Probabilistic analyses using Latin Hypercube Sampling method

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ABSTRACT: The Latin Hypercube Sampling (LHS) method is a numerical simulation method of the Monte Carlo type convenient for realisation of probabilistic analyses. The paper is focused on brief characterisation of algorithm of LHS method. It deals with method modifications and implementation of statistical correlation among random variables based on the optimisation of the sequence of particular samples in the columns of input variable matrix. LHS converges to the correct solution significantly faster than the Monte Carlo method and in this way substantially reduces the number of simulations and thus calculation time-demands. At the same time LHS preserves high accuracy of estimates of statistical characteristics. Further paper summarizes the LHS applications on solutions of geotechnical problems in Czech Republic and shortly characterises prepared software focused on probabilistic analyses by LHS method. The software is based on LHS *mean* method cooperating with simulated annealing method to take the statistical dependency of input variables into consideration.

1 INTRODUCTION

Mechanical parameters of rock mass and soils obtained from geotechnical investigation often display significant scatter. This fact follows not only from the natural development of the geological environment, but it is also caused by inaccuracies arising from the laboratory experiments and field tests.

Probabilistic calculations have been becoming a more available tool for solving numerical geotechnical problems. Their spreading in the common praxis is prevented first of all by the time-demanding calculations, requirements for outputs from geotechnical investigation and, in addition, due to the absence of the implementation of probabilistic methods in a commonly used software. The present paper therefore deals with the Latin Hypercube Sampling reduction probabilistic method, which is an alternative to the time-consuming Monte Carlo simulation method.

2 PROBABILISTIC CHARACTER OF PARAMETERS

Without regard to selected solution of the geotechnical problem (numerical, analytical solution) the analyses results are sensitive to values of input parameters. In case of variability of these values it is advisable to take into consideration their character of random quantities, described by the statistical or probabilistic characteristics. Random input quantities are represented in probabilistic calculations by a set of deterministic values (the so-called realisations, samples), which as a whole forms one of deterministic tasks which form the solved random problem (e.g. geomechanical model). The response of the random problem is a data set at which we seek statistical and probabilistic characteristics.

From the practical point of view, the paper further takes into consideration only continuous random quantities, which can assume all values from a final or endless interval and mentions only the most used characteristics.

A continuous random quantity X is characterised by the probability density function f(x) and the cumulative distribution function F(x):

$$F(x) = \int_{-\infty}^{+\infty} f(x)dx \tag{1}$$

The position of the values of random quantity X is best fitted by the mean or expected value denoted as $E(X)$ *(also* $\mu(X)$*)*, data variability (scatter) is expressed by variance $Var(X)$, also $\sigma^2(X)$:

$$\mu(X) = \int_{-\infty}^{+\infty} xf(x)dx \tag{2}$$

$$\sigma^2(X)\int_{-\infty}^{+\infty}(x-\mu_X)^2 f(x)dx \quad (3)$$

The square root of variance is titled as standard deviation ($\sigma_X = \sqrt{\sigma_X^2}$). Other characteristics (third and fourth moment) of the random quantities suitable for the determination of the probability distribution asymmetry are skewness and kurtosis.

An important feature of random variables is the degree of their dependency. The dependency is characterised by covariance *cov* (X_i,X_j), or rather the correlation coefficient *corr* (X_i, X_j) (3), which, in contrast with covariance, does not change when variables are being linearly transformed. The correlation coefficient assumes values from –1 to 1.

$$cov(X,Y) = E[(X-\mu_x)(Y-\mu_y)] \quad (4)$$

$$corr(X,Y) = \frac{cov(X,Y)}{\sigma_X \sigma_Y} \quad (5)$$

For the statistic processing of variable input parameters is necessary, first of all, to describe these parameters by probability density functions. There are several appropriate tests on agreement of experimental data with probability distribution, for example the χ^2 test, Kolmogorov - Smirnov test, MLE, or other advanced statistical analyses implemented into user programs. If the amount of input data is insufficient or we know only the interval of the values, it is difficult to determine the relevant distribution.

