Numerical Study of Algebraic Problems Using Stochastic Arithmetic

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Abstract. A widely used method to estimate the accuracy of the numerical solution of real life problems is the CESTAC Monte Carlo type method. In this method, a real number is considered as an N-tuple of Gaussian random numbers constructed as Gaussian approximations of the original real number. This N-tuple is called a "discrete stochastic number" and all its components are computed synchronously at the level of each operation so that, in the scope of granular computing, a discrete stochastic number is considered as a granule. In this work, which is part of a more general one, discrete stochastic numbers are modeled by Gaussian functions defined by their mean value and standard deviation and operations on them are those on independent Gaussian variables. These Gaussian functions are called in this context *stochastic numbers* and operations on them define *continuous stochastic arithmetic (CSA)*. Thus operations on stochastic numbers are used as a model for operations on imprecise numbers. Here we study some new algebraic structures induced by the operations on stochastic numbers in order to provide a good algebraic understanding of the performance of the CESTAC method and we give numerical examples based on the Least squares method which clearly demonstrate the consistency between the CESTAC method and the theory of stochastic numbers.

Keywords: stochastic numbers, stochastic arithmetic, standard deviations, least squares approximation.

1 Introduction

A widely used method to estimate the accuracy of the numerical solution of real life problems is the CESTAC method, see for example [4,6,8,13,14,15,16,17]. In this method, real numbers are considered as vectors of N Gaussian random numbers constructed to be Gaussian approximations of the same value. This vector is called a "discrete stochastic number". The CESTAC method has been implemented in a software called CADNA in which discrete stochastic numbers are computed one operation after the other. In other words all their components are computed synchronously at the level of each operation so that, in the

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scope of granular computing [19], a discrete stochastic number is considered as a granule. Moreover in CADNA the components of a the discrete stochastic numbers are randomly rounded up or down with same probability to take into account the rounding of floating point operators in the same way that directed rounding is used in softwares implementing interval arithmetic. In this work, which is part of a more general one, discrete stochastic numbers are modeled by Gaussian functions defined by their mean value and standard deviation and operations on them are those on independent Gaussian variables. These Gaussian functions are called in this context “stochastic numbers” and operations on them define *continuous stochastic arithmetic (CSA)* also called more briefly *stochastic arithmetic*. Operations on stochastic numbers are used as a model for operations on imprecise numbers. Some fundamental properties of stochastic numbers are considered in [5,18]. Here we study numerically the performance of the CESTAC method [1,2,3,10,11] using numerical examples based on the Least squares method. Our experiments clearly demonstrate the consistency between the CESTAC method and the theory of stochastic numbers and present one more justification for both the theory and the computational practice.

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. [10,11].

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

2 Stochastic Arithmetic Theory (SAT) Approach

A *stochastic number* a is written in the form $a = (m, s)$. The first component m is interpreted as *mean value*, and the second component s is the *standard deviation*. A stochastic number of the form $(m; 0)$ has zero standard deviation and represents a (pure) mean value, whereas a stochastic number of the form $(0; s)$ has zero mean value and represents a (pure) standard deviation. In this work we shall always assume $s \geq 0$. Denote by $\mathbb{S}$ the set of all stochastic numbers, $\mathbb{S} = \{(m; s) \mid m \in \mathbb{R}, s \in \mathbb{R}^+\}$. For two stochastic numbers $(m_1; s_1),\ (m_2; s_2) \in \mathbb{S}$, we define addition by

$$(m_1; s_1) + (m_2; s_2) \stackrel{def}{=} \left(m_1 + m_2;\ \sqrt{s_1^2 + s_2^2}\right), \tag{1}$$

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

$$\gamma * (m_1; s_1) \stackrel{def}{=} (\gamma m_1;\ |\gamma| s_1). \tag{2}$$

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

$$-1 * (m_1; s_1) = (-m_1;\ s_1), \tag{3}$$

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

$$(m_1; s_1) - (m_2; s_2) \stackrel{def}{=} (m_1; s_1) + (-1) * (m_2; s_2) = \left(m_1 - m_2;\ \sqrt{s_1^2 + s_2^2}\right). \tag{4}$$

Symmetric stochastic numbers. A symmetric (centered) stochastic number has the form $(0; s), s \in \mathbb{R}$. The arithmetic operations (1)–(4) 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 (1) by "$\oplus$" and multiplication by scalars by "$*$", that is:

$$s_1 \oplus s_2 = \sqrt{s_1^2 + s_2^2}, \quad \gamma * s_1 = |\gamma| s_1,$$

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 $s_1 \oplus s_2 \oplus ... \oplus s_n = t$ is equivalent to $s_1^2 + ... + s_n^2 = t^2$.

