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Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems

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Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems

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Abstract

The following techniques for uncertainty and sensitivity analysis are briefly summarized: Monte Carlo analysis, differential analysis, response surface methodology, Fourier amplitude sensitivity test, Sobol' variance decomposition, and fast probability integration. Desirable features of Monte Carlo analysis in conjunction with Latin hypercube sampling are described in discussions of the following topics: (i) properties of random, stratified and Latin hypercube sampling, (ii) comparisons of random and Latin hypercube sampling, (iii) operations involving Latin hypercube sampling (i.e., correlation control, reweighting of samples to incorporate changed distributions, replicated sampling to test reproducibility of results), (iv) uncertainty analysis (i.e., cumulative distribution functions, complementary cumulative distribution functions, box plots), (v) sensitivity analysis (i.e., scatterplots, regression analysis, correlation analysis, rank transformations, searches for nonrandom patterns), and (vi) analyses involving stochastic (i.e., aleatory) and subjective (i.e., epistemic) uncertainty.

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1. Introduction

The assessment and presentation of the effects of uncertainty are now widely recognized as important parts of analyses for complex systems.[1-6] At the simplest level, such analyses can be viewed as the study of functions of the form

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

where the function **f** represents the model or models under study, $\mathbf{x} = [x_1, x_2, \ldots]$ is a vector of model inputs, and $\mathbf{y} = [y_1, y_2, \ldots]$ is a vector of model predictions. The goal of an uncertainty analysis is to determine the uncertainty in the elements of **y** that results from uncertainty in the elements of **x**. A typical adjunct to an uncertainty analysis is a sensitivity analysis, which attempts to determine how the uncertainty in individual elements of **x** affects the uncertainty in the elements of **y**. In practice, **f** can be quite complex (e.g., one or more computer programs involving complex algorithms and many thousands of lines of programming); further, **x** and **y** are often of high dimension.

To carry out uncertainty and sensitivity analyses, the uncertainty in the elements of **x** must be characterized. For this presentation, the uncertainty in the elements of **x** is assumed to be characterized by a sequence of distributions

$$D_1, D_2, \ldots, D_{nX}, \tag{1.2}$$

where D_j is the distribution associated with the element x_j of **x** and nX is the number of elements contained in **x** (i.e., $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$). Various correlations and additional relationships between the elements of **x** are also possible. Initially, the distributions in Eq. (1.2) will be assumed to characterize a degree of belief with respect to where the appropriate values for the elements of **x** are located for use in the evaluation of the function **f** in Eq. (1.1). When used in this manner, these distributions are providing a quantitative representation for what is commonly referred to as subjective or epistemic uncertainty.[7, 8] Such distributions are often developed through an expert review process.[9-29]

For notational convenience, the function **f**, and hence **y**, in Eq. (1.1) will be assumed to be real-valued, although such simplicity is almost never the case in real analyses. With this assumption, the representation in Eq. (1.1) becomes

$$y = f(\mathbf{x}). \tag{1.3}$$

Further, again for notational convenience and also for ease in distinguishing between different uses of probability at later points in this presentation, the distributions in Eq. (1.2) and any additional relationships imposed on the elements of **x** will be represented by a probability space $(\mathcal{S}_{su}, \mathcal{\delta}_{su}, p_{su})$, where the subscript "*su*" is used as a designator for "subjective." As a reminder, a probability space $(\mathcal{S}, \mathcal{\delta}, p)$, consists of three elements: a set $\mathcal{S}$ that contains everything that could occur in the particular universe under consideration; a collection $\mathcal{\delta}$ of subsets of $\mathcal{S}$ for which probability will be defined; and a function p that actually defines probability for the elements of $\mathcal{\delta}$ (Sect. IV.4, Ref. 30). In the terminology of probability theory, the set $\mathcal{S}$ is the sample space; the elements of $\mathcal{S}$ (i.e., the vectors **x** in Eqs. (1.1) and (1.3)) are elementary events; the elements of $\mathcal{\delta}$ are events; and the function p is a probability measure.

