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Extension of Latin Hypercube Samples with Correlated Variables

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Abstract

A procedure for extending the size of a Latin hypercube sample (LHS) with rank correlated variables is described and illustrated. The extension procedure starts with an LHS of size m and associated rank correlation matrix $\mathbf{C}$ and constructs a new LHS of size $2m$ that contains the elements of the original LHS and has a rank correlation matrix that is close to the original rank correlation matrix $\mathbf{C}$. The procedure is intended for use in conjunction with uncertainty and sensitivity analysis of computationally demanding models in which it is important to make efficient use of a necessarily limited number of model evaluations.

Key Words: Experimental design, Latin hypercube sample, Monte Carlo analysis, Rank correlation, Sample size extension, Sensitivity analysis, Uncertainty analysis.

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1. Introduction

The evaluation of the uncertainty associated with analysis outcomes is now widely recognized as an important part of any modeling effort.[1-11] A number of approaches to such evaluations are in use, including differential analysis,[12-17] response surface methodology,[18-26] variance decomposition procedures,[27-31] and Monte Carlo (i.e., sampling-based) procedures.[32-42] Additional information is available in a number of reviews.[43-51] Monte Carlo analysis employing Latin hypercube sampling[52, 53] is one of the most popular and effective approaches for the evaluation of the uncertainty associated with analysis outcomes and is the focus of this presentation.

Conceptually, an analysis can be formally represented by a function of the form

$$\mathbf{y} = f(\mathbf{x}), \tag{1.1}$$

where

$$\mathbf{x} = [x_1, x_2, \ldots, x_n] \tag{1.2}$$

is a vector of analysis inputs and

$$\mathbf{y} = [y_1, y_2, \ldots, y_p] \tag{1.3}$$

is a vector of analysis results. In turn, uncertainty with respect to the appropriate values to use for the elements of $\mathbf{x}$ leads to uncertainty with respect to the values for the elements of $\mathbf{y}$. Most analyses use probability to characterize the uncertainty associated with the elements of $\mathbf{x}$ and hence the uncertainty associated with the elements of $\mathbf{y}$. In particular, a sequence of probability distributions

$$D_1, D_2, \ldots, D_n \tag{1.4}$$

is used to characterize the uncertainty associated with the elements of $\mathbf{x}$, where the distribution D_j characterizes the uncertainty associated with the element x_j of $\mathbf{x}$. The definition of the preceding distributions is often accomplished through an expert review process and can be accompanied by the specification of correlations and other restrictions involving the interplay of the possible values for the elements of $\mathbf{x}$.[54-69]

In a Monte Carlo (i.e., sampling-based) analysis, a sample

$$\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{in}], i = 1, 2, \ldots, m, \tag{1.5}$$

is generated from the possible values for $\mathbf{x}$ in consistency with the distributions indicated in Eq. (1.4) and any associated restrictions. In turn, the evaluations

$$\mathbf{y}_i = f(\mathbf{x}_i), i = 1, 2, \ldots, m, \tag{1.6}$$

create a mapping

$$[\mathbf{x}_i, \mathbf{y}_i], i = 1, 2, \ldots, m, \tag{1.7}$$

between analysis inputs and analysis outcomes that forms the basis for uncertainty analysis (i.e., the determination of the uncertainty in the elements of $\mathbf{y}$ that derives from uncertainty in the elements of $\mathbf{x}$) and sensitivity analysis (i.e., the determination of how the uncertainty in individual elements of $\mathbf{x}$ contributes to the uncertainty in elements of $\mathbf{y}$).

As previously indicated, Latin hypercube sampling is a very popular method for the generation of the sample indicated in Eq. (1.5). Further, this generation is often performed in conjunction with a procedure introduced by Iman and Conover to induce a desired rank correlation structure on the resultant sample.[70, 71] As a result of this popularity, the original paper introducing Latin hypercube sampling was recently declared a *Technometrics* classic in experimental design.[72] The effectiveness of Latin hypercube sampling, and hence the cause of its popularity, derives from the fact that it provides a dense stratification over the range of each uncertain variable with a relatively small sample size while preserving the desirable probabilistic features of simple random sampling. More specifically, Latin hypercube sampling combines the desirable features of simple random sampling with the desirable features of a multilevel, highly fractionated fractional factorial design. Latin hypercube sampling accomplishes this by using a highly structured, randomized procedure to generate the sample indicated in Eq. (1.5) in consistency with the distributions indicated in Eq. (1.4).

A drawback to Latin hypercube sampling is that its highly structured form makes it difficult to increase the size of an already generated sample while simultaneously preserving the stratification properties that make Latin hypercube sampling so effective. Unlike simple random sampling, the size of a Latin hypercube sample (LHS) cannot be increased simply by generating additional sample elements as the new sample containing the original LHS and the additional sample elements will no longer have the structure of an LHS. For the new sample to also be an LHS, the additional sample elements must be generated with a procedure that takes into account the existing LHS that is being increased in size and the definition of Latin hypercube sampling.

The purpose of this presentation is to describe a procedure for the extension of the size of an LHS that results in a new LHS with a correlation structure close to that of the original LHS. The basic idea is to start with an LHS

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, \ldots, x_{in}\right], i = 1, 2, \ldots, m, \tag{1.8}$$

of size m and then to generate a second sample

$$\tilde{\mathbf{x}}_i = \left[\tilde{x}_{i1}, \tilde{x}_{i2}, \ldots, \tilde{x}_{in}\right], i = 1, 2, \ldots, m, \tag{1.9}$$

of size m such that

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_i & \text{for } i = 1, 2, \ldots, m \\ \tilde{\mathbf{x}}_{i-m} & \text{for } i = m+1, m+2, \ldots, 2m \end{cases} \tag{1.10}$$

is an LHS of size $2m$ and also such that the correlation structures associated with the original LHS in Eq. (1.8) and the extended LHS in Eq. (1.10) are similar. A related extension technique for LHSs has been developed by C. Tong[73] but does not consider correlated variables. Extensions to other integer multiples of the original sample size are also possible.

There are at least three reasons why such extensions of the size of an LHS might be desirable. First, an analysis could have been performed with a sample size that was subsequently determined to be too small. The extension would permit the use of a larger LHS without the loss of any of the already performed, and possibly quite expensive, calculations. Second, the implementation of the Iman and Conover procedure to induce a desired rank correlation structure on an LHS of size m requires the inversion of an $m \times m$ matrix. This inversion can be computationally demanding when a large sample is to be generated. The presented extension procedure provides a way to generate an LHS of size $2m$ with a specified correlation structure at a computational expense that is approximately equal to that of generating two LHSs of size m with the desired correlation structure. Third, the extension procedure provides a way to perform replicated Latin hypercube sampling[74, 75] to test the stability of results that enhances the quality of results obtained when the replicates are pooled.

2. Definition of Latin Hypercube Sampling

Latin hypercube sampling operates in the following manner to generate a sample of size m from n variables with the distributions $D_1, D_2, \ldots, D_n$ indicated in Eq. (1.4). The range $\mathcal{X}_j$ of each variable x_j is divided into m contiguous intervals

$$\mathcal{X}_{ij},\ i = 1, 2, \ldots, m, \tag{2.1}$$

of equal probability in consistency with the corresponding distribution D_j. A value for the variable x_j is selected at random from the interval $\mathcal{X}_{ij}$ in consistency with the distribution D_j for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. Then, the m values for x_1 are combined at random and without replacement with the m values for x_2 to produce the ordered pairs

$$\left[x_{i1}, x_{i2}\right],\ i = 1, 2, \ldots, m. \tag{2.2}$$

Then, the preceding pairs are combined at random and without replacement with the m values for x_3 to produce the ordered triples

$$\left[x_{i1}, x_{i2}, x_{i3}\right],\ i = 1, 2, \ldots, m. \tag{2.3}$$

The process continues in the same manner through all n variables. The resultant sequence

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, \ldots, x_{in}\right],\ i = 1, 2, \ldots, m, \tag{2.4}$$

is an LHS of size m from the n variables $x_1, x_2, \ldots, x_n$ generated in consistency with the distributions $D_1, D_2, \ldots, D_n$.

