Control and Cybernetics

vol. 39 (2010) No. 2

On probabilistic bounds inspired by interval arithmetic^{*}

by

Antanas Žilinskas and Julius Žilinskas

Institute of Mathematics and Informatics Akademijos 4, LT-08663 Vilnius, Lithuania e-mail: antanasz@ktl.mii.lt, julius.zilinskas@mii.lt

Abstract: A randomized method aimed at evaluation of probabilistic bounds for function values is considered. Stochastic intervals tightly covering ranges of function values with probability close to one are modelled by a randomized method inspired by interval arithmetic. Statistical properties of the modelled intervals are investigated experimentally. The experimental results are discussed with respect to application of this method in the construction of a branch and bound type randomized algorithm for global optimization.

Keywords: global optimization, branch and bound method, randomized computing, interval arithmetic.

1. Introduction

The branch and bound method is an important tool for solving global optimization (GO) problems (Horst, Pardalos and Thoai, 1995). Efficiency of this method crucially depends on availability of tight bounds concerning objective function values on subsets of the feasible region comprising the branching tree; for general discussion on this subject we refer to Floudas et al. (2005) and for an experimental investigation of influence of bounds tightness on the efficiency of the corresponding algorithms we refer to Žilinskas and Žilinskas (2006). In some cases tight bounds can be evaluated owing to the structural or analytical properties of objective functions (Floudas et al., 2005). Suitable bounds over rectangular regions can be calculated for a rather broad class of functions by means of interval arithmetic, and the corresponding GO methods are indeed efficient for those classes of objective functions (Hansen and Walster, 2003). Recently the interval arithmetic based GO methods have been developed for the optimization problems with general constraints (Markot et al., 2006; Sun and Johnson, 2005). However, the efficiency of interval methods can be degraded by the dependency of variables; dependency means multiple occurrences

^{*}Submitted: July 2007; Accepted: January 2010

of the same variables in the expression/algorithm of the considered objective function. We are interested in developing a method for the construction of tight stochastic bounds for the values of objective function, whose properties do not suggest a specific method for computation of tight bounds, and whose structure conditions strong dependency implying the degradation of the bounds evaluated by means of interval arithmetic. We make the same general assumptions about the analytical properties of objective functions as in development of interval methods, since our method is based on a stochastic mixture of two versions of interval arithmetic.

The idea of randomization has proven successful in various computational problems (Rajasekaran et al., 2001). Many algorithms of "black box" optimization include randomized subroutines. For example, the method of branch and probabilistic bounds (Zhigljavsky, 1990) is implemented as a standard branch and bound method but including a randomized procedure for evaluation of bounds. Let us briefly explain this procedure. In a subset of the feasible region, corresponding to a node of the branching tree, a number of points is generated at random independently and with uniform distribution. The set of function values at these random points is considered a random sample with special theoretical distribution, and the lower bound for function values is estimated as minimum of the theoretical distribution (Zhigljavsky, 1990; Zhigljavsky and Žilinskas, 2008).

Alt and Lamotte (2001) proposed another idea for the randomized evaluation of bounds, where random bounds for function values are obtained as the result of computations by using random interval arithmetic. Unlike the "black box" model, where only function values are available, the random interval arithmetic model is applicable where an algorithm for computing function values is available. Randomization is inserted into the structure of the algorithm: the current operation of random interval arithmetic is chosen at random with equal probabilities from two corresponding operations of inner and outer interval arithmetic. The result of the computation is a random interval shorter than the result obtained by the outer interval arithmetic; this advantage of random interval arithmetic is gained for the price of loss of guaranteed inclusion of function values in the resulting interval. The length and the probability of inclusion can be balanced by means of changing the probability of two possible alternatives, i.e. operations of outer or inner interval arithmetic. By choosing an appropriate balance, a good performance of the branch and bound type algorithm based on balanced random arithmetic has been achieved in some practical problems; see e.g. (Žilinskas and Bogle, 2004). However, in some cases the statistical assumptions justifying balanced random interval arithmetic are rejected by statistical consistency testing (Žilinskas and Bogle, 2003). In the present paper a new version of probabilistic bounds inspired by interval arithmetic is investigated experimentally, and it is shown that in this case the statistical model fits well to the experimental data collected in testing experiments.