When viewed in its most general form, uncertainty analysis simply involves determination of the distribution for y that results from the function f in Eq. (1.3) and the distributions $D_1, D_2, \ldots, D_{nX}$ in Eq. (1.2), which define probability space $(\mathcal{S}_{su}, \mathcal{\delta}_{su}, p_{su})$. Further, the distribution for y can be presented as a cumulative distribution function (CDF) or as a complementary cumulative distribution function (CCDF), which is simply one minus the CDF (Fig. 1.1). The CCDF is typically used when it is desired to display small probabilities associated with large values of y or when it is desired to answer the question "How likely is y to be this large or larger?" Given that it can be determined, the CDF, or equivalently the CCDF, in Fig. 1.1 provides a complete representation of the uncertainty in y. A density function can also be used to summarize the uncertainty in y; however, CDFs and CCDFs provide more convenient and informative summaries in sampling-based studies.

The CCDF in Fig. 1.1 can be formally defined by the integral

$$prob(y > Y) = \int_{\mathcal{S}_{su}} \delta_Y[f(\mathbf{x})] d_{su}(\mathbf{x}) dV_{su}, \tag{1.4}$$

where $prob(y > Y)$ is the probability that a value larger than Y will occur, d_{su} represents the density function corresponding to the distributions in Eq. (1.2) and hence to the probability space $(\mathcal{S}_{su}, \mathcal{\delta}_{su}, p_{su})$, the differential dV_{su} is selected for mnemonic purposes because integration will typically be over a high-dimension (i.e., nX) volume, and

$$\delta_Y[f(\mathbf{x})] = \begin{cases} 1 & \text{if} \quad f(\mathbf{x}) > Y \\ 0 & \text{if} \quad f(\mathbf{x}) \le Y. \end{cases} \tag{1.5}$$

Similarly, the corresponding CDF is defined by

$$\begin{aligned} prob(y \le Y) &= 1 - prob(y > Y) \\ &= 1 - \int_{S_{su}} \delta_Y[f(\mathbf{x})] d_{su}(\mathbf{x}) dV_{su}, \end{aligned} \tag{1.6}$$

where $prob(y \le Y)$ is the probability that a value less than or equal to Y will occur. Although the integral in Eqs. (1.4) and (1.6) formally defines the CCDF and CDF associated with y, in practice this integral is not amenable to a closed-form evaluation; rather, some type of approximation procedure must be used. In particular, the focus of this presentation is on the use of Latin hypercube sampling[31, 32] in the approximation of this integral.

As just indicated, uncertainty analysis is simple in concept and involves evaluation of the integral in Eq. (1.4) to obtain the CDF and CCDF in Fig. 1.1. Sensitivity analysis involves the determination of the effects of the individual elements of $\mathbf{x}$ on $y = f(\mathbf{x})$. Although sensitivity analysis is closely tied to uncertainty analysis, it tends to be a more complex undertaking due to both the variety of possible measures of sensitivity and the additional computational procedures required to evaluate these measures. This presentation will emphasize sensitivity measures that can be obtained when Latin hypercube sampling is used to evaluate the integral in Eq. (1.4).

One formal way to look at sensitivity analysis is to view it as an analysis of variance problem. Specifically, the variance $V(y)$ of y is given by

$$V(y) = \int_{S_{su}} [E(y) - f(\mathbf{x})]^2 d_{su}(\mathbf{x}) dV_{su}, \tag{1.7}$$

where $E(y)$ denotes the expected value of y and is given by

$$E(y) = \int_{S_{su}} f(\mathbf{x}) d_{su}(\mathbf{x}) dV_{su}. \tag{1.8}$$

Sensitivity analysis can then be viewed as a decomposition of $V(y)$ into components due to the individual elements of $\mathbf{x}$, with the size of these components then providing an indication of variable importance. However, as will be discussed, not all sensitivity analysis procedures are mathematically equivalent to a variance decomposition problem. A variety of sensitivity measures based on Latin hypercube sampling will be presented.