The Iman and Conover restricted pairing procedure[70, 71] provides a way to generate an LHS with a rank correlation structure close to a correlation structure specified by a matrix

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix}, \tag{2.5}$$

where c_{rs} is the desired rank (i.e., Spearman) correlation between x_r and x_s. The details of this procedure are not needed in the development of the extension algorithm and therefore will not be presented. Additional information on this procedure is available in the original article[70] and also in a recent review on Latin hypercube sampling.[52]

When the LHS indicated in Eq. (2.4) is generated with the Iman and Conover procedure with a target correlation structure defined by the matrix $\mathbf{C}$ in Eq. (2.5), the resultant rank correlation structure can be represented by the matrix

$$\mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1n} \\ d_{21} & d_{22} & \cdots & d_{2n} \\ \vdots & \vdots & & \vdots \\ d_{n1} & d_{n2} & \cdots & d_{nn} \end{bmatrix}, \tag{2.6}$$

where d_{rs} is the rank correlation between x_r and x_s in the sample. Specifically,

$$d_{rs} = \frac{\sum_{i=1}^{m}\left[r(x_{ir})-\bar{r}(x_r)\right]\left[r(x_{is})-\bar{r}(x_s)\right]}{\left\{\sum_{i=1}^{m}\left[r(x_{ir})-\bar{r}(x_r)\right]^2\right\}^{1/2}\left\{\sum_{i=1}^{m}\left[r(x_{is})-\bar{r}(x_s)\right]^2\right\}^{1/2}}$$

$$= \frac{\sum_{i=1}^{m}\left[r(x_{ir})-(m+1)/2\right]\left[r(x_{is})-(m+1)/2\right]}{m\left(m^2-1\right)/12}, \tag{2.7}$$

where $r(x_{ir})$ and $r(x_{is})$ denote the rank-transformed values of x_{ir} and x_{is}, respectively. Use of the Iman and Conover procedure results in the correlation matrix **D** being similar to, but usually not equal to, the target correlation matrix **C**.

3. Extension Algorithm

The extension algorithm starts with an LHS of size m of the form indicated in Eq. (2.4) and an associated rank correlation matrix $\mathbf{D}_1$ as indicated in Eq. (2.6) generated with the Iman and Conover procedure so that $\mathbf{D}_1$ is close to the target correlation matrix $\mathbf{C}$. The problem under consideration is how to extend this sample to an LHS of size $2m$ with a rank correlation matrix $\mathbf{D}$ that is again close to $\mathbf{C}$. This extension can be accomplished by application of the following algorithm:

Step 1. Let k_j be a discrete variable with a uniform distribution on the set $\mathcal{K}_j = \{1, 2, \ldots, m\}$ for $j = 1, 2, \ldots, n$. Use the Iman and Conover procedure to generate an LHS

$$\mathbf{k}_i = \left[k_{i1}, k_{i2}, \ldots, k_{in}\right], i = 1, 2, \ldots, m, \tag{3.1}$$

from $k_1, k_2, \ldots, k_n$ with a rank correlation matrix $\mathbf{D}_2$ close to the candidate correlation matrix $\mathbf{C}$. In turn, the vectors $\mathbf{k}_i = [k_{i1}, k_{i2}, \ldots, k_{in}]$ define n-dimensional rectangular solids

$$\begin{aligned} \mathcal{S}_i &= \mathcal{X}_{k_{i1}1} \times \mathcal{X}_{k_{i2}2} \times \ldots \times \mathcal{X}_{k_{in}n} \\ &= \mathcal{E}_{i1} \times \mathcal{E}_{i2} \times \ldots \times \mathcal{E}_{in} \end{aligned} \tag{3.2}$$

in the space $\mathcal{X}_1 \times \mathcal{X}_2 \times \ldots \times \mathcal{X}_n$, where the sets $\mathcal{E}_{ij} = \mathcal{X}_{k_{ij}j}$, $j = 1, 2, \ldots, n$, correspond to strata indicated in Eq. (2.1) and used in the generation of the original LHS. In essence, an LHS

$$\mathbf{s}_i = \left[\mathcal{E}_{i1}, \mathcal{E}_{i2}, \ldots, \mathcal{E}_{in}\right], i = 1, 2, \ldots, m, \tag{3.3}$$

with a rank correlation matrix $\mathbf{D}_2$ close to the specified correlation matrix $\mathbf{C}$ is being generated from the strata used to obtain the original LHS.

Step 2. For each i, divide the n-dimensional rectangular solid $\mathcal{S}_i$ defined in Eq. (3.2) into 2^n equal probability rectangular solids by dividing each edge $\mathcal{E}_{ij}$ of $\mathcal{S}_i$ into two nonoverlapping intervals of equal probability on the basis of the corresponding probability distribution D_j. Specifically, $\mathcal{S}_i = \mathcal{E}_{i1} \times \mathcal{E}_{i2} \times \ldots \times \mathcal{E}_{in}$ as indicated in Eq. (3.2), and each of the 2^n equal probability sets is of the form

$$\mathcal{T}_{i\mathbf{l}} = \mathcal{E}_{i1l_1} \times \mathcal{E}_{i2l_2} \times \ldots \times \mathcal{E}_{inl_n}, \tag{3.4}$$

where $\mathcal{E}_{ij1} \cup \mathcal{E}_{ij2} = \mathcal{E}_{ij}$, $\mathcal{E}_{ij1} \cap \mathcal{E}_{ij2} = \varnothing$, $prob(\mathcal{E}_{ij1}) = prob(\mathcal{E}_{ij2}) = prob(\mathcal{E}_{ij})/2$ with $prob(\sim)$ denoting probability, and $\mathbf{l} = [l_1, l_2, \ldots, l_n]$ is an element of $\mathcal{L} = \mathcal{L}_1 \times \mathcal{L}_2 \times \ldots \times \mathcal{L}_n$ with $\mathcal{L}_j = \{1, 2\}$. In turn,

$$\mathcal{S}_i = \cup_{\mathbf{l} \in \mathcal{L}} \mathcal{T}_{i\mathbf{l}}, \tag{3.5}$$

where the $\mathcal{T}_{i\mathbf{l}}$ are disjoint, equal probability rectangular solids.

Step 3. For each i, identify the n-dimensional rectangular solid

$$\mathcal{T}_i = \mathcal{T}_{i\mathbf{l}} = \mathcal{E}_{i1l_1} \times \mathcal{E}_{i2l_2} \times \ldots \times \mathcal{E}_{inl_n} \tag{3.6}$$

constructed in Step 2 such that $x_{ij} \notin \mathcal{E}_{ijl_j}$ for $j = 1, 2, \ldots, n$. For each i, there is exactly one such set $\mathcal{T}_i$.

Step 4. For each i, obtain the vector

$$\tilde{\mathbf{x}}_i = \left[\tilde{x}_{i1}, \tilde{x}_{i2}, \ldots, \tilde{x}_{in}\right] \tag{3.7}$$

by randomly sampling $\tilde{x}_{ij}$ from the interval $\mathcal{E}_{ijl_j}$ in consistency with the distribution D_j for $j = 1, 2, \ldots, n$.

Step 5. Extend the original LHS in Eq. (2.4) by

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_i & \text{for } i = 1, 2, \ldots, m \\ \tilde{\mathbf{x}}_{i-m} & \text{for } i = m+1, m+2, \ldots, 2m \end{cases} \tag{3.8}$$

to obtain the desired LHS of size $2m$.

For an integer $k > 2$, minor modifications of the preceding algorithm can be used to extend an LHS of size m to an LHS of size $k \times m$.

4. Illustration of Extension Algorithm

The extension algorithm is illustrated for the generation of LHSs from

$$\mathbf{x} = [x_1, x_2], \tag{4.1}$$

with (i) x_1 having a triangular distribution on [0, 1] with mode at 0.5, (ii) x_2 having a triangular distribution on [1, 10] with mode at 7.0, and (iii) x_1 and x_2 having a rank correlation of −0.7. Thus, $n = 2$ in Eq. (1.2); the distributions D_1 and D_2 in Eq. (1.4) correspond to triangular distributions; and

$$\mathbf{C} = \begin{bmatrix} 1.0 & -0.7 \\ -0.7 & 1.0 \end{bmatrix} \tag{4.2}$$

is the correlation matrix in Eq. (2.5). The extension of an LHS of size $m = 10$ to an LHS of size $2m = 20$ is illustrated.

The illustration starts with the generation of the LHS

$$\mathbf{x}_i = [x_{i1}, x_{i2}], i = 1, 2, \ldots, m = 10, \tag{4.3}$$

from $\mathbf{x} = [x_1, x_2]$ consistent with the distributions D_1 and D_2 and the specified rank correlation between x_1 and x_2. The resulting sample matrix $\mathbf{S}_1$, rank transformed sample matrix $\mathbf{RS}_1$ and rank correlation matrix $\mathbf{D}_1$ are given by

$$\mathbf{S}_1 = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_9 \\ \mathbf{x}_{10} \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \vdots & \vdots \\ x_{91} & x_{92} \\ x_{10,1} & x_{10,2} \end{bmatrix} = \begin{bmatrix} 0.297 & 8.726 \\ 0.358 & 8.147 \\ \vdots & \vdots \\ 0.404 & 4.020 \\ 0.728 & 6.924 \end{bmatrix}, \tag{4.4}$$

$$\mathbf{RS}_1 = \begin{bmatrix} r(\mathbf{x}_1) \\ r(\mathbf{x}_2) \\ \vdots \\ r(\mathbf{x}_9) \\ r(\mathbf{x}_{10}) \end{bmatrix} = \begin{bmatrix} r(x_{11}) & r(x_{12}) \\ r(x_{21}) & r(x_{22}) \\ \vdots & \vdots \\ r(x_{91}) & r(x_{92}) \\ r(x_{10,1}) & r(x_{10,2}) \end{bmatrix} = \begin{bmatrix} 2 & 10 \\ 3 & 9 \\ \vdots & \vdots \\ 4 & 2 \\ 9 & 6 \end{bmatrix}, \tag{4.5}$$