The overwhelming majority of studies and works dealing with the probabilistic analysis of geotechnical problems (e.g. Hamm et al. 2006, Flores 2010, Suchomel 2011, Choi 1997) point out the fact that it is recommendable to describe rock (soil) mass parameters by a normal or log-normal distribution.

The input parameters of solved probabilistic analyses we can regard as random variables

3 LATIN HYPERCUBE SAMPLING METHOD

The Monte Carlo method is commonly used numerical simulation method for solution of random problems in which we require statistical and probabilistic information on the problem response. However, for their exact estimates the Monte Carlo method usually requires many trials (program runs, simulations) to achieve the required error. To reduce the number of simulations and the significant time demands on calculations several reduction methods have been developed. The Latin Hypercube Sampling Method appertains to these methods.

The first implementation of the Latin Hypercube Sampling method is associated with the solving and processing of uncertainties in analyses of the safety of nuclear power plants in the United States of America. The method was published for the first time by Conover and his colleagues in 1979 and its practical use was first described in the work by Iman and Conover (1982). The LHS is a very efficient tool for executing statistical analyses which are focused on the determination of lower statistical moments of resulting variables. LHS converges to the correct solution significantly faster than the Monte Carlo method and this way significantly reduces the number of simulations with preservation of high accuracy estimates of probability density function parameters (the number of simulations N is in the order of tens to several hundreds). The advantage of this method follows from the manner of the selection of realisations (samples), where the entire scope of the input random variable is uniformly covered with respect to the distribution function. No real value is a priori excluded. The current method preserves the identified (estimated) probability density functions for individual random variables and the determined correlation coefficients between them. To attain these advantages LHS produce the highly dependent joint probability density function of random values vector.

3.1 *Samples generation and their form*

The method principle is N multiple generation of samples of each random variable. The domain of the cumulative distribution function *F(x)* corresponding to the probability density function *f(x)* for the particular variable is divided into N disjunctive intervals (layers). Individual intervals assume identical probabilities of 1/N. One value is selected from each layer to represent the entire interval and is to be used only once in the simulation. It is therefore a case of a stratification method. In major cases the representative value of the random variable is derived by means of the inverse transformation of the distribution function.

There are more methods available for the selection of samples from individual intervals within the domain of the distribution function. One of the methods lies in generating N random numbers *n* from the uniformly distributed interval (0, 1). These numbers are subsequently assigned to corresponding intervals using linear transformation. The values of samples $x_{i,k}$ of the variable X_i are determined by means of the inverse distribution function:

$$x_{i,k} = F_i^{-1}\left(\frac{n+(k-1)}{N}\right) \quad (4)$$

Where k is the k[th] sample (also layer, interval) of the i^{th} random variable X_i, F_i^{-1} is the inverse distribution function of this variable, n is a randomly generated number from the interval (0, 1), N is the number of intervals and, at the same time, the number of simulations. The manner of the selection and the method itself are often referred to as „LHS *random*".

Another method of generating samples of a random variable which is applied in the majority of studies is selecting a value from the mid-point (median) of the interval 1/N on the distribution function. This method is again associated with the direct use of the inverse distribution function:

$$x_{i,k} = F_i^{-1}\left(\frac{k-0{,}5}{N}\right) \tag{5}$$

This method is sometime referred to as the „LHS *median*". Fig. 1 depicts the cumulative distribution function $F(x)$, which is divided into eight intervals with equal probability of 1/N. Points on the vertical axis represent medians of these intervals and subsequently mark the corresponding values of the variable X_i.