A branch and bound type GO algorithm is developed using stochastic interval arithmetic. The method is aimed for problems with simplest (interval) constraints, and does not include such frequently used enhancements as the interval Newton method. A "pure" version of the algorithm seems best suited for the assessment of the applicability of the considered stochastic bounds for further development of GO algorithms aimed at special classes of real world problems. An example of problems of the probable future interest is included: it is an optimization problem of statistics. This problem, although simple from the optimization point of view, well illustrates the fact that despite the common words in the title with "interval arithmetic", the "stochastic interval arithmetic" is oriented at estimating the bounds for functions, which are different from functions aimed by interval arithmetic.

2. Stochastic interval arithmetic

For the practical efficiency of branch and bound global optimization (GO) algorithms it is important that information about the range of function values over the considered set be as precise as possible, while the procedure for extracting such an information should be as cheap as possible. We consider a possibility of tightening bounds by means of randomization, thus accepting the loss of guaranteed bounding. The considered version of stochastic interval arithmetic is a modification of random interval arithmetic proposed by Alt and Lamotte (2001). In spite of the similarity of the widely used term "stochastic arithmetic" (Alt, Lamotte and Markov, 2006; Markov, Alt and Lamotte, 2004) and the title of this section "stochastic interval arithmetic", the research goals related to both terms are quite different. The latter title describes a rather narrow theme on probabilistic bounds meant for use in branch and bound type GO, while the former term is used in a much broader context.

The operations of stochastic interval arithmetic are defined by combining the operations of overestimating standard (outer) interval arithmetic and semiunderestimating operations of inner interval arithmetic. Methodologically, it would be more appropriate to apply not semi-underestimating but strictly underestimating interval operations. However, in this research, the inner interval arithmetic was used for the sake of comparability of the experimental results with those of Alt and Lamotte (2001), Žilinskas and Bogle (2003, 2004). For the discussion about underestimating interval arithmetic we refer to Kreinovich, Nesterov and Zheludeva (1996), Žilinskas and Žilinskas (2005), Žilinskas (2006), and for an example illustrating relations between the interval values defined by various interval arithmetics we refer to Žilinskas and Žilinskas (2005).

Let us consider computation of an arithmetic expression using random interval arithmetic proposed by Alt and Lamotte (2001). The arithmetic operations are performed according to the normal priority order, and the standard vs inner mode of every interval operation is chosen randomly with equal probabilities. An interval value computed in this way is a random interval. To get a reliable

approximation of the range of values of the considered arithmetic expression, a sample of random intervals is generated. Intervals are parameterized by centers and radii. It is assumed that the standard deviation of centers of the generated intervals is negligibly small, and the distribution of their radii is normal. The range is estimated using the sample mean of the centers of generated random intervals, and the sample mean and the sample standard deviation of radii of these intervals. The slight modification of Alt and Lamotte (2001), where the sequence of interval arithmetic operations is performed by choosing standard/inner modes randomly with predefined probabilities, is called balanced random arithmetic and was investigated by Žilinskas and Bogle (2003). Some advantage of balanced random interval arithmetic with respect to its predecessor (Alt and Lamotte, 2001) can be explained by the flexibility of choosing the mixing probability, and more realistic distributions: the standard deviation of centers is not assumed to be small and the distribution of radii is assumed to be folded normal (Leone, Nelson and Notingham, 1961). Nevertheless, the experiments (Zilinskas and Bogle, 2003) show that the hypotheses about the above mentioned distributions are frequently rejected by statistical consistency tests. This happens, e.g. in the case when balanced random interval arithmetic is applied to compute interval values of GO test functions defined by simple formulas.

We propose stochastic interval arithmetic where the result of the arithmetic operation $\tilde{\circ}$ is defined as a random convex combination of the results of standard and inner interval operations:

$$[x]\tilde{\circ}[y] = \frac{a([x]\hat{\circ}[y]) + b([x]\check{\circ}[y])}{a+b}$$

where $[x] \circ [y]$ denotes the result of standard interval arithmetic operation, $[x] \circ [y]$ denotes the result of inner interval arithmetic operation, and a and b are random coefficients. The distributions of random coefficients a and b are uniform; their ranges are defined by the predefined coefficient $pc: a \in [0, pc]$, $b \in [0, (1 - pc)]$. The implemented distribution of coefficients has been found empirically by searching for an appropriate distribution where densities of a and b were positive over the entire interval [0, 1], a + b = 1, and mean values of a and b would be easily controllable. In this case the coefficient pc controls the balance between the underestimating and overestimating components: for pcclose to 0, the results of stochastic interval arithmetic are close to the results of inner interval arithmetic, and for pc close to 1, the results of stochastic interval arithmetic are close to the results of standard interval arithmetic. However, we are most interested in the case of an intermediate pc value. Let stochastic interval arithmetic with $pc \sim 0.5$ be repeatedly applied to compute an interval value of a function. From a sample of centers and radii of the stochastic intervals the information on the range of function values can be extracted using the confidence interval technique. The results would be theoretically sound, if the distributions of centers and radii of generated stochastic intervals were known.