Inclusion. Inclusion of stochastic numbers plays important roles in applications. Inclusion relation "$\subseteq_s$" between two stochastic numbers $X_1 = (m_1; s_1)$, $X_2 = (m_2; s_2) \in \mathbb{S}$ is defined by [3]

$$X_1 \subseteq_s X_2 \Longleftrightarrow (m_2 - m_1)^2 \le s_2^2 - s_1^2. \tag{5}$$

Relation (5) is called *stochastic inclusion*, briefly: s-inclusion.

It is easy to prove [3] that addition and multiplication by scalars are (inverse) s-inclusion isotone (invariant with respect to s-inclusion), that is

$$X_1 \subseteq X_2 \Longleftrightarrow X_1 + Y \subseteq X_2 + Y, \quad X_1 \subseteq X_2 \Longleftrightarrow \gamma * X_1 \subseteq \gamma * X_2$$

3 The CESTAC Method

Suppose that some mathematical value r has to be computed with a numerical method implemented on a computer. The initial data are imprecise and the computer uses floating point number representation. In the CESTAC method a real number r, intermediate or final result, is considered as a Gaussian random variable with mean value m and standard deviation σ that have to be approximated. So r is a stochastic number.

In practice a stochastic number is approximated by an N-tuple with components $r_j,\ j = 1, ..., N$, which are empirical samples representing the same theoretical value. As seen before, this vector is called *discrete stochastic number*. The operations on these samples are those of the computer in use followed by a random rounding. The samples corresponding to imprecise initial values are randomly generated with a Gaussian distribution in a known confidence interval.

Following the classical rules of statistics, the mean value m is the best approximation of the exact value r and the number of significant digits on m is computed by:

$$C_m = log_{10}\left(\frac{\sqrt{N}\,|\overline{r}|}{\sigma\ \tau_\eta}\right), \tag{6}$$

wherein $m = N^{-1}\ \ \sum_{j=1}^{N} r_j,\ \ \sigma^2 = (N-1)^{-1}\sum_{j=1}^{N}(r_j - m)^2$ and τ_η is the value of Student's distribution for $k-1$ degrees of freedom and a probability level p. Most of the time p is chosen to be $p = 0.95$ so that $\tau_\eta = 4.303$. This type of computation on samples approximating the same value is called *Discrete Stochastic Arithmetic* (*DSA*).

It has been shown [5] that if one only wants the accuracy of r, i.e., its number of significant decimal digits, then $N = 3$ suffices. This is what is chosen in the software named CADNA [20] which implements the CESTAC method. But if one wants a good estimation of the error on r then a greater value for N, experimentally at least $N = 5$ must be chosen. The experiments given below use $N = 5$ and $N = 20$ showing that the two series of results are very close and that a large value for N is unnecessary.

The goal of next section 4 is to compare the results obtained with *Continuous Stochastic Arithmetic (CSA)* and the theory developed in this paper with results obtained with the CESTAC method implementing *Discrete Stochastic Arithmetic (DSA)*.

It should be remarked that DSA which is used in the CESTAC method takes into account round-off errors at the level of each floating point operation because of the random rounding done at this level. On the contrary CSA is a theoretical model in which data are imprecise but arithmetic operations are supposed exact. This is why in our experiments relative errors on data are chosen to be of order 10^{-2}–10^{-3} whereas the computations are done using double presision arithmetic. Thus experiments on computer can be considered very close to the theoretical CSA model.

4 Application: Linear Regression

As said before, in the CESTAC method, each stochastic variable is represented by an N-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 N-tuples.