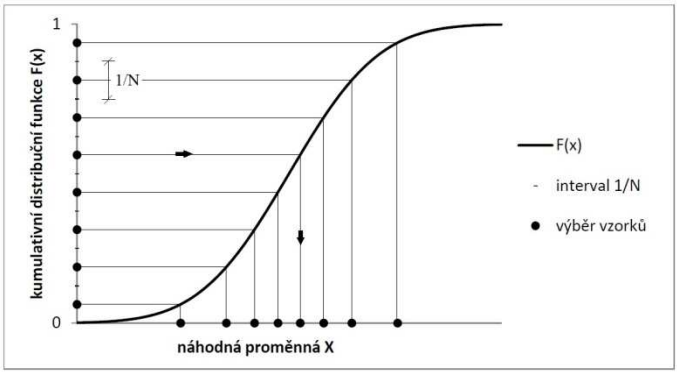

Fig. 1: Sampling by LHS *median* method

Authors Huntington & Lyrintzis (1998), Keramat & Kielbasa (1999), Vořechovský (2009) point out disadvantages of this stratification method. These disadvantages are first of all related to marginal layers of the distribution function domain, which most of all affect the variance, skewness and kurtosis of input variables. Whilst this method provides the adequate or a very close mean value to the required value, the variance differs mostly significantly.

Huntington and Lyrintzis make a suggestion the selection of representative samples $x_{i,k}$ to be solved as a mean value of the interval defined on the probability density function of a particular variable X_i.

$$x_{i,k} = N\int_{y_{i,k-1}}^{y_{i,k}} xf(x)dx \tag{6}$$

Limits of integration $y_{i,k}$ can be determined from the relationship (7):

$$y_{i,k} = F_i^{-1}\left(\frac{k}{N}\right) \tag{7}$$

The method referred to as the LHS *mean* (Fig. 2) better captures the probability density function, where the mean value is determined exactly and the variance estimate of the particular variable is significantly closer to the required variance. The LHS *mean* converges to a correct solution faster than the LHS *median*, therefore it requires smaller number of simulations.

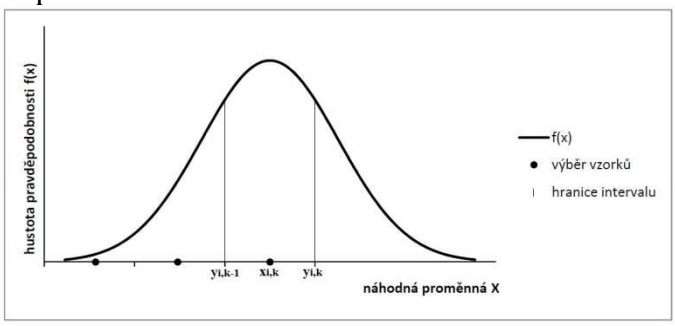

Fig. 2: Sampling by LHS *mean* method.

Evaluation and recommendation in favour of stratification methods generally in relation to random methods (Monte Carlo) is a part of paper by Flores et al. (2010), Helton & Davis (2003), Olsson et al. (2003) and others.

When the LHS method is applied, one of the two forms of samples arranged in sets for individual deterministic simulations is usually taken into consideration. In the first form, after generating representative samples for all random variables, samples for individual simulations are selected in the form of random permutations of whole numbers 1, 2, … to N.

Tab. 1: Permutační tabulka – počet simulací 1 až N vzhledem k počtu veličin X_1 až X_i

N/X_i	X_1	X_2	X_3	X_4	…	X_i
1	3	1	6	3	2	6
2	5	2	2	1	4	4
3	1	6	3	5	5	1
4	4	3	5	2	1	3
:	6	4	4	6	3	5
N	2	5	1	4	6	2

The permutation table lines define the number of simulations N and their sequence, whilst the columns define the number of variables X_i taken into account when solving the random problem. Individual elements, numbers in the permutation table, determine the k^{th} layer (interval) which the sample $x_{i,k}$ of the variable X_i is selected from. As soon as the sequence (order) numbers are replaced by samples, we can speak about an **X** K x N samples matrix, where the K denotes the number

of variables and N is for the number of simulations.

The second form considers standardised elements arranged in a **U** K x N normalised samples matrix.

$$u_{i,j} = \frac{x_{i,j} - u_j}{\sigma_j} \tag{8}$$

where u_j and σ_j are the mean value and standard deviation of the j^{th} variable respectively. This transformation will ensure that all columns (variables) have a zero mean value and unit variance. Other options are to work directly with the values of samples of individual variables or with random variables from the uniform distribution (0,1) generated in the columns of a K x N matrix.