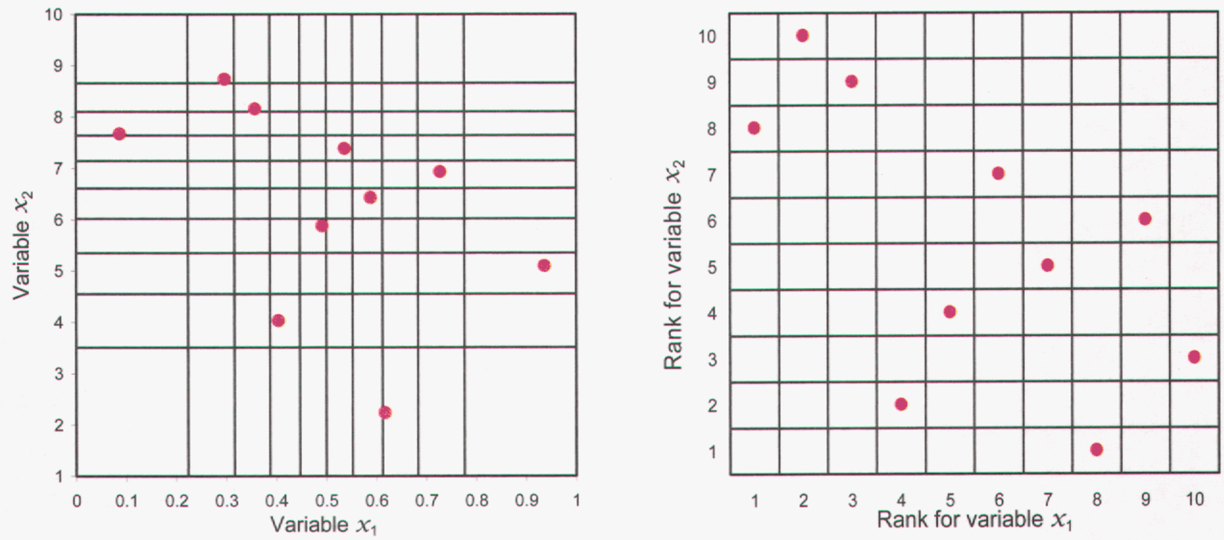
and

$$\mathbf{D}_1 = \begin{bmatrix} 1.000 & -0.612 \\ -0.612 & 1.000 \end{bmatrix}. \tag{4.6}$$

The full sample is shown in Fig. 1. The object is now to extend this sample to an LHS of size $2m = 20$ with an associated rank correlation matrix close to the correlation matrix $\mathbf{C}$ in Eq. (4.2).

Step 1. The Iman and Conover procedure is used to generate an LHS

$$\mathbf{k}_i = [k_{i1}, k_{i2}], i = 1, 2, \ldots, m = 10, \tag{4.7}$$



Key: ● $\mathbf{x}_i$, Initial sample

Fig. 1. Generation of LHS of size $m = 10$: (a) raw (i.e., untransformed) values, and (b) rank transformed values.

from discrete variables k_1 and k_2 that are uniformly distributed on $\{1, 2, \ldots, 10\}$ and have a rank correlation of -0.7. The resulting sample matrix $\mathbf{RS}_2$ and rank correlation matrix $\mathbf{D}_2$ are given by

$$\mathbf{RS}_2 = \begin{bmatrix} \mathbf{k}_1 \\ \mathbf{k}_2 \\ \vdots \\ \mathbf{k}_9 \\ \mathbf{k}_{10} \end{bmatrix} = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \\ \vdots & \vdots \\ k_{91} & k_{92} \\ k_{10,1} & k_{10,2} \end{bmatrix} = \begin{bmatrix} 7 & 6 \\ 10 & 1 \\ \vdots & \vdots \\ 4 & 5 \\ 8 & 2 \end{bmatrix} \tag{4.8}$$

and

$$\mathbf{D}_2 = \begin{bmatrix} 1.000 & -0.758 \\ -0.758 & 1.000 \end{bmatrix}. \tag{4.9}$$

In turn, the vectors $\mathbf{k}_i = [k_{i1}, k_{i2}]$ define rectangles (in the general case, n-dimensional rectangular solids)

$$S_i = \mathcal{X}_{k_{i1}1} \times \mathcal{X}_{k_{i2}2} = \mathcal{E}_{i1} \times \mathcal{E}_{i2} \tag{4.10}$$

as indicated in Eq. (3.2) and illustrated in Fig. 2. In particular, the sets S_i correspond to the shaded areas in Fig. 2, and the sets $\mathcal{E}_{i1}$ and $\mathcal{E}_{i2}$ correspond to the edges of S_i along the x_1 and x_2 axes, respectively.

Step 2. Each rectangle S_i defined in Eq. (4.10) and illustrated in Fig. 2a is divided into $2^2 = 4$ equal probability rectangles by dividing each edge of S_i (i.e., $\mathcal{E}_{i1}$ and $\mathcal{E}_{i2}$) into two nonoverlapping intervals of equal probability on the basis of the corresponding probability distributions D_1 and D_2 (Fig. 3). As a result of this division, each S_i can be expressed as

$$S_i = \mathcal{T}_{i,[1,1]} \cup \mathcal{T}_{i,[1,2]} \cup \mathcal{T}_{i,[2,1]} \cup \mathcal{T}_{i,[2,2]}, \tag{4.11}$$

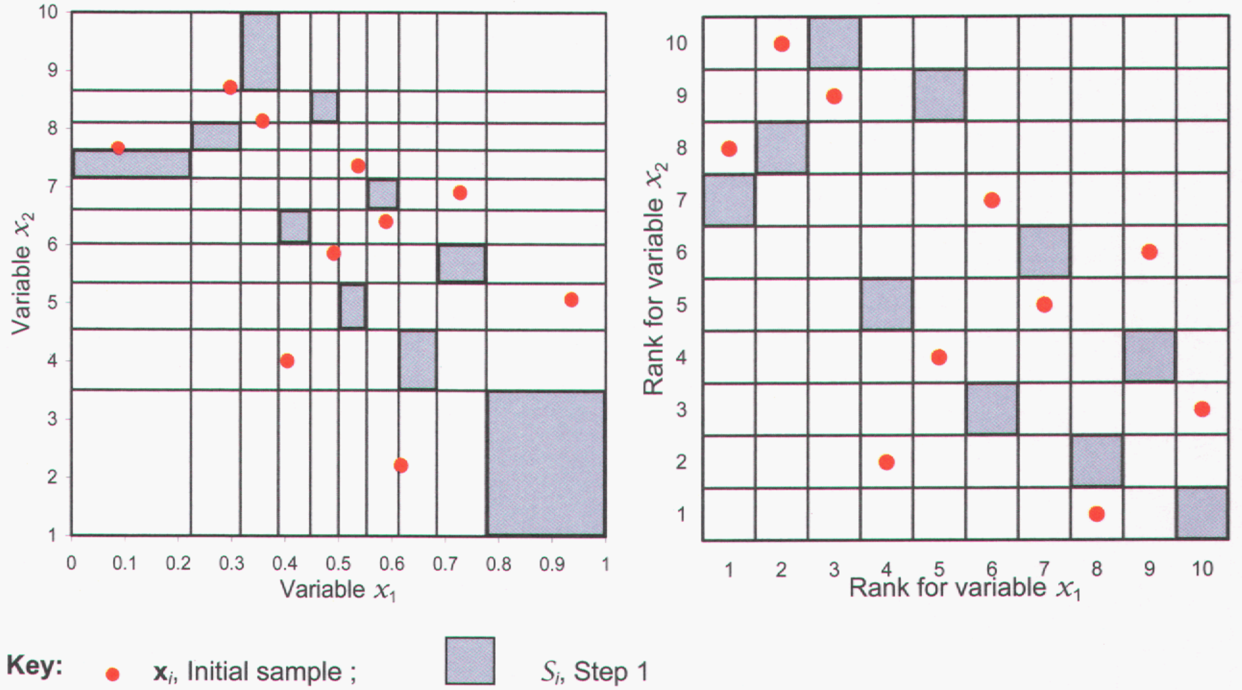


Fig. 2. Overlay of initial LHS $\mathbf{x}_i = [x_{i1}, x_{i2}]$, $i = 1, 2, \ldots, 10$, and rectangles $\mathcal{S}_i = \mathcal{E}_{i1} \times \mathcal{E}_{i2}$ generated in Step 1 of extension algorithm.

where (i) $\mathcal{E}_{i11}$ and $\mathcal{E}_{i12}$ are the equal probability intervals into which $\mathcal{E}_{i1}$ is divided, (ii) $\mathcal{E}_{i21}$ and $\mathcal{E}_{i22}$ are the equal probability intervals into which $\mathcal{E}_{i2}$ is divided, and (iii) $\mathcal{T}_{i,[1,1]} = \mathcal{E}_{i11} \times \mathcal{E}_{i21}$, $\mathcal{T}_{i,[1,2]} = \mathcal{E}_{i11} \times \mathcal{E}_{i22}$, $\mathcal{T}_{i,[2,1]} = \mathcal{E}_{i12} \times \mathcal{E}_{i21}$, and $\mathcal{T}_{i,[2,2]} = \mathcal{E}_{i12} \times \mathcal{E}_{i22}$. Thus, the rectangles interior to the $\mathcal{S}_i$ in Fig. 3 correspond to the sets $\mathcal{T}_{i,[1,1]}$, $\mathcal{T}_{i,[2,1]}$, $\mathcal{T}_{i,[2,1]}$ and $\mathcal{T}_{i,[2,2]}$, which in turn are defined by the intervals (i.e., edges) $\mathcal{E}_{i11}$, $\mathcal{E}_{i12}$, $\mathcal{E}_{i21}$ and $\mathcal{E}_{i22}$.