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 done on the one-dimensional linear regression method for numeric input data.

4.1 Derivation of a Formula for Regression

Let $(x_i,\ y_i)$, $i = 1, ..., n$, be a set of n pairs of numbers where all x_i are different, $x_1 < x_2 < ... < x_n$. As well-known the regression line that fits the (numeric) input data (x, y), $x = (x_1, x_2, ..., x_n) \in \mathbb{R}^n$, $y = (y_1, y_2, ..., y_n) \in \mathbb{R}^n$, is

$$l : \eta = (S_{xy}/S_{xx})(\xi - \overline{x}) + \overline{y}, \tag{7}$$

wherein $\overline{x} = (\sum x_i)/n$, $\overline{y} = (\sum y_i)/n$ (all sums run from 1 to n), and

$$S_{xx} = \sum (x_i - \overline{x})^2 > 0, \qquad S_{xy} = \sum (x_i - \overline{x})(y_i - \overline{y}) = \sum (x_i - \overline{x}) y_i.$$

Note that that l passes through the point $(\overline{x}, \overline{y})$.

The expression in the right hand-side of (7) can be rewritten in the form:

$$\begin{aligned} L : \eta &= (S_{xy}/S_{xx})(\xi - \overline{x}) + \overline{y} \\ &= (1/S_{xx}) \left(\sum (x_i - \overline{x}) y_i \right) (\xi - \overline{x}) + \left(\sum y_i \right) /n \\ &= \sum ((x_i - \overline{x})(\xi - \overline{x})/S_{xx} + 1/n)\ y_i. \end{aligned}$$

Thus the line (7) can be represented in the form

$$l : \eta = \sum \gamma_i(\xi)\ y_i, \tag{8}$$

wherein the functions

$$\gamma_i(\xi) = \gamma_i(x; \xi) = (x_i - \overline{x})(\xi - \overline{x})/S_{xx} + 1/n, \ \ i = 1, 2, ..., n, \tag{9}$$

depend only on x and not on y.

Since γ_i is linear, it may have at most one zero. Denoting by ξ_i the zero of the linear function $\gamma_i(\xi)$, we have

$$\xi_i = \overline{x} + S_{xx}/(n(\overline{x} - x_i)),\ i = 1, ..., n. \tag{10}$$

If $x_i = \overline{x}$, then $\gamma_i = 1/n > 0$.

In every interval $[\xi_j, \xi_{j+1}]$ the signs of γ_i do not change and can be easily calculated [9].

Table 1. Results obtained with $\varepsilon = 0$, $\delta = 0.01$

u_i	*DSA* 5 samples	*DSA* 20 samples	*CSA*	CADNA
(0;ε)	(2.98587;0.000930)	(2.99719;0.009134)	(3.00000;0.009591)	0.298E+001
(1.5;ε)	(5.99914;0.003732)	(6.00011;0.005948)	(6.00000;0.006164)	0.599E+001
(2.5;ε)	(8.00291;0.005348)	(7.99994;0.006061)	(8.00000;0.004690)	0.800E+001

4.2 Experiments

As said above, the results obtained with *CSA* and those obtained with the CESTAC method with N samples, i.e., with *DSA* have to be compared. Here the successive values $N = 5$ and $N = 20$ have been chosen to experiment the efficiency of the CESTAC method with different sizes of discrete stochastic numbers. The *CSA* is based on operations defined on Gaussian random variable $(m; \sigma)$.

The regression method (8) has been implemented with *CSA* and *DSA*. We consider the situation when the values of the function y_i are imprecise and abscissas x_i are considered exact.

For all examples presented below, we take the couples of values from the line $v = 2u + 3$. The values chosen for abscissas are $x_1 = 1,\ x_2 = 2,\ x_3 = 2.5,\ x_4 = 4,\ x_5 = 5.5$, and the values y_i considered as imprecise are obtained as follows:

In the case of *CSA* they are chosen as $y_1 = (5; \delta),\ y_2 = (7; \delta),\ y_3 = (8; \delta),\ y_4 = (11; \delta),\ y_5 = (14; \delta)$ and δ is chosen as $\delta = 0.01$.