Since they are not known, we used the approximations: normal distribution for centers, and folded normal distribution for radii, as proposed by Žilinskas and Bogle (2004). The applicability of these approximations is analyzed below by means of the technique of testing statistical hypotheses.

Let an interval value of a function be computed several times using stochastic interval arithmetic, and a sample of intervals be produced. We want to estimate the range of function values using the corresponding centers and radii of the sampled intervals. The idea is to approximate the range by a confidence interval of a random variable, defined by the sum of hypothetical random variables *center* and $\pm radius$. We assume that centers and radii are distributed according to normal and folded normal distributions, correspondingly. It is well known that the randomly generated values of normally distributed random variable with parameters (μ, σ), belong to the interval $\mu \pm 3\sigma$ with probability higher than 0.997. The probability of the similar event for a folded normal random variable is even higher than 0.997. These arguments suggest the approximation of the range by the interval

$$\left[\mu_{centers} \pm \left(3.0\sigma_{centers} + \mu_{radii} + 3.0\sigma_{radii}\right)\right],\tag{1}$$

where the theoretical parameters are replaced by their estimates based on a sample of intervals obtained by repeated computation of interval function value by means of stochastic interval arithmetic. Proposed estimates of ranges and stochastic interval arithmetic have been implemented in C++ modifying a C++ interval library filib++ (Lerch et al., 2001; Žilinskas, 2005).

An experimental investigation has been performed to test how much the actual properties of stochastic interval arithmetic are close to the hypothetical ones: do the samples of centers and radii pass the test of compatibility with the theoretical distributions, and is the accuracy of the approximation (1) acceptable? The results of similar experiments with balanced random interval arithmetic are also presented below for comparison.

For the experiments the following GO test functions were used: Rosenbrock, Six Hump Camel Back, and Goldstein and Price; these functions have been used in experiments with balanced random interval arithmetic (Žilinskas and Bogle, 2003).

Interval function values (parameterized by centers and radii) were computed using balanced random and stochastic interval arithmetics. The value pc = 0.55has been used for stochastic interval arithmetic. Such a pc value corresponds to the value of the mixing probability adopted in balanced random interval arithmetic; in the sequence of alternating standard/inner interval operations the probability of an operation in the standard mode equal to ps = 0.55 was shown appropriate (Žilinskas and Bogle, 2004). The histograms of samples of 1000 values of centers and radii of are presented in Figs. 1 through 4. The values computed using standard and inner interval arithmetics are shown as vertical lines denoted by 'inn' and 'st'. The sample means and the sample standard deviations are presented in the titles of x-axes. The graphs of normal distributions for centers and folded normal distributions for radii with the evaluated sample means and standard deviations are also shown in Figs. 1 through 4. The Kolmogorov-Smirnov test was used to test the compatibility of samples with the corresponding hypothetical distributions. P-values of tests, denoted QKS, are presented below the figures.

The interval values of the Rosenbrock function were computed for a randomly generated $X = [0.521, 1.52] \times [-0.817, 0.183]$. The histograms of centers and radii of a sample of 1000 interval function values, computed using balanced random and stochastic interval arithmetics are presented in Fig. 1. The histograms of the samples generated using balanced random interval arithmetic severely differ from the hypothetical distributions indicating the concentration of samples at the results of standard and inner arithmetic. This phenomenon is implied by the extremely simple formula of the Rosenbrock function:

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

In this case four random intervals are computed using balanced random interval arithmetic, and their probabilities depend on ps

$$\begin{split} \mathbf{P}\left\{f(X) &= 100(x_2 - \hat{x}_1^2)^2 + (1 - x_1)^2\right\} &= ps \times ps, \\ \mathbf{P}\left\{f(X) &= 100(x_2 - \hat{x}_1^2)^2 + (1 - x_1)^2\right\} &= ps \times (1 - ps), \\ \mathbf{P}\left\{f(X) &= 100(x_2 - \hat{x}_1^2)^2 + (1 - x_1)^2\right\} &= (1 - ps) \times ps, \\ \mathbf{P}\left\{f(X) &= 100(x_2 - \hat{x}_1^2)^2 + (1 - x_1)^2\right\} &= (1 - ps) \times (1 - ps). \end{split}$$