Step 3. For each i, the rectangle

$$\mathcal{T}_i = \mathcal{T}_{i,[r,s]} = \mathcal{E}_{i1r} \times \mathcal{E}_{i2s} \tag{4.12}$$

constructed at Step 2 is identified such that $x_{i1} \notin \mathcal{E}_{i1r}$ and $x_{i2} \notin \mathcal{E}_{i1s}$ (Fig. 4). This selection excludes intervals that contain values for x_1 and x_2 in the original LHS.

Step 4. For each i, the vector

$$\tilde{\mathbf{x}}_i = \left[\tilde{x}_{i1}, \tilde{x}_{i2}\right] \tag{4.13}$$

is obtained by randomly sampling $\tilde{x}_{i1}$ and $\tilde{x}_{i2}$ from the intervals $\mathcal{E}_{i1r}$ and $\mathcal{E}_{i2s}$, respectively, associated with the definition of the rectangle $\mathcal{T}_i$ in Eq. (4.12). The resulting sample matrix $\mathbf{S}_2$ is

$$\mathbf{S}_2 = \begin{bmatrix} \tilde{\mathbf{x}}_1 \\ \tilde{\mathbf{x}}_2 \\ \vdots \\ \tilde{\mathbf{x}}_9 \\ \tilde{\mathbf{x}}_{10} \end{bmatrix} = \begin{bmatrix} \tilde{x}_{11} & \tilde{x}_{12} \\ \tilde{x}_{21} & \tilde{x}_{22} \\ \vdots & \vdots \\ \tilde{x}_{91} & \tilde{x}_{92} \\ \tilde{x}_{10,1} & \tilde{x}_{10,2} \end{bmatrix} = \begin{bmatrix} 0.571 & 6.860 \\ 0.816 & 2.993 \\ \vdots & \vdots \\ 0.429 & 6.056 \\ 0.662 & 4.096 \end{bmatrix}, \tag{4.14}$$

the corresponding rank correlation matrix $\mathbf{D}_2$ is shown in Eq. (4.9), and the full sample is shown in Fig. 5.

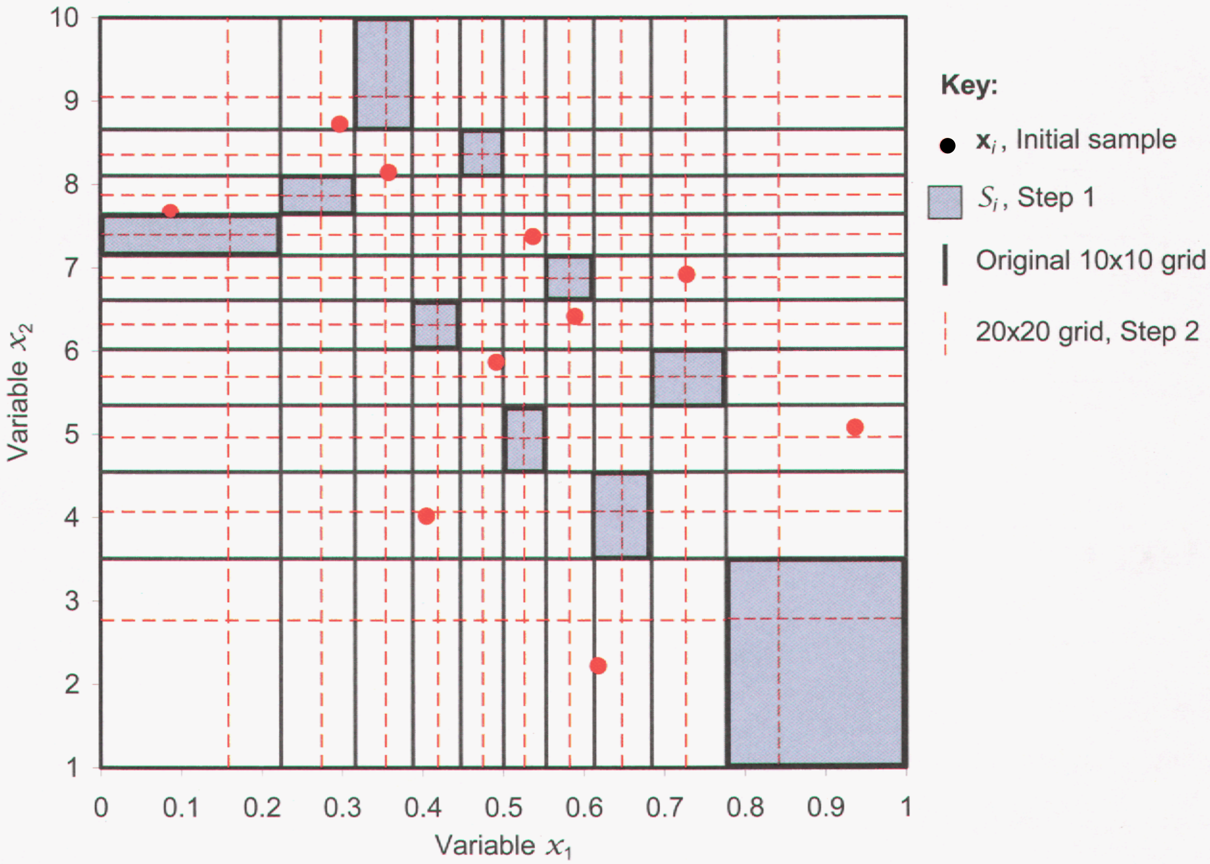


Fig. 3. Division of each rectangle S_i into $2^2 = 4$ equal probability rectangles $\mathcal{T}_{i,[1,1]}$, $\mathcal{T}_{i,[1,2]}$, $\mathcal{T}_{i,[2,1]}$ and $\mathcal{T}_{i,[2,2]}$ in Step 2 of the extension algorithm.

Step 5. The original LHS $\mathbf{x}_i$, $i = 1, 2, \ldots, 10$, in Eq. (4.3) is combined with the LHS $\tilde{\mathbf{x}}_i$, $i = 1, 2, \ldots, 10$, in Eq. (4.13) to produce the extended LHS

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_i & \text{for } i = 1, 2, \ldots, 10 \\ \tilde{\mathbf{x}}_{i-m} & \text{for } i = 11, 12, \ldots, 20 \end{cases} \tag{4.15}$$

of size 20. The associated rank correlation matrix

$$\mathbf{D} = \begin{bmatrix} 1.000 & -0.654 \\ -0.654 & 1.000 \end{bmatrix} \tag{4.16}$$

is reasonably close to the desired correlation matrix $\mathbf{C}$ in Eq. (4.2). The individual elements of the extended LHS correspond to the points shown in Fig. 5.