In the case of the CESTAC method *(DSA)* the data for the y_i are randomly generated with Gaussian distributions whose mean values are the centers of the above stochastic numbers and standard deviation δ.

From formula (8), three values of v_i corresponding to three input values considered as imprecise $u_i = (0; \varepsilon);\ (1.5; \varepsilon);\ (2.5; \varepsilon)$ are computed with *DSA* and with *CSA* and different values of ε. They are reported in tables 1–3.

The tables show that the mean values obtained with *CSA* are very close to the mean values obtained with *DSA*.

Let us now call $(m_v; \sigma_v)$ the values provided by *CSA* for the above least squares approximation at some point u.

CSA can be considered a good model of *DSA* if the mean value $\overline{v}$ of the samples obtained at point u with the *DSA* is in the theoretical confidence interval provided by *CSA*, in other words if:

$$m_v - 2\sigma_v \le \overline{v} \le m_v + 2\sigma_v \tag{11}$$

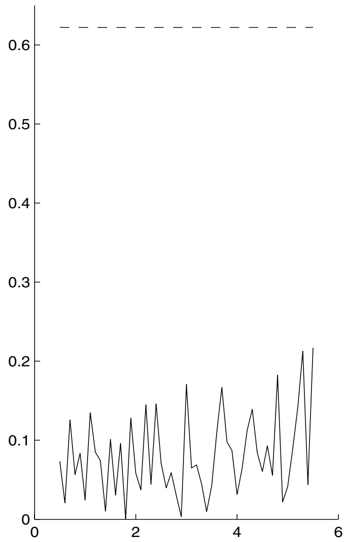
with a probability of 0.95. This formula can be rewritten as: $-2\sigma_v \le \overline{v} - m_v \le +2\sigma_v$, $|\overline{v} - m_v| \le +2\sigma_v$.

Table 2. Results obtained with $\varepsilon = 0.01$, $\delta = 0.01$

u_i	*DSA* 5 samples	*DSA* 20 samples	*CSA*	CADNA
(0;ε)	(2.99372;0.021080)	(3.00001;0.018596)	(3.00000;0.032542)	0.29E+001
(1.5;ε)	(5.99043;0.015064)	(5.99956;0.024394)	(6.00000;0.031702)	0.59E+001
(2.5;ε)	(8.01482;0.017713)	(7.99296;0.017689)	(8.00000;0.031449)	0.80E+001

Table 3. Results obtained with $\varepsilon = 0.1$, $\delta = 0.01$

u_i	*DSA* 5 samples	*DSA* 20 samples	*CSA*	CADNA
(0;ε)	(2.76260;0.122948)	(3.03062;0.213195)	(3.00000;0.311120)	Non significant
(1.5;ε)	(5.86934;0.205126)	(6.11816;0.179552)	(6.00000;0.311033)	0.5E+001
(2.5;ε)	(7.97106;0.219142)	(8.07687;0.229607)	(8.00000;0.311008)	0.7E+001



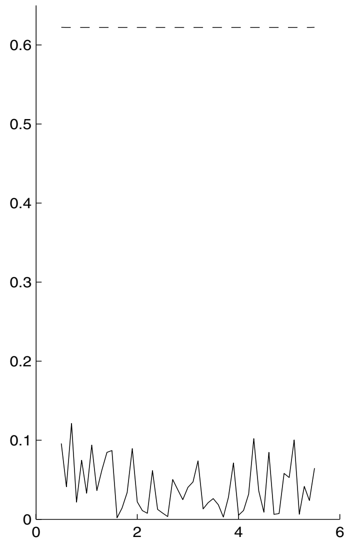


Fig. 1. The dash line represents $2\sigma_v$ and the full line $|\overline{v}-m_v|$, the left figure is computed with $N = 5$ and the right one with $N = 20$

The regression line has been computed with the previous data and $\varepsilon = 0.01$ and from $u = 0.5$ to $u = 5.5$ with a step of 0.1. Figure 1 shows the curves $|\overline{v}-m_v|$ and $2\sigma_{v_i}$ for N=5 and N=20. On our samples formula (11) is always respected.

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 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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