As the numerical value of the second operand of addition in most cases is much smaller than of the first one, we get interval values similar to standard interval with the probability ps, and interval values similar to inner interval with the probability 1 - ps. Therefore, the histograms look like if in ps cases only standard interval arithmetic was used, and in 1 - ps cases only inner interval arithmetic was used. The discrete distribution is, of course, far from the normal distribution. On the other hand, the histograms of the samples generated using stochastic interval arithmetic are similar to the theoretical distributions. The Kolmogorov-Smirnov test supports our observation: at the standard significance level 0.05 the hypothetical distributions are acceptable for the results of stochastic interval arithmetic, but definitely not acceptable for the results of balanced random interval arithmetic. Similar results for the Six Hump Camel Back function for a randomly generated $X = [2.56, 3.56] \times [-1.45, -0.451]$ are presented in Fig. 2.

The histograms for the Goldstein and Price function for $X = [0.521, 1.52] \times [-0.817, 0.183]$ are presented in Fig. 3. Although in this case the Kolmogorov-Smirnov test rejects the theoretical hypotheses, visually the histograms of centers and radii of the random intervals generated using stochastic interval arithmetic seem closer to the theoretical distributions than those of balanced random interval arithmetic.



a) balanced random interval arithmetic

 $[2.56, 3.56] \times [-1.45, -0.451]$



Figure 1. The histograms of centers and radii of balanced random and stochastic intervals for the Rosenbrock function over randomly generated $X = [0.521, 1.52] \times [-0.817, 0.183]$



Figure 2. The histograms of centers and radii of balanced random and stochastic intervals for the Six Hump Camel Back function over randomly generated X =



Figure 3. The histograms of centers and radii of balanced random and stochastic intervals for the Goldstein and Price function over randomly generated $X = [0.521, 1.52] \times [-0.817, 0.183]$



Figure 4. The histograms of centers and radii of balanced random and stochastic intervals for objective function of optimization problem related to the evaluation of parameters in statistics over randomly generated X = [1.72, 3.72]

Similar results for the objective function of the optimization problem related to the evaluation of parameters in statistics (see description in the next section) for a randomly generated X = [1.72, 3.72] are presented in Fig. 4. The histograms of the samples generated using balanced random interval arithmetic severely differ from the hypothetical distributions. The histograms of the samples generated using stochastic interval arithmetic are similar to the theoretical distributions. The Kolmogorov-Smirnov test supports our observation: at the standard significance level 0.05 the hypothetical distributions are acceptable for the results of stochastic interval arithmetic, but definitely not acceptable for the results of balanced random interval arithmetic.

An alternative method for the construction of global optimization oriented probabilistic bounds for function values is based on extreme value statistics (Zhigljavsky, 1990; Zhigljavsky and Žilinskas, 2008). Let x_i , i = 1, ..., n, be a sample of random vectors uniformly distributed in X, and let \tilde{y}_i , i = 1, ..., n, denote increasingly ordered function values $f(x_i)$. We refer to Zhigljavsky (1990), Zhigljavsky and Žilinskas (2008) for a discussion of assumptions concerning properties of $f(\cdot)$, related to the estimation of minimum/maximum of $f(x), x \in X$, using information about $f(x_i)$. The ordered statistics based estimates of extreme values normally involve some first/last members of the sequence \tilde{y}_i , i = 1, ..., n. For example, the following simple estimate of minimum

$$f_{min} = \tilde{y}_1 - a_k (\tilde{y}_k - \tilde{y}_1), \tag{2}$$

is discussed by Zhigljavsky and Žilinskas (2008), p. 68, where it is emphasized that k should be relatively small with respect to the sample size; the multiplier a_k depends on behavior of $f(\cdot)$ in the vicinity of the minimizer. We are interested in small samples, e.g. in the experiments below the samples of size n = 20are considered. Therefore the value k = 2 seems most appropriate. Assuming that the minimizer is on the border of the feasible region X, the function in the vicinity of the minimizer can be approximated by a linear function; these assumptions suggest for functions of two variables the choice of $a_2 = 2$ (Zhigljavsky and Žilinskas, 2008). Applying the estimate of maximum f_{max} , obtained by means of an obvious reformulation of (2), the interval $[f_{min}, f_{max}]$ can be considered a stochastic estimate of the range for function values. Stochastic estimates of ranges for function values obtained using extreme value statistics, balanced random interval arithmetic, and stochastic interval arithmetic were compared experimentally. The ranges for the Rosenbrock, Six Hump Camel Back, and Goldstein and Price functions were estimated over the feasible region shown in the captions of Figs. 1-3. Samples of 1000 stochastic estimates of ranges were generated by the competing methods for all three test cases. Two criteria were used for comparison: failure (if an estimate did not cover the range) percentage, and average length of stochastic intervals. Estimates of ranges were computed by means of balanced random arithmetic and stochastic arithmetic using random samples of size equal to 5. Estimates from the method based on extreme value statistics were computed using samples of size 20, in