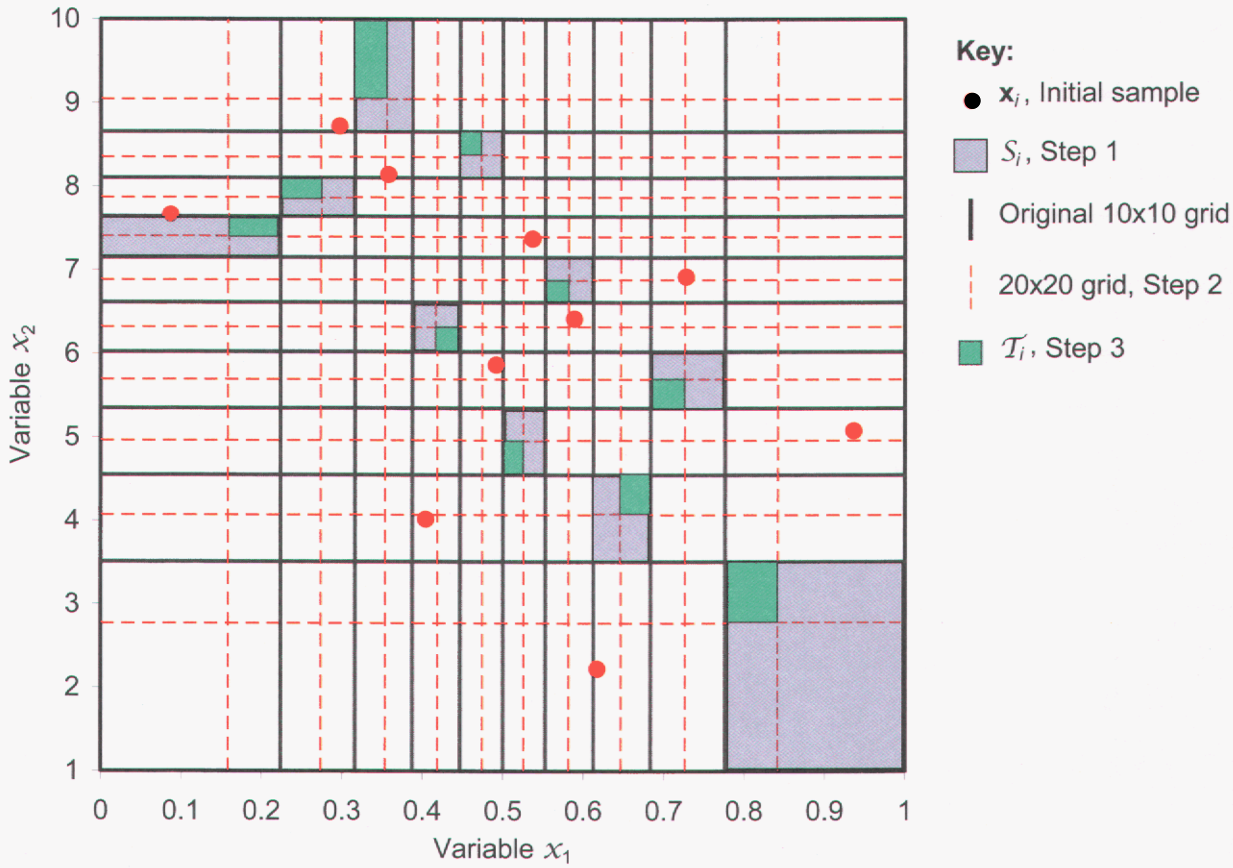


Fig. 4. Rectangles $\mathcal{T}_i = \mathcal{T}_{i,[r,s]} = \mathcal{E}_{i1r} \times \mathcal{E}_{i2s}$ constructed at Step 2 and identified at Step 3 of the extension algorithm with property that $x_{i1} \notin \mathcal{E}_{i1r}$ and $x_{i2} \notin \mathcal{E}_{i2s}$.

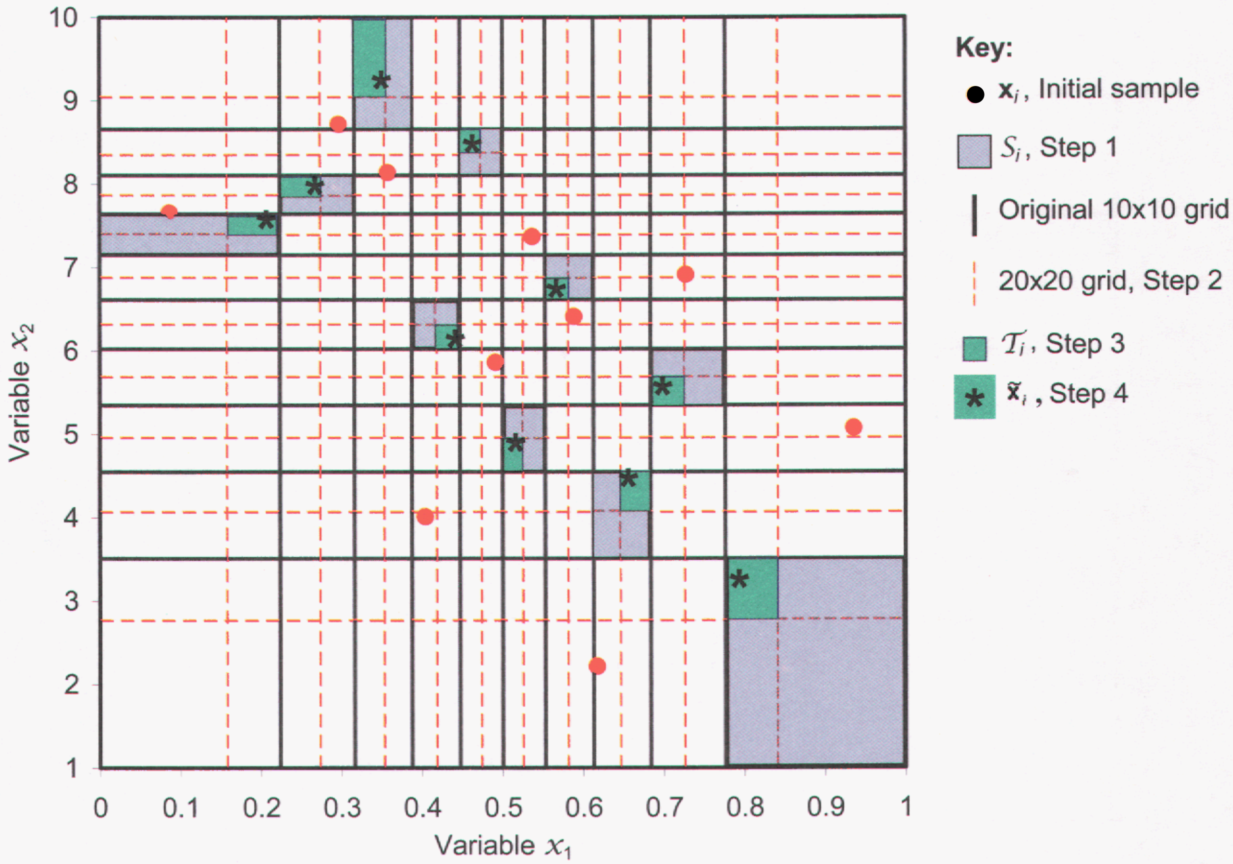


Fig. 5. Sample elements $\tilde{\mathbf{x}}_i = [\tilde{x}_{i1}, \tilde{x}_{i2}]$, $i = 1, 2, \ldots, 10$, obtained at Step 4 of the extension algorithm.

5. Correlation

The extension algorithm described in Sect. 3 and illustrated in Sect. 4 starts with an initial LHS of size m with a rank correlation matrix $\mathbf{D}_1$, generates a second LHS of size m with a rank correlation matrix $\mathbf{D}_2$, and then constructs an LHS of size $2m$ that includes the elements of the first LHS and has a rank correlation matrix $\mathbf{D}$ close to $(\mathbf{D}_1 + \mathbf{D}_2)/2$. This section demonstrates that the resultant rank correlation matrix $\mathbf{D}$ is indeed close to $(\mathbf{D}_1 + \mathbf{D}_2)/2$.

This demonstration is based on considering variables u and v that are elements of the vector $\mathbf{x}$ in Eq. (1.2) and the results of using the extension algorithm to extend an LHS of size m from $\mathbf{x}$ to an LHS of size $2m$. In this extension,

$$\left[u_i, v_i\right], i = 1, 2, \ldots, m, \tag{5.1}$$

are the values for u and v in the first LHS;

$$\left[\tilde{u}_i, \tilde{v}_i\right], i = 1, 2, \ldots, m, \tag{5.2}$$

are the values for u and v in the second LHS, and

$$\left[u_i, v_i\right] = \begin{cases} \left[u_i, v_i\right] & \text{for } i = 1, 2, \ldots, m \\ \left[\tilde{u}_{i-m}, \tilde{v}_{i-m}\right] & \text{for } i = m+1, m+2, \ldots, 2m \end{cases} \tag{5.3}$$

are the values for u and v in the extended LHS.

The rank correlations associated with the samples in Eqs. (5.1) – (5.3) are given by

$$\rho_1 = \sum_{i=1}^{m} \left[r_1(u_i) - (m+1)/2\right]\left[r_1(v_i) - (m+1)/2\right] \Big/ \left[m\left(m^2 - 1\right)/12\right], \tag{5.4}$$

$$\rho_2 = \sum_{i=1}^{m} \left[r_2(\tilde{u}_i) - (m+1)/2\right]\left[r_2(\tilde{v}_i) - (m+1)/2\right] \Big/ \left[m\left(m^2 - 1\right)/12\right] \tag{5.5}$$

and

$$\rho = \sum_{i=1}^{2m} \left[r(u_i) - (2m+1)/2\right]\left[r(v_i) - (2m+1)/2\right] \Big/ \left[m\left(4m^2 - 1\right)/6\right], \tag{5.6}$$

respectively, where r_1, r_2 and r denote the rank transforms associated with the individual samples. The object of this section is to show that ρ is close to $(\rho_1 + \rho_2)/2$.