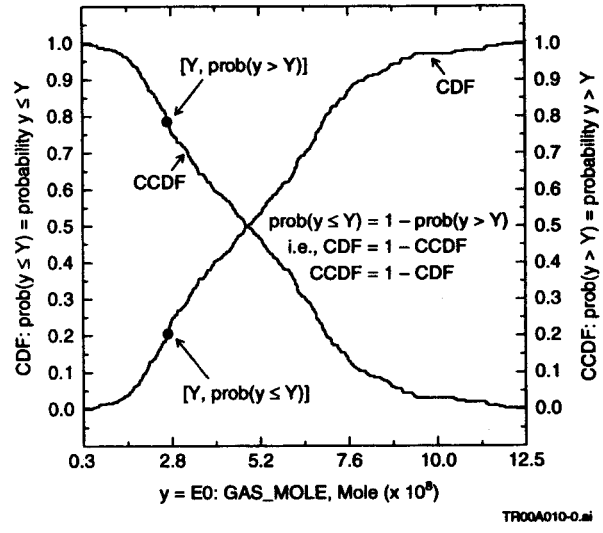

Fig. 1.1. Use of CDFs and CCDFs to represent uncertainty in model predictions.

2. Techniques for Uncertainty and Sensitivity Analysis

The use of Latin hypercube sampling constitutes part of what is often called a Monte Carlo procedure for the propagation of uncertainty. In addition, there exist a number of other procedures that are also used for the propagation of uncertainty, including differential analysis, response surface methodology, the Fourier amplitude sensitivity test (FAST) and the closely related Sobol' variance decomposition, and fast probability integration. To provide perspective on, and a context for, the use of Latin hypercube sampling, the preceding procedures are briefly summarized in this section.

2.1 Monte Carlo Analysis

In Monte Carlo analysis, a probabilistically based sampling procedure is used to develop a mapping from analysis input to analysis results. This mapping then provides a basis for both the evaluation of the integral in Eq. (1.4) (i.e., uncertainty analysis) and the evaluation of the effects of individual elements of $\mathbf{x}$ on $y = f(\mathbf{x})$ (i.e., sensitivity analysis). Specifically, a sample

$$\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{i,nX}], \; i = 1, 2, \ldots, nS, \tag{2.1}$$

of size nS is generated from $\mathcal{S}_{su}$ in consistency with the distributions in Eq. (1.2) (i.e., in consistency with the definition of the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$). A number of possible sampling procedures exist, including random sampling, stratified sampling, and Latin hypercube sampling (see Sect. 3). The preceding sampling procedures are probabilistically based in the sense that weights

$$w_i, \; i = 1, 2, \ldots, nS, \tag{2.2}$$

exist such that the result obtained with sample element $\mathbf{x}_i$ can be used in conjunction with the weight w_i to obtain quantities such as expected values, variances and other entities that derive from integration over $\mathcal{S}_{su}$. For random sampling and also Latin hypercube sampling, w_i is the reciprocal of the sample size (i.e., $w_i = 1/nS$); for stratified sampling, w_i is determined by the probability of the stratum (i.e., subset of $\mathcal{S}_{su}$) from which $\mathbf{x}_i$ was sampled and the number of samples taken from that stratum.

Once the sample in Eq. (2.1) is generated, evaluation of f creates the following mapping from analysis inputs to analysis results:

$$[\mathbf{x}_i, y_i], \; i = 1, 2, \ldots, nS, \tag{2.3}$$

where $y_i = f(\mathbf{x}_i)$. Then, the integrals in Eqs. (1.4), (1.7) and (1.8) can be approximated by

$$prob(y > Y) \doteq \widehat{prob}(y > Y) = \sum_{i=1}^{nS} \delta_Y(y_i) w_i \tag{2.4}$$

$$E(y) \doteq \hat{E}(y) = \sum_{i=1}^{nS} y_i w_i \tag{2.5}$$

$$V(y) \doteq \hat{V}(y) = \sum_{i=1}^{nS} [\hat{E}(y) - y_i]^2 w_i. \tag{2.6}$$

The distribution function approximated in Eq. (2.4) provides the most complete representation of the uncertainty in y that derives from the distributions in Eq. (1.2) and hence from the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. The expected value and variance approximated in Eqs. (2.5) and (2.6) provide a summary of this distribution but with the inevitable loss of resolution that occurs when the information contained in 2 nS numbers (i.e., in the y_i and w_i) is mapped into two numbers. For random sampling, use of $w_i = 1/(nS - 1)$ in Eq. (2.6) results in an unbiased estimate for $V(y)$.