Table 1. Results of experimental testing where 'Stochastic' is a shorthand for the method of stochastic interval arithmetic, 'Random' is a shorthand for the method of balanced random arithmetic, and 'Extremal' is a shorthand for the method based on extreme value statistics; 'Length' denotes the average lengths of generated stochastic intervals, and 'Failure' denotes the percentage of failures to cover real range of function values

Rosenbrock function							
Method	Stochastic	Random	Extremal				
Length	960	965	1095				
Failure $(\%)$	2.5	2.3	4.8				
Six Hump Camel Back function							
Method	Stochastic	Random	Extremal				
Length	847	881	912				
Failure $(\%)$	0.1	0.2	14.4				
Goldstein and Price function							
Method	Stochastic	Random	Extremal				
Length	115380	316596	266370				
Failure $(\%)$	0.8	5.9	8.4				

order to account for the 4 times higher complexity of computing an estimate by stochastic interval arithmetic than by the method based on extreme value statistics.

A foremost conclusion from the experimental results concerning the method based on extreme value statistics was that the theoretically justified value $a_2 = 2$ is too small, implying high failure probability. Therefore, the values of a_2 were tuned for test cases individually to get average lengths of intervals similar to those obtained by stochastic interval arithmetic; thus different methods can be compared with respect to percentage of failures.

The experimental results presented in Table 1 clearly show that both versions of randomized interval arithmetic clearly outperform the method based on extreme value statistics. The results of stochastic interval arithmetic are better than the results of balanced random arithmetic. The deficiency of the method based on extreme value statistics can be explained by the inadequacy of its asymptotic nature to small size of samples used for estimation. This method is also sensitive to the behavior of the considered function in the vicinities of both kinds of extremum points, which is difficult to assess a priori.

The statistical model of stochastic interval arithmetic seems sufficiently adequate to the experimental data; at least the adequacy of this model is much better than the adequacy of the model of balanced random interval arithmetic. However, a much better adequacy of the model does not necessarily imply a much higher accuracy of the approximation (1). The results of experiments, designed to assess the accuracy of (1) for both randomized interval arithmetics, are presented below.

For the experimental assessment of the approximation (1) the precise values of the considered ranges are desirable. However, their computation is a difficult task. Therefore, their statistical estimates were used: the range of function values corresponding to a randomly chosen multidimensional interval of variables is estimated using 2000 function values computed at uniformly distributed random points. The size of samples, used to compute the approximations (1), was chosen equal to N = 30 and N = 5. The approximation is called successful if the statistical estimate of a range is a sub-interval of the corresponding approximation (1). The success rate is estimated taking into account the approximations of ranges corresponding to 1000 randomly chosen multidimensional intervals of variables. The accuracy of approximation is measured by the mean ratio of widths of approximation (1) and of the standard interval enclosure, i.e. the interval computed using standard interval arithmetic. The ratio of widths shows how much approximation (1) is narrower than bounds computed using standard interval arithmetic. When approximation (1) is used in global optimization, the success rate influences the reliability of the branch and bound algorithm. The ratio of widths determines the efficiency of the algorithm: for a smaller ratio the approximation is narrower, and the algorithm is faster since sub-regions are discarded earlier.

The inter-relationship between the success rate and the ratio of widths is obtained by estimating both parameters for different values of the coefficient pc in the case of stochastic interval arithmetic. Similarly, in the case of balanced random interval arithmetic both parameters are estimated for different values of probability to choose the mode of standard interval arithmetic ps. The curves showing these inter-relationships for both versions of interval arithmetic, and for two sizes of samples (N = 30 and N = 5), are presented in Figs. 5 and 6.

The considered inter-relationships for the Goldstein and Price function are shown in Fig. 5. The results can be summarized as follows. First: the intervals obtained using stochastic interval arithmetic more reliably cover the corresponding ranges of function values than the intervals of the same average length obtained using balanced random interval arithmetic. Second: the difference is more evident for a small sample. The second conclusion is especially important for global optimization, since small sample sizes are preferable to save time on computing approximations.