Among individual variables usually arise significant undesired correlations affecting the accuracy and quality of results. The random permutation described above represents the simplest permutation method. The assumption is adopted that the generated vectors of the **X** matrix (or **U**) are independent, or the dependences are sufficiently small.

3.2 *Statistical dependency introducing*

It is advisable to verify the measure of statistical dependency of individual vectors (columns of the permutation table) using a Pearson's linear correlation coefficient or a Spearman's rank correlation coefficient. The majority of works solve the implementation of statistical correlation in the form of rearranging the sequence of samples at individual variables and do not change their values. In this way, the probability distribution of each random quantity is preserved.

There are several methods proposed for the simulation of correlated random variables with assigned arbitrary probability distribution function and values of correlation coefficients. This paper is further focused on a brief description and assessment of a few methods which are based on the optimisation of the sample sequence in the columns of a K x N matrix, which were generated without taking correlations into consideration.

The orthogonal transformation of independent random variables into correlated variables represents the most widely spread method for introducing correlation in the LHS method. Iman and Conover (1982) described a method using Spearman's coefficient of correlation (9) for the description of statistical dependence between columns of an order matrix and the Cholesky decomposition of a correlation matrix (10). Disadvantage of this method is the assumption of uncorrelated input variables and a persisting significant error in correlation between variables with respect to the required correlation matrix.

The method referred to as the Updated Latin Hypercube Sampling (ULHS) (Florian 1992) arising from the Iman and Conover procedure was developed for the reduction of undesired correlation with the aim of obtaining uncorrelated variables. Spearman's correlation coefficient describes the dependence among columns of an order matrix **R** (K x N):

$$c_{i,j} = 1 - \frac{6\sum_k (R_{ki} - R_{kj})^2}{N(N-1)(N+1)} \tag{9}$$

where coefficients $c_{i,j}$ are Spearman's correlation coefficients among variables i and j within the interval (-1, 1) and R are individual elements of matrix **R**. The correlation matrix **C** is symmetrical and positively definite and in the case of the UHLS, the **C** has the shape of a unit matrix.

$$\boldsymbol{C} = \boldsymbol{L}^T \boldsymbol{L} \tag{10}$$

L is a lower triangular matrix. The modified matrix of order $\mathbf{R}^*$ is derived from the relationship:

$$\boldsymbol{R}^* = \boldsymbol{R}\boldsymbol{L}^{-1} \tag{11}$$

The order numbers in each column of the matrix **R** are subsequently ordered in such a way that their sequence is identical to orders in corresponding columns of matrix $\mathbf{R}^*$. This modification of order matrix can be realised iteratively and it theoretically allows significant reduction of correlation. However, other authors (e.g. Huntington & Lyrintzis 1998) caution that the ULHS method tends to converge to sequences which still give the correlation error between some variables. In the case of the simulation of correlated variables, the technique described above, faces with significant problems.

Huntington and Lyrintzis (1998) propose an optimisation method called „*single-switch*". Instead of using orders this method directly rearranges modified samples and uses Pearson's correlation coefficient for the determination of correlations. The subsequent procedure is solved step-by-step for each column m of matrix **R** with samples R. The vector **T** contains actual correlation coefficients between the m^{th} column and each previous column (m -1):

$$T_j = \frac{1}{N}\sum_{i=1}^{N} R_{ij} R_{im} \tag{12}$$

where $1 \le j \le m$-1. The error of correlation coefficients E:

$$E = \sum_{j=1}^{m-1} \left(T_j - T_{jm}^{'}\right)^2 \tag{13}$$

where T' is a matrix containing required (target) correlation coefficients. The principle of the optimisation method is the calculation of the change in E for each pair of samples of the m^{th} variable, which occurs when they are switched. The pair providing the greatest reduction in E is switched. This procedure is realised for the m^{th} variable iteratively until no further improvement is possible or the correlation coefficients are found inside the defined intervals. The procedure is repeated step by step for all variables. The "*single-switch*" method provides significantly higher correlation accuracy at a lower number of in comparison with the UHLS.