Associated with the first LHS are pairs

$$\left[\mathcal{U}_i, \mathcal{V}_i\right], i = 1, 2, \ldots, m, \tag{5.7}$$

of equal probability intervals such that $u_i \in \mathcal{U}_i$ and $v_i \in \mathcal{V}_i$. In turn, $\mathcal{U}_i$ and $\mathcal{V}_i$ can be subdivided into nonoverlapping left and right equal probability subintervals $\mathcal{U}_{il}$, $\mathcal{U}_{ir}$, $\mathcal{V}_{il}$, $\mathcal{V}_{ir}$ such that

$$\mathcal{U}_i = \mathcal{U}_{il} \cup \mathcal{U}_{ir} \text{ and } \mathcal{V}_i = \mathcal{V}_{il} \cup \mathcal{V}_{ir}. \tag{5.8}$$

The first LHS can then be more specifically associated with the sequence

$$[\mathcal{U}_{i1}, \mathcal{V}_{i1}],\ i = 1, 2, \ldots, m, \tag{5.9}$$

where

$$\mathcal{U}_{i1} = \begin{cases} \mathcal{U}_{il} & \text{if } u_i \in \mathcal{U}_{il} \\ \mathcal{U}_{ir} & \text{if } u_i \in \mathcal{U}_{ir} \end{cases} \text{ and } \mathcal{V}_{i1} = \begin{cases} \mathcal{V}_{il} & \text{if } v_i \in \mathcal{V}_{il} \\ \mathcal{V}_{ir} & \text{if } v_i \in \mathcal{V}_{ir}. \end{cases}$$

Similarly, the second LHS can be associated with the sequence

$$[\mathcal{U}_{i2}, \mathcal{V}_{i2}],\ i = 1, 2, \ldots, m, \tag{5.10}$$

where

$$\mathcal{U}_{i2} = \begin{cases} \mathcal{U}_{jl} & \text{if } \tilde{u}_i \in \mathcal{U}_{jl} \\ \mathcal{U}_{jr} & \text{if } \tilde{u}_i \in \mathcal{U}_{jr} \end{cases} \text{ and } \mathcal{V}_{i2} = \begin{cases} \mathcal{V}_{jl} & \text{if } \tilde{v}_i \in \mathcal{V}_{jl} \\ \mathcal{V}_{jr} & \text{if } \tilde{v}_i \in \mathcal{V}_{jr}. \end{cases}$$

If desired, the second LHS can be ordered so that either $\mathcal{U}_i = \mathcal{U}_{i1} \cup \mathcal{U}_{i2}$ for $i = 1, 2, \ldots, m$ or $\mathcal{V}_i = \mathcal{V}_{i1} \cup \mathcal{V}_{i2}$ for $i = 1, 2, \ldots, m$; however, it is not possible to have both equalities hold.

The rank transforms associated with the three samples are related by

$$r(u_i) = 2r_1(u_i) - \delta_{ui},\ r(\tilde{u}_i) = 2r_2(\tilde{u}_i) - \tilde{\delta}_{ui} \tag{5.11}$$

$$r(v_i) = 2r_1(v_i) - \delta_{vi},\ r(\tilde{v}_i) = 2r_2(\tilde{v}_i) - \tilde{\delta}_{vi} \tag{5.12}$$

for $i = 1, 2, \ldots, m$, where

$$\delta_{ui} = \begin{cases} 1 & \text{if } \mathcal{U}_{i1} = \mathcal{U}_{il} \\ 0 & \text{if } \mathcal{U}_{i1} = \mathcal{U}_{ir} \end{cases},\ \tilde{\delta}_{ui} = \begin{cases} 1 & \text{if } \mathcal{U}_{i2} = \mathcal{U}_{jl} \\ 0 & \text{if } \mathcal{U}_{i2} = \mathcal{U}_{jr} \end{cases}$$

$$\delta_{vi} = \begin{cases} 1 & \text{if } \mathcal{V}_{i1} = \mathcal{V}_{rl} \\ 0 & \text{if } \mathcal{V}_{i1} = \mathcal{V}_{ir} \end{cases},\ \tilde{\delta}_{vi} = \begin{cases} 1 & \text{if } \mathcal{V}_{i2} = \mathcal{V}_{jl} \\ 0 & \text{if } \mathcal{V}_{i2} = \mathcal{V}_{jr} \end{cases}.$$

Specifically, $\delta_{ui} = 1$ if u_i is in the left interval $\mathcal{U}_{il}$ associated with $\mathcal{U}_i$, and $\delta_{ui} = 0$ if u_i is the right interval $\mathcal{U}_{ir}$ associated with $\mathcal{U}_i$. The variables $\tilde{\delta}_{ui}$, δ_{vi} and $\tilde{\delta}_{vi}$ are defined similarly for $\tilde{u}_i$, v_i and $\tilde{v}_i$.

If the second sample is ordered so that $\mathcal{U}_i = \mathcal{U}_{i1} \cup \mathcal{U}_{i2}$, then

$$\tilde{\delta}_{ui} = 1 - \delta_{ui} \tag{5.13}$$

Similarly, if the second sample is ordered so that $\mathcal{V}_i = \mathcal{V}_{i1} \cup \mathcal{V}_{i2}$, then

$$\tilde{\delta}_{vi} = 1 - \delta_{vi}. \tag{5.14}$$

However, as previously indicated, the concurrent existence of both orderings is not possible.

The representation for ρ in Eq. (5.6) can now be written as

$$\rho = \left\{ \sum_{i=1}^{m} \left[2r_1(u_i) - \delta_{ui} - (2m+1)/2 \right] \left[2r_1(v_i) - \delta_{vi} - (2m+1)/2 \right] \right.$$

$$\left. + \sum_{i=1}^{m} \left[2r_2(\tilde{u}_i) - \tilde{\delta}_{ui} - (2m+1)/2 \right] \left[2r_2(\tilde{v}_i) - \tilde{\delta}_{vi} - (2m+1)/2 \right] \right\} \left\{ m\left(4m^2 - 1\right)/6 \right\}^{-1}$$

$$= \left\{ \sum_{i=1}^{m} \left[r_1(u_i) - (m + \delta_{ui} + 1/2)/2 \right] \left[r_1(v_i) - (m + \delta_{vi} + 1/2)/2 \right] \right.$$

$$\left. + \sum_{i=1}^{m} \left[r_2(\tilde{u}_i) - \left(m + \tilde{\delta}_{ui} + 1/2\right)/2 \right] \left[r_2(\tilde{v}_i) - \left(m + \tilde{\delta}_{vi} + 1/2\right)/2 \right] \right\} \left\{ m\left(4m^2 - 1\right)/24 \right\}^{-1}, \tag{5.15}$$

where the first equality results from the representations for $r(u_i)$, $r(v_i)$, $r(\tilde{u}_i)$ and $r(\tilde{v}_i)$ in Eqs. (5.11) – (5.12) and the second equality results from factoring 4 out of the numerator.

Because the ratio

$$q = \left\{ m\left(m^2 - 1\right)/12 \right\} / \left\{ m\left(4m^2 - 1\right)/24 \right\} = 2\left(m^2 - 1\right)/\left(4m^2 - 1\right) \tag{5.16}$$

converges to 1/2 very rapidly (e.g., $q = 0.496$ for $m = 10$ and $q = 0.499$ for $m = 20$), a very good approximation to the representation for ρ in Eq. (5.15) is given by

$$\rho \cong \frac{1}{2} \left\{ \sum_{i=1}^{m} \frac{\left[r_1(u_i) - (m + \delta_{ui} + 1/2)/2 \right] \left[r_1(v_i) - (m + \delta_{vi} + 1/2)/2 \right]}{m\left(m^2 - 1\right)/12} \right.$$

$$\left. + \sum_{i=1}^{m} \frac{\left[r_2(\tilde{u}_i) - \left(m + \tilde{\delta}_{ui} + 1/2\right)/2 \right] \left[r_2(\tilde{v}_i) - \left(m + \tilde{\delta}_{vi} + 1/2\right)/2 \right]}{m\left(m^2 - 1\right)/12} \right\} \tag{5.17}$$

$$= \frac{1}{2} \left\{ \sum_{i=1}^{m} \frac{\left[\left(r_1(u_i) - \delta_{ui}/2 + 1/4 \right) - (m+1)/2 \right] \left[\left(r_1(v_i) - \delta_{vi}/2 + 1/4 \right) - (m+1)/2 \right]}{m\left(m^2 - 1\right)/12} \right.$$

$$\left. + \sum_{i=1}^{m} \frac{\left[\left(r_2(\tilde{u}_i) - \tilde{\delta}_{ui}/2 + 1/4 \right) - (m+1)/2 \right] \left[\left(r_2(\tilde{v}_i) - \tilde{\delta}_{vi}/2 + 1/4 \right) - (m+1)/2 \right]}{m\left(m^2 - 1\right)/12} \right\} \tag{5.18}$$

$$= \left(\hat{\rho}_1 + \hat{\rho}_2 \right)/2, \tag{5.19}$$

where $\hat{\rho}_1$ and $\hat{\rho}_2$ correspond to the preceding summations involving r_1 and r_2, respectively.