The results of the experiments with the objective function of a practical process network synthesis problem from Csendes (1998), presented in Fig. 6, are similar to the results of experiments with the Goldstein and Price function. Narrower approximations are obtained more reliably using stochastic interval arithmetic than using balanced random interval arithmetic; the difference is more evident for a small sample.



Figure 5. Interrelationship between success rate and mean ratio of widths for the Goldstein and Price function; solid line corresponds to balanced random interval arithmetic, and dashed line corresponds to stochastic interval arithmetic



Figure 6. Interrelationship between success rate and mean ratio of widths for objective function of process network synthesis problem; solid line corresponds to balanced random interval arithmetic, and dashed line corresponds to stochastic interval arithmetic

3. Global optimization using stochastic interval arithmetic

The tightness of bounds is an important factor of efficiency in branch and bound based GO. On the other hand, a branch and bound approach based algorithm can fail if the bounds are underestimated.

For the experimental comparison of the efficiency of interval GO with different versions of interval arithmetic, a branch and bound algorithm has been implemented, where lower and upper bounds for function values can be computed by a chosen version of interval arithmetic. Three versions of interval arithmetic are included: standard, balanced random, and stochastic. The smallest value of the function at the middle points of the considered sub-regions is used as an estimate of the upper bound for the minimum.

GO algorithms based on the balanced random and stochastic interval arithmetics are randomized algorithms because of stochastic bounds used in branch and bound procedures. Therefore, the efficiency and the reliability of optimization were assessed by averaging the results of 100 runs. Experiments were performed with different values of pc for stochastic interval arithmetic. Stochastic bounds for function values were estimated from the samples of random intervals where sample size was equal to 5. An optimization problem related to a process network synthesis problem (Csendes, 1998) was used for testing. The termination condition was defined by the relative tolerance equal to 10^{-2} . For different values of pc the reliability and the efficiency of the algorithm were assessed. The reliability was measured by success rate equal to the ratio of runs where the global minimum was estimated with the predefined accuracy. The efficiency was measured by the ratio between the mean number of objective function calls by the algorithm using stochastic (balanced random) interval arithmetic, and number of objective function calls by the algorithm using standard interval arithmetic. The results summarized in Fig. 7 show that the efficiency of stochastic and balanced random interval arithmetics, measured in function calls ratio for success rate close to 1, is approximately 10 times better than that of standard interval arithmetic. The algorithm with stochastic interval arithmetic uses fewer function calls for the same success rate than the algorithm with balanced random interval arithmetic.

The time of optimization has also been measured. Average relative optimization time is computed averaging the ratios of time of GO using stochastic (balanced random) and standard interval arithmetics; the results are presented in Fig. 8. When the desired success rate is less than 99%, the algorithms with stochastic bounds are faster than the algorithm with standard interval arithmetic. When 90% success rate is required, the algorithms are more than five times faster, when 80% – six times faster. The speed of optimization algorithms with stochastic bounds computed from balanced random intervals and stochastic intervals is similar, although the computation of interval function value using balanced random arithmetic takes approximately twice shorter time than such a computation using stochastic interval arithmetic.



Figure 7. The relationship between success rate and function calls ratio for the problem of optimal synthesis of process network; solid line corresponds to balanced random interval arithmetic, and dashed line corresponds to stochastic interval arithmetic



Figure 8. The relationship between success rate and average relative time for the problem of optimal synthesis of process network; solid line corresponds to balanced random interval arithmetic, and dashed line corresponds to stochastic interval arithmetic

The optimization problems related to the evaluation of parameters in statistics have frequently the properties favorable to the application of the proposed GO method. The 100% success rate in these problems is not necessary, since estimates anyway are random variables as functions of a random sample. Moreover, for the small and medium samples an increase of the minimization precision does not necessarily improve the quality of estimates with respect to statistical criteria, e.g. bias and standard deviation. The problem of estimation of parameters of the three-parameter lognormal models (Wingo, 1984) illustrates well the properties of the typical optimization problems of interest: the number of variables is small, the formulas of computations according to these formulas are large, causing strong dependency of variables.