A very effective and accurate procedure for the implementation of required correlations is represented by the Simulated Annealing Method (e.g. Morris & Mitchel 1995, Minasny & McBratney 2006, Vořechovský 2009). It prefers the norm E for assessing the quality of statistical dependences allowing for deviations of all correlation coefficients with a square (14), unlike the maximum difference, which is not suitable for direct minimisation.

$$E = \sum_{i=1}^{N_V} \sum_{j=1}^{N_V} (A_{i,j} - T_{i,j})^2 \tag{14}$$

where N_V is the number of variables and in brackets there is the difference between actual correlation coefficients $A_{i,j}$ and required (target) $T_{i,j}$ for quantities i and j. The method arises from a simple probabilistic method which swaps the orders of a random pair of samples of a randomly selected variable in matrix **X** (e.g. normalised samples, order numbers). In the case of E norm reduction, the matrix **X** was adopted as a new generation, i.e. the initial matrix. But the abovementioned procedure in the majority of cases ends in a state when no change brings the reduction of the norm and the new matrix cannot be adopted. The method therefore finds the so-called local minimums, without a chance of finding the actual global minimum (Vořechovský 2009). The principle of the Simulated Annealing Method is therefore based on the violation of the condition that a new generation of samples may be adopted only in the case of E norm reduction. In an every iteration a new generation is produced, it is ether adopted or not. The simulated annealing comes on in the second case and the new vector with a higher energy configuration ($\Delta E > 0$) is adopted with a certain probability which follows Boltzmann's distribution:

$$P \approx exp\left(\frac{-\Delta E}{t}\right) \tag{15}$$

This distribution takes into consideration a system which is found in temperature equilibrium t and has its energy in terms of probability distributed among possible energy states ΔE. The non-zero probability in the adoption of a new generation of samples increases the chance of finding a configuration which will avoid the local minimum.

Other selected permutation method, mentioned in smaller detail, is the Symmetric Latin Hypercubes Design (SLHD) method (Ye et al. 2000), arising from a symmetric matrix N x K. The SLHD is based on a "Columnwise-Pairwise" (CP) algorithm. Within an optimum symmetric matrix searching process this algorithm simultaneously swaps the orders of two pairs within a column in each step of a particular iteration. The swap which is best with respect to the minimisation criterion is selected at the end of the iteration and is used for the matrix modification. The shape of the resultant matrix is significantly sensitive to the initial random generation of the permutation matrix, therefore the whole algorithm should be repeated several times with different initial permutations. The authors have evaluated the method on the basis of a comparison with the simulated annealing algorithm and Cholesky decomposition. Whereas the CP method is primarily suitable for small-size designs (e.g. 2 variables x 12 simulations), the simulated annealing for more extensive concepts (e.g. 4 variables x 25 simulations). The authors have pointed out that simulated annealing in conjunction with symmetric matrix gave more accurate results in majority of cases.

There are several other methods available based on the optimisation of the samples order, which were implemented into the LHS method with the aim of allowing for correlations among variables and are not described in this paper in more detail. Anyway, their principle is very similar to the algorithms described above (e.g. Gram - Schmidt order orthogonalisation).

4 THE LHS APPLICATION TO SOLVING GEOTECHNICAL PROBLEMS IN THE CZECH REPUBLIC

4.1 *General overview*

The use of the LHS method in geotechnical practise in the Czech Republic is not too frequent, the majority of works dealing with this topic was carried out on university field.

The statistical analysis of the Mrázovka tunnel numerical model is part of the work of Hilar (2000), where the LHS was used for assessing the influence of five basic parameters of the Mohr-Coulomb model on deformations of the lining and ground surface. Another example is the use of

the LHS method for the Valík tunnel calculations (Hrubešová et al. 2003), where the LHS is applied to the appraising of the influence of 10 input parameters (e.g. the anisotropy coefficient, dip of discontinuities etc.). Vaněčková (2008) uses the LHS method for solving problems of stability of a rock slope intersected by a system of discontinuities. Geotechnical parameters and other properties of discontinuities can assume four different probability distribution functions. Part of the Parák study (2008) is focused on the LHS application to the determination of the influence of ground geotechnical parameters, parameters of sprayed concrete and initial conditions on structural forces of a circular tunnel lining. Doc. J. Pruška devotes to the using of the LHS in geotechnics in the long term (e.g. Pruška, Šedivý 2010).