The first summation in Eqs. (5.17) and (5.18), which corresponds to $\hat{\rho}_1$, is an approximation to ρ_1 in Eq. (5.4); similarly, the second summation in Eqs. (5.17) and (5.18), which corresponds to $\hat{\rho}_2$, is an approximation to ρ_2 in Eq. (5.5). The quantities δ_{ui}, $\tilde{\delta}_{ui}$, δ_{vi} and $\tilde{\delta}_{vi}$ randomly vary between 0 and 1, with each of these values being equally likely. As shown in Eq. (5.17), this causes the term $(m + 1)/2$ in Eqs. (5.4) and (5.5) that corresponds to the mean of the rank transformed variables to randomly oscillate between $(m + 1/2)/2$ and $(m + 3/2)/2$; further, the expected value of these oscillations is $(m + 1)/2$. An alternate, but equivalent, representation is given in Eq. (5.18). In this representation, the term corresponding to the rank transformed value of a variable oscillates between the correct value minus 1/4 and the correct value plus 1/4, with the expected value of these oscillations being the correct rank transformed value. As a result,

$$\rho \cong (\hat{\rho}_1 + \hat{\rho}_2)/2 \cong (\rho_1 + \rho_2)/2, \tag{5.20}$$

which is the desired outcome of the extension algorithm.

A more formal assessment of the relationship between ρ and $(\rho_1 + \rho_2)/2$ is also possible. This assessment is based on considering the statistical behavior of $\hat{\rho}_1 - \rho_1$ and $\hat{\rho}_2 - \rho_2$.

The difference $\hat{\rho}_1 - \rho_1$ can be expressed as

$$\begin{aligned}\hat{\rho}_1 - \rho_1 &= \sum_{i=1}^{m} \frac{\left[\left(r_1(u_i) - \delta_{ui}/2 + 1/4\right) - (m+1)/2\right]\left[\left(r_1(v_i) - \delta_{vi}/2 + 1/4\right) - (m+1)/2\right]}{m\left(m^2-1\right)/12} \\ &\quad - \sum_{i=1}^{m} \frac{\left[r_1(u_i) - (m+1)/2\right]\left[r_1(v_i) - (m+1)/2\right]}{m\left(m^2-1\right)/12} \\ &= [A+B]/\left[m\left(m^2-1\right)/12\right],\end{aligned} \tag{5.21}$$

where

$$A = \sum_{i=1}^{m}\left[r_1(u_i) - (m+1)/2\right]\left[1/4 - \delta_{vi}/2\right] + \sum_{i=1}^{m}\left[r_1(v_i) - (m+1)/2\right]\left[1/4 - \delta_{ui}/2\right]$$

$$B = \sum_{i=1}^{m}\left[1/4 - \delta_{vi}/2\right]\left[1/4 - \delta_{ui}/2\right].$$

The terms A and B are now considered individually.

There exist sequences of integers j_i, $i = 1, 2, \ldots, m$, and k_i, $i = 1, 2, \ldots, m$, such that

$$r_1\left(u_{j_i}\right) = i \text{ and } r_1\left(v_{k_i}\right) = i \tag{5.22}$$

for $i = 1, 2, \ldots, m$. As a result, the term A in Eq. (5.21) can be written in the form

$$
\begin{aligned}
A &= \sum_{i=1}^{m}\left[r_1\left(u_{j_i}\right)-(m+1)/2\right]\left[1/4-\delta_{vj_i}/2\right]+\sum_{i=1}^{m}\left[r_1\left(v_{k_i}\right)-(m+1)/2\right]\left[1/4-\delta_{uk_i}/2\right] \\
&= \sum_{i=1}^{m}\left[i-(m+1)/2\right]\left[1/4-\delta_{vj_i}/2\right]+\sum_{i=1}^{m}\left[i-(m+1)/2\right]\left[1/4-\delta_{uk_i}/2\right] \\
&= \sum_{i=1}^{m}\left[i-(m+1)/2\right]s_i \\
&= \sum_{i=1}^{m}A_i, \qquad (5.23)
\end{aligned}
$$

where

$$
s_i = 1/2-\delta_{uk_i}/2-\delta_{vj_i}/2=\left(1-\delta_{uk_i}-\delta_{vj_i}\right)/2
$$

and

$$
A_i = \left[i-(m+1)/2\right]s_i .
$$

The terms δ_{uk_i} and δ_{vj_i} are mutually independent and independent of their subscripts; further, s_i takes on values of $-1/2$, 0, and 1/2 with probabilities of 1/4, 1/2, and 1/4, respectively, and thus has an expected value of $E(s_i) = 0$ and a variance of $V(s_i) = 1/8$. In turn, the expected value and variance for each A_i are given by

$$
E\left(A_i\right)=0 \qquad (5.24)
$$

and

$$
V\left(A_i\right)=\left[i-(m+1)/2\right]^2 V\left(s_i\right)=\left[i-(m+1)/2\right]^2/8, \qquad (5.25)
$$

respectively.

The variance $V(A)$ of A can be expressed in terms of the variances $V(A_i)$ for the A_i and is given by

$$
\begin{aligned}
V(A) &= \sum_{i=1}^{m}V\left(A_i\right) \\
&= \sum_{i=1}^{m}\left[i-(m+1)/2\right]^2/8 \\
&= \left[m\left(m^2-1\right)/12\right]/8 \\
&= m\left(m^2-1\right)/96. \qquad (5.26)
\end{aligned}
$$

Now, by the Lindeberg generalization of the central limit theorem (see Theorem 3, p. 262, Ref. 76),

$$A\Big/\sqrt{V(A)} = A\Big/\sqrt{m\left(m^2-1\right)/96} \tag{5.27}$$

asymptotically approaches a standard normal distribution as m increases.

The term B in Eq. (5.21) is now considered. Specifically, the expected value $E(B)$ and $V(B)$ for B are given by

$$E(B) = 0 \text{ and } V(B) = m/256, \tag{5.28}$$

respectively. As a result, $V(B)/V(A)$ goes to zero as m increases, and thus B is asymptotically inconsequential in Eq. (5.21).

The difference $\hat{\rho}_2 - \rho_2$ can be handled similarly to the difference $\hat{\rho}_1 - \rho_1$ in Eq. (5.21). Specifically, $\hat{\rho}_2 - \rho_2$ can be expressed as

$$\begin{aligned}
\hat{\rho}_2 - \rho_2 &= \sum_{i=1}^{m} \frac{\left[\left(r_2(\tilde{u}_i) - \tilde{\delta}_{ui}/2 + 1/4\right) - (m+1)/2\right]\left[\left(r_2(\tilde{v}_i) - \tilde{\delta}_{vi}/2 + 1/4\right) - (m+1)/2\right]}{m\left(m^2-1\right)/12} \\
&\quad - \sum_{i=1}^{m} \frac{\left[r_2(\tilde{u}_i) - (m+1)/2\right]\left[r_2(\tilde{v}_i) - (m+1)/2\right]}{m\left(m^2-1\right)/12} \\
&= \left[\tilde{A} + \tilde{B}\right]\Big/\left[m\left(m^2-1\right)/12\right],
\end{aligned} \tag{5.29}$$

where $\tilde{A}$ and $\tilde{B}$ are defined analogously to A and B in Eq. (5.21). Similarly to the development for A and B, it follows that

$$\tilde{A}\Big/\sqrt{V(\tilde{A})} = \tilde{A}\Big/\sqrt{m\left(m^2-1\right)/96} \tag{5.30}$$

asymptotically approaches a standard normal distribution and that $\tilde{B}$ is asymptotically inconsequential in Eq. (5.29).

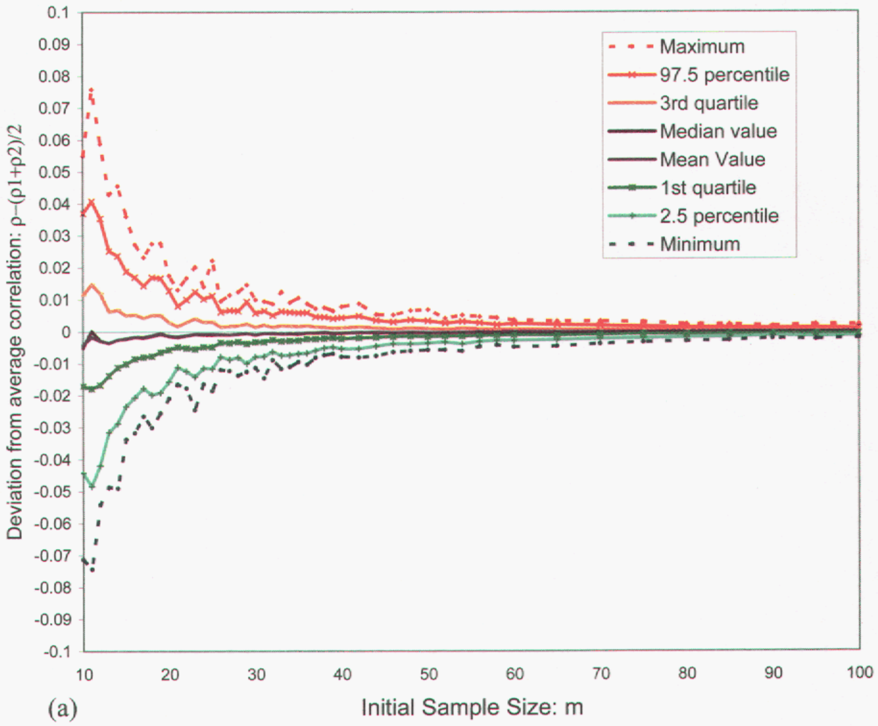
The statistical behavior of the difference $\rho - (\rho_1 + \rho_2)/2$ can now be assessed. Specifically,

$$\begin{aligned}
\rho - (\rho_1 + \rho_2)/2 &\cong (\hat{\rho}_1 + \hat{\rho}_2)/2 - (\rho_1 + \rho_2)/2 \\
&= \left[(\hat{\rho}_1 - \rho_1) + (\hat{\rho}_2 - \rho_2)\right]/2 \\
&= \left\{[A+B]\Big/\left[m\left(m^2-1\right)/12\right] + \left[\tilde{A} + \tilde{B}\right]\left[m\left(m^2-1\right)/12\right]\right\}\Big/2 \\
&\cong \left[A + \tilde{A}\right]\Big/\left[m\left(m^2-1\right)/24\right] \\
&= \left[A/V(A) + \tilde{A}/V(\tilde{A})\right]\Big/4\sqrt{m\left(m^2-1\right)/96},
\end{aligned} \tag{5.31}$$