The probability density of the lognormal distribution is defined by the formula

$$p(y) = \frac{1}{\sqrt{2\pi\beta(y-\gamma)}} \exp\left(-\frac{(\ln(y-\gamma)-\mu)^2}{2\beta}\right),\tag{3}$$

where $y > \gamma$, $-\infty < \gamma < \infty$, and $\beta > 0$. The number of parameters of p(y) is equal to three, and these parameters can be estimated by the method of maximum likelihood as described in Wingo (1984):

$$\min_{10 \le \theta \le 10} [\mu(\theta) + \frac{1}{2} \ln(\beta(\theta))], \tag{4}$$

$$\mu(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ln(y_i - \gamma(\theta)), \tag{5}$$

$$\beta(\theta) = \frac{1}{n-1} \sum_{i=1}^{n} [\ln(y_i - \gamma(\theta)) - \mu(\theta)]^2, \tag{6}$$

 $\gamma(\theta) = y_{\min} - \exp(-\theta),$

where y_i , i = 1, ..., n, is a sample of n observations, and y_{\min} denotes the minimum observed value.

Although the optimization problem (4) seems rather simple, it has been considered in several research papers, e.g. cited by Wingo (1984); for the more recent results related to this statistical problem and further references we refer to Basak, Basak and Balakrishnan (2008). The GO algorithms based on balanced random arithmetic and on stochastic arithmetic have been tested using 100 random samples (of size equal to 100) from the distribution (3) with parameters $\gamma = 10$, $\mu = 1$, and $\beta = 0.5$; these values for the parameters have been chosen following Wingo (1984). The averaged results are presented in Fig. 9, showing some advantage of stochastic interval arithmetic based algorithm.

To assess the performance of the stochastic arithmetic based GO algorithm in the estimation of parameters of (3), the statistics of the testing is presented in Table 2; see the row "stochastic". One hundred random samples of size 100



Figure 9. The relationship between success rate and function calls ratio (left) as well as average relative time (right) for the problem (4) where the tolerance of termination condition was equal to 10^{-3} ; solid line corresponds to balanced random interval arithmetic, and dashed line corresponds to stochastic interval arithmetic

were considered. The estimate of γ was obtained as $\gamma_o = y_{\min} - \exp(-\theta_o)$ where y_{\min} was minimum sample value, and θ_o was the minimizer in (4). The estimates of two other parameters were obtained by replacing γ with γ_o in (5) and (6), respectively. The means and the standard deviations of the estimates are denoted by $\bar{\gamma}, \bar{\beta}, \bar{\mu}$ and std. γ , std. β , std. μ , respectively. For comparison, the statistics of estimates obtained using standard interval arithmetic are presented in the row "standard" of Table 2. The considered problem of estimation is difficult because one of the parameters estimated, namely the parameter γ , is minimum of the distribution density p(y), and

$$\lim_{y \to \gamma+0} p(y) = \lim_{y \to \gamma+0} p'(y) = 0.$$
⁽⁷⁾

If the parameter γ were known, then the estimation problem would be reduced to a trivial one where the estimates of the remaining two parameters could be computed using formulas (5) and (6). The statistics of estimates of β and μ , obtained for the case of known γ ($\gamma = 10$) are presented in the row "analytical" of Table 2. These statistics can be considered as the desirable limit for the corresponding statistics of estimates obtained for the case of unknown γ .

The results of Table 2 show that the estimates obtained using the stochastic interval arithmetic are as good as those obtained using the standard interval arithmetic, but the former are obtained using a considerably smaller number of function calls.

Table 2. The results of estimation of parameters of the lognormal distribution

algorithm	calls ratio	$\overline{\gamma}$	std. γ	$\overline{\mu}$	std. μ	$\overline{\beta}$	std. β
analytical	0.000	10.000	0.000	1.015	0.067	0.466	0.015
standard	1.000	10.022	0.292	0.984	0.147	0.514	0.138
stochastic	0.033	9.837	0.156	1.074	0.100	0.428	0.092

To improve the efficiency, different enhancements are included into the state of the art GO algorithms based on interval arithmetic, e.g. the interval Newton method. In contrast, very simple versions of GO algorithms based on stochastic interval arithmetic were considered in the present paper so as to exclude confusing factors in the assessment of the newly proposed stochastic interval arithmetic. Simple test functions were used, adequate for the (simple) tested version of the algorithm. The obtained results of experimental testing encourage the development of a sophisticated (parallel) version of GO algorithm based on stochastic interval arithmetic and oriented at the optimization problems in statistics.

4. Conclusions

In computing probabilistic bounds for function values, the stochastic interval arithmetic outperforms the balanced random arithmetic as well as the method based on extreme value statistics; the methods were compared with respect to application in branch and bound type methods for global optimization. The parameter estimation problems in statistics seem a proper field to be aimed at in the further development of the proposed approach.