The above-mentioned works and studies assume linearly independent input geotechnical parameters which means, they did not deal with their correlation. In addition, all works consider the LHS *median* method type (the mid-point of an interval within the domain of the distribution function). This method, in comparison with the LHS *mean*, converges to the result significantly slower and higher number of simulations is recommended for achieving a satisfactory accuracy. Further, normal probability distribution of input parameters is usually assumed in the majority of works.

The LHS method finds significant use in the Czech Republic in the field of reinforced concrete structures. The Institute of Construction Mechanics of the Faculty of Civil Engineering of the University of Technology in Brno, represented by Prof. Novák, doc. Vořechovský and others, deals with modifications and improvements of the LHS method for practical applications in the long term.

4.2 *LHS software*

In a framework of an applied research project the present paper authors have prepared software, and continue in its further developing, focused on probabilistic analyses by LHS method. This chapter devotes to brief feature description of the program implemented into simple graphic projection.

Program considers four different basic probability distributions (normal, log-normal, exponential and Weibull distribution) to be assigned to random variables. Selection of representative samples of each random variable is based on LHS *mean* method. As mentioned in Chapter 3.2., this method selects samples as a mean value of intervals defined on probability density function of particular random variable. Implemented method, in comparison with standard LHS versions, better captures the probability density function and variance estimate of particular random variable is substantially closer to required value (Fig. 3 – example of convergence of Young modulus variance).

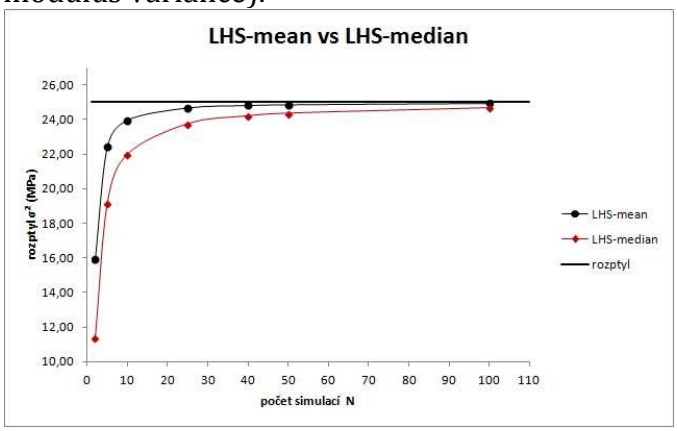

Fig. 3: Evaluation of variance convergence of samples genrated by LHS *mean* and LHS *median* method to required value in relation to simulation number.

This feature allows further reduction of simulation number, in conjunction with accuracy preservation, and concurrently lowers time demands of analyses in this way. Occurrence of undesired correlations and introduction of required correlations among random variables is being solved by Simulated Annealing method cooperating with simple "smoothing" algorithm.

Software and LHS *mean* method itself has been verifying by numerical models of underground construction realised in Czech Republic recently (e.g. cross sections of Brusnice tunnel).

5 SUMMARY

The Latin Hypercube Sampling (LHS) method represents an effective probabilistic method of the Monte Carlo type for statistical processing of input variables and estimation of statistical moments of the solved problem response. The greatest advantage lies in the possibility of significant reducing the number of simulations in comparison with the standard Monte Carlo method with preservation of the high accuracy of estimates. The LHS method maintains the probability distribution assigned to all variables and allows for the degree of correlation among them. Several modifications improving the method accuracy and at the same time reducing the time-demands of simulations were developed and adopted. The LHS method finds its use in many branches, including geotechnics with underground constructions. The LHS use for structural analyses of underground structures may significantly improve the accuracy of the concept of the anticipated behaviour of a structure (first of all the occurrence probability of limit states).

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