(t_i)} \leq \overline{P(t_i)} \leq m_{P(t_i)} + 2\sigma_{P(t_i)}$. Thus the numerical experiment shows clearly that the continuous stochastic arithmetic is a good model for the CESTAC method.

4 Computation of a polynomial

In the above section it has been shown experimentally that the theory of stochastic numbers is consistent with the CESTAC method for linear computation. We show now that it is also true in the non-linear case with the computation of the value of a polynomial. Anyhow it must be noted that an hypothesis of the theory is that the stochastic numbers involved in the operations are independent. This





Fig. 1. Lagrange, Interval computations Fig. 2. Lagrange, Interval+CSA



Fig. 3. Lagrange DSA 3 samples+CSA Fig. 4. Lagrange DSA 5 samples+CSA



Fig. 5. Lagrange DSA 10 samples+CSA Fig. 6. Lagrange DSA 30 samples+CSA

hypothesis is clearly not fulfilled in the case of the computation of a polynomial. So one can expect that the order of magnitude of the results are the same for the theoretical and experimental result but that there may be anyhow some differences. In fact these differences may exist but are rather small.

A great number of polynomials have been tested for which the results are always consistent. As an example the results obtained with DSA (experimental), CSA (theoretical) and the values provided by the CADNA software for the two simple polynomials:

$$p(x) = x^{2} - 2x + 1,$$

$$q(x) = x^{3} - 3x^{2} + 3x - 1$$

are reported in Table 1 and Table 2. The values of the polynomials have been computed for several values of x with the CADNA software implementing the CESTAC method (i. e. with the *DSA*) and with the *CSA*. In the *DSA* case, the mean value and standard deviation of the result are reported for k = 3 and k = 20 samples. The values provided by the CADNA software are those obtained with the *DSA* with k = 3 which are printed with as many significant digits as computed by the software, i. e. according to formula (1).

When the value is non-significant then the symbol @.0 is printed.

x	DSA 3 samples	DSA 20 samples	CSA	CADNA3
(2; 0.0001)	(1.000015; 0.000232)	(0.999896; 0.000197)	(1.000000; 0.000346)	0.100E + 001
(2; 0.001)	(0.999401; 0.003352)	(0.999789; 0.002116)	(1.000000; 0.003464)	0.10E + 001
(2; 0.01)	(0.999779; 0.018623)	(1.000769; 0.020472)	(1.000000; 0.034641)	0.90E + 000
(2; 0.1)	(0.853213; 0.104408)	(0.961586; 0.131396)	(1.000000; 0.346411)	@.0
(10; 0.01)	(80.92840; 0.023482)	(81.02938; 0.165771)	(81.00000; 0.142832)	0.81E + 002
(10; 0.1)	(81.58815; 1.031574)	(81.58087; 1.851930)	(81.00000; 1.428320)	0.8E + 002

Table 1. Values of $p(x) = x^2 - 2x + 1$ computed with DSA and CSA

x	DSA 3 samples	DSA 20 samples	CSA	CADNA3
(2; 0.0001)	(0.999796; 0.000196)	(1.000075; 0.000374)	(1.000000; 0.001136)	0.999E + 000
(2; 0.001)	(1.001783; 0.002189)	(0.999558; 0.002989)	(1.000000; 0.011367)	0.10E + 001
(2; 0.01)	(1.018297; 0.029464)	(0.989954; 0.028460)	(1.000000; 0.113670)	0.1E + 001
(2; 0.1)	(1.361246; 0.503563)	(1.013540; 0.313214)	(1.000000; 1.136706)	@.0
(10; 0.01)	(728.7242; 4.028841)	(729.4479; 1.780299)	(729.0000; 1.783594)	0.72E + 003
(10; 0.1)	(720.1993; 23.03887)	(726.4653; 22.87894)	(729.0000; 17.83594)	0.7E + 003

Table 2. Values of $q(x) = x^3 - 3x^2 + 3x - 1$ computed with DSA and CSA

5 Conclusion

Starting from a minimal set of empirically known facts related to stochastic numbers, we formally deduce a number of properties and relations. We investigate the set of all stochastic numbers and show that this set possesses nice algebraic properties. We point out to the distinct algebraic nature of the spaces of mean-values and standard deviations. Based on the algebraic properties of the stochastic numbers we propose a natural relation for inclusion, called stochastic inclusion. Numerical examples based on Lagrange interpolation and polynomial computation demonstrate the consistency between the CESTAC method and the presented theory of stochastic numbers. This is one more justification for the practical use of the CADNA software.

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