Acknowledgement

The authors acknowledge the support of the Agency for International Science and Technology Development Programmes in Lithuania via COST programme.

References

- ALT, R. and LAMOTTE, J.L. (2001) Experiments on the evaluation of functional ranges using random interval arithmetic. *Mathematics and Computers in Simulation*, 56 (1), 17–34.
- ALT, R., LAMOTTE, J.L. and MARKOV, S. (2006) On the numerical solution to linear problems using stochastic arithmetic. *Proc. ACM Symposium* on Applied Computing, 3, Dijon, France, 1055–1059.
- BASAK, P., BASAK, I. and BALAKRISHNAN, N. (2009) Estimation for threeparameter lognormal distribution based on progressively censored data. *Computational Statistics and Data Analysis*, 53 (10), 3580–3592.

- CSENDES, T. (1998) Optimization methods for process network synthesis a case study. In: C. Carlsson and I. Eriksson, eds., *Global & Multiple Criteria Optimization and Information Systems Quality.* Abo Academy, Turku, 113–132.
- FLOUDAS, C.A., AKROTIRIANAKIS, I.G., CARATZOULAS, S., MEYER, C.A. and KALLRATH, J. (2005) Global optimization in the 21st century: Advances and challenges. *Computers & Chemical Engineering*, **29**(6), 1185–1202.
- HANSEN, E. and WALSTER, G.W. (2003) *Global Optimization Using Interval* Analysis, 2nd. edn. Marcel Dekker, New York.
- HORST, R., PARDALOS, P. and THOAI, N. (1995) Introduction to Global Optimization. Kluwer, Dodrecht.
- KREINOVICH, V., NESTEROV, V.M. and ZHELUDEVA, N.A. (1996) Interval methods that are guaranteed to underestimate (and the resulting new justification of Kaucher arithmetic). *Reliable Computing*, 2(2), 119–124.
- LEONE, P., NELSON, L. and NOTINGHAM, R. (1961) The folded normal distribution. *Technometrics*, 3(4), 543–550.
- LERCH, M., TISCHLER, G., VON GUDENBERG, J.W., HOFSCHUSTER, W. and KRÄMER, W. (2001) The Interval Library filib++ 2.0 - Design, Features and Sample Programs. Preprint 2001/4, Universität Wuppertal.
- MARKOT, M.C., FERNANDEZ, J., CASADO, L.G. and CSENDES, T. (2006) New interval methods for constrained global optimization. *Math. Programming, Ser. A*, **106**, 287–318.
- MARKOV, S., ALT, R. and LAMOTTE, J. (2004) Stochastic arithmetic: s-spaces and some applications. *Numerical Algorithms*, **37**, 275-284.
- RAJASEKARAN, S., PARDALOS, P.M., REIF, J.H. and ROLIM, J.D. (2001) Handbook of Randomized Computing, 1 and 2. Kluwer, Dodrecht.
- SUN, M., and JOHNSON, A.W. (2005) Interval branch and bound with local sampling for constrained global optimization. *Journal of Global Optimization*, 33, 61–82.
- WINGO, D. (1984) Fitting three-parameter lognormal models by numerical global optimization – an improved algorithm. *Computational Statistics* and Data Analysis, 2, 13–25.
- ZHIGLJAVSKY, A. (1990) Branch and probability bound methods for global optimization. *Informatica*, 1, 125–140.
- ZHIGLJAVSKY, A. and ZILINSKAS, A. (2008) *Stochastic Global Optimization*. Springer, New York.
- ŽILINSKAS, A. and ŽILINSKAS, J. (2006) On efficiency of tightening bounds in interval global optimization. LNCS 3732. Springer, 197–205.
- ŽILINSKAS, A. and ŽILINSKAS, J. (2005) On underestimating in interval computations. BIT Numerical Mathematics, 45(2), 415–427.
- ŽILINSKAS, J. and BOGLE, I.D.L. (2003) Evaluation ranges of functions using balanced random interval arithmetic. *Informatica*, 14(3), 403–416.

- ŽILINSKAS, J. and BOGLE, I.D.L. (2004) Balanced random interval arithmetic. Computers & Chemical Engineering, 28(5), 839–851.
- ŽILINSKAS, J. (2005) Comparison of packages for interval arithmetic. Informatica, 16(1), 145–154.
- ŽILINSKAS, J. (2006) Estimation of functional ranges using standard and inner interval arithmetic. *Informatica*, **17**(1), 125–136.