The mapping in Eq. (2.3) can be explored with various techniques to determine the effects of the individual elements of $\mathbf{x}$ on y. For example, scatterplots based on the points

$$[x_{ij}, y_i], \; i = 1, 2, \ldots, nS, \tag{2.7}$$

for each element x_j of $\mathbf{x}$ may completely reveal the relationships between the x_j and y (Fig. 2.1). Another possibility is to use the results in Eq. (2.3) and least squares techniques to construct a regression model of the form

$$y = b_0 + \sum_{j=1}^{nX} b_j x_j \tag{2.8}$$

that relates y to the x_j. Various aspects of this model and the construction process that produced it can then be used to infer the relationships between the x_j and y. The preceding and other techniques for sensitivity analysis in conjunction with Monte Carlo procedures are discussed in more detail in Sect. 6.

Monte Carlo procedures for the propagation of uncertainty are very popular and many examples of their

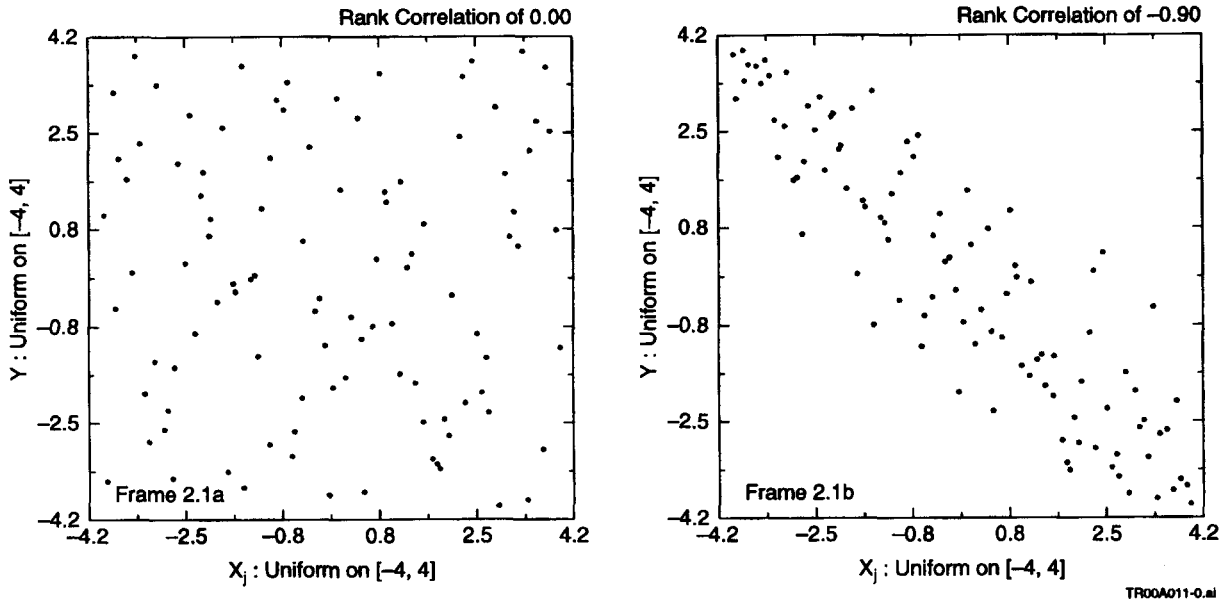

Fig. 2.1. Scatterplots produced in a Monte Carlo analysis with a Latin hypercube sample of size $nS = 100$: (a) no relationship between x_j and y, and (b) well-defined relationship between x_j and y (see Sect. 5.1 for a discussion of rank correlation).

use exist.[33-47] Further, Monte Carlo procedures find a wide variety of applications in the sciences and a very extensive literature exists.[48-60]

2.2 Differential Analysis

Differential analysis is based on the partial derivatives of f with respect to the elements of $\mathbf{x}$. In its simplest form, differential analysis involves approximating the model by the Taylor series

$$y(\mathbf{x}) \doteq f(\mathbf{x}_0) + \sum_{j=1}^{nX} [\partial f(\mathbf{x}_0)/\partial x_j][x_j - x_{j0}], \tag{2.9}$$

where $\mathbf{x}_0 = [\mathbf{x}_{10}, \mathbf{x}_{20}, \ldots, \mathbf{x}_{nX,0}]$ is a vector of base-case values for the x_j (e.g., the expected values for the x_j defined by the distributions in Eq. (1.2)).