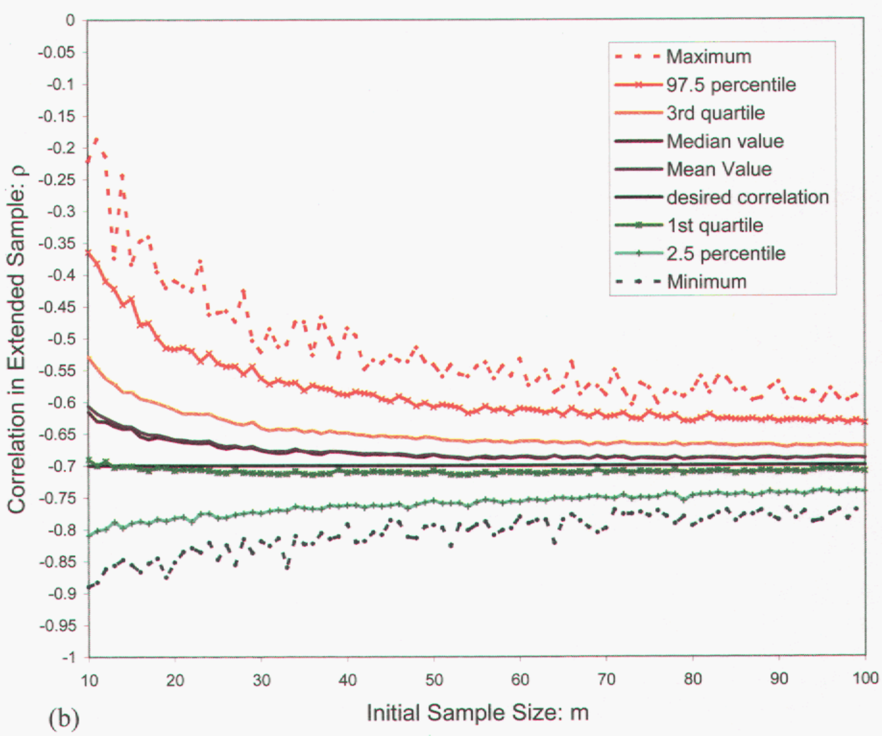
where (i) the first approximation follows from Eq. (5.19), (ii) the first equality is the result of an algebraic rearrangement of the preceding expression, (iii) the second equality follows from the representations in Eqs. (5.21) and

(5.29), (iv) the following approximate relationship results from the asymptotic disappearance of the effects associated with B and $\tilde{B}$, and (v) the final equality is the result of an algebraic rearrange of the preceding expression to isolate the asymptotically standard normal variables $A/V(A)$ and $\tilde{A}/V(\tilde{A})$. Thus, it follows from the final expression in Eq. (5.31) that $\rho - (\rho_1 + \rho_2)/2$ approximately follows a normal distribution with mean zero with increasing values for m; further, the variance associated with this distribution decreases rapidly with increasing values for m.

In consistency with the normality results associated with Eq. (5.31), numerical simulations show that the potential differences between ρ and $(\rho_1 + \rho_2)/2$ are small and decrease rapidly as the initial sample size m increases. As an example, results obtained for the doubling of samples with initial sizes from 10 to 100 for two correlated variables are shown in Fig. 6. For each sample size considered, a target rank correlation of −0.7 is used and a sample of the desired size is generated for the target correlation. Then, the extension algorithm is used to generate a sample of twice the initial size. To obtain an assessment of the stability of the results, the extension procedure is repeated 1000 times. As shown in Fig. 6, the difference between the rank correlation coefficient in an extended sample of size $2m$ and the average of the rank correlation coefficients for the two underlying samples of size m (i.e., $\rho - (\rho_1 + \rho_2)/2$ is small and decreases as m increases (Fig. 6a), and the rank correlation coefficient in an extended sample of size $2m$ (i.e., ρ) is close to the target rank correlation and the variability around the target correlation decreases as m increases (Fig. 6b).



(a)



(b)

Fig. 6. Variation of rank correlation coefficients in extended LHSs with increasing sample size: (a) Difference between rank correlation coefficient in extended sample of size $2m$ and average of rank correlations in two underlying samples of size m (i.e., $\rho - (\rho_1 + \rho_2)/2$, and (b) Rank correlation coefficient in extended sample of size $2m$ (i.e., ρ).

6. Discussion

Latin hypercube sampling is the preferred sampling procedure for the assessment of the implications of epistemic uncertainty in complex analyses because of its probabilistic character (i.e., each sample element has a weight equal to the reciprocal of the sample size that can be used in estimating probability-based quantities such as means, standard deviations, distribution functions, and standardized regression coefficients) and efficient stratification properties (i.e., a dense stratification exists over the range of each sampled variable). As a result, Latin hypercube sampling has been used in a number of large and computationally demanding analyses, including (i) the U.S. Nuclear Regulatory Commission's (NRC's) reassessment of the risk from commercial nuclear power plants (i.e., the NUREG-1150 analyses),[77-82] (ii) an extensive probabilistic risk assessment for the La Salle Nuclear Power Plant carried out as part of the NRC's Risk Methods Integration and Evaluation Program (RMEIP),[83] (iii) the U.S. Department of Energy's (DOE's) performance assessment for the Waste Isolation Pilot Plant (WIPP) in support of a compliance certification application to the U.S. Environmental Protection Agency (EPA),[84, 85] and (iv) performance assessments carried out in support of the DOE's development of a repository for high-level radioactive waste at Yucca Mountain, Nevada.[86, 87] Analyses of this type involve multiple complex, computationally demanding models, from 10's to 100's of uncertain analysis inputs, and large numbers of analysis outcomes of interest.

Because of the large computational cost associated with analyses of the type just indicated, the sample size that can be used is necessarily limited. Further, the determination of an adequate sample size is complicated by the large number of uncertain analysis inputs and the potentially large number of analysis results to be studied. As a result, it is difficult to determine an appropriate sample size before an analysis is carried out. If too small a sample is used, the analysis can lack the necessary resolution to provide the desired uncertainty and sensitivity analysis results. If the sample size is too large, the analysis will incur unnecessary computational cost. Indeed, if the estimated size of the required sample is too large, the entire analysis may be abandoned owing to the anticipated computational cost. Fortunately, the necessary sample size for most analyses is not as large as is often thought.[88-90]

The extension procedure for LHSs described in this presentation provides a way to address the sample size problem sequentially. Specifically, an analysis can be performed initially with a relatively small sample size. If acceptable results are obtained with this sample, the analysis is over. However, if the results are felt to lack adequate resolution, the extension procedure can be used to generate a larger LHS. This approach is computationally efficient because the original sample elements are part of the extended LHS, and thus all of the original, and potentially expensive, calculated results remain part of the analysis. If necessary, the extension procedure could be employed multiple times until an acceptable level of resolution was obtained.

An approach to assessing the adequacy of an LHS of size m is to generate k replicated (e.g., $k = 3$) LHSs of size m and then check for consistency of results obtained with the replicated samples.[74, 75] For example, the t-test can be used to obtain confidence intervals for mean results. A minor modification of the extension algorithm described in Sect. 3 can be used to generate the k replicated LHSs of size m so that their pooling will result in an LHS of size $k \times m$. Then, after an assessment of sample size adequacy is made, a final presentation uncertainty and sensitivity analysis can be performed with the results of the pooled samples, which corresponds to using an LHS of size $k \times m$. This approach permits an assessment of sample size adequacy and also provides final results with a higher resolution than obtained from any of the individual replicated samples.

The extension procedure can also be used in the generation of very large LHSs with a specified correlation structure. For example, if an LHS of size $k \times m$ is desired, a possible implementation strategy is to use the extension procedure to generate k LHSs of size m so that their pooling will result in an LHS of size $k \times m$. As a result of the inversion of a large matrix in the Iman/Conover correlation control procedure, the approach of generating and pooling k LHSs of size m can require less computational effort than generating a single LHS of size $k \times m$.

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7. References

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