Once the approximation in Eq. (2.9) is determined, variance propagation formulas can be used to determine the uncertainty in y that results from the distributions in Eq. (1.2). In particular,

$$E(y) \doteq y(\mathbf{x}_0) + \sum_{j=1}^{nX} [\partial f(\mathbf{x}_0)/\partial x_j] E(x_j - x_{j0}) = y(\mathbf{x}_0) \tag{2.10}$$

and

$$V(y) \doteq \sum_{j=1}^{nX} [\partial f(\mathbf{x}_0)/\partial x_j]^2 V(x_j) + 2\sum_{j=1}^{nX}\sum_{k=j+1}^{nX} [\partial f(\mathbf{x}_0)/\partial x_j][\partial f(\mathbf{x}_0)/\partial x_k]\, Cov(x_j, x_k), \tag{2.11}$$

where E, V and Cov denote expected value, variance and covariance, respectively. If the x_j are uncorrelated, then

$$V(y) \doteq \sum_{j=1}^{nX} [\partial f(\mathbf{x}_0)/\partial x_j]^2 V(x_j). \tag{2.12}$$

Thus, the Taylor series in Eq. (2.9) leads to approximations of the expected value and variance for y that result from the distributions in Eq. (1.2). Differential analysis does not lead very naturally to an approximation for the CDF or CCDF for y, although such approximations could be obtained by using a Monte Carlo simulation of the Taylor series in Eq. (2.9).

The determination of expected values, variances and possibly CDFs or CCDFs constitutes the uncertainty analysis component of differential analysis. Sensitivity analysis is based on the use of the partial derivatives associated with a Taylor series to determine the effects of the individual elements of $\mathbf{x}$ on y. For example, if the Taylor series in Eq. (2.9) is used and the ele-

ments of $\mathbf{x}$ are independent, then the fractional contribution of x_j to the variance of y can be approximated by

$$V(y|x_j) \doteq [\partial f(\mathbf{x}_0)/\partial x_j]^2 V(x_j)/V(y), \tag{2.13}$$

with $V(y)$ being obtained from the approximation in Eq. (2.12). An ordering of the x_j on the basis of the size of the fractional contributions $V(y|x_j)$ provides a ranking of variable importance on the basis of how much of the variance of y can be accounted for by each element of $\mathbf{x}$.

Normalization of the partial derivatives in the Taylor series in Eq. (2.9) provides a basis for another approach to assessing the importance of individual elements of $\mathbf{x}$. In particular, the following normalizations are possible:

$$\frac{y(\mathbf{x})-y(\mathbf{x}_0)}{y(\mathbf{x}_0)} \doteq \sum_{j=1}^{nX}\left[\frac{\partial f(\mathbf{x}_0)}{\partial x_j}\frac{x_{j0}}{y(\mathbf{x}_0)}\right]\left[\frac{x_j-x_{j0}}{x_{j0}}\right] \tag{2.14}$$

and

$$\frac{y(\mathbf{x})-y(\mathbf{x}_0)}{SD(y)} \doteq \sum_{j=1}^{nX}\left[\frac{\partial f(\mathbf{x}_0)}{\partial x_j}\frac{SD(x_j)}{SD(y)}\right]\left[\frac{x_j-x_{j0}}{SD(x_j)}\right], \tag{2.15}$$

where SD denotes standard deviation, $SD(y)$ is estimated from Eq. (2.12), and no problem with respect to division by zero exists. The normalized coefficients

$$C_{bc}(x_j) = [\partial f(\mathbf{x}_0)/\partial x_j][x_{j0}/y(\mathbf{x}_0)],\ j = 1, 2, \ldots, nX, \tag{2.16}$$

from Eq. (2.14) provide a ranking of variable importance based on equal fractional changes from base-case values x_{j0} and thus incorporate no distributional information about the elements of $\mathbf{x}$. The normalized coefficients

$$C_{sd}(x_j) = [\partial f(\mathbf{x}_0)/\partial x_j][SD(x_j)/SD(y)],\ j = 1, 2, \ldots, nX, \tag{2.17}$$

from Eq. (2.15) provide a ranking of variable importance based on changes from base-case values x_{j0} that are equal fractions of the standard deviation $SD(x_j)$ of x_j. Thus, unlike rankings of variable importance with the coefficients in Eq. (2.16), rankings with the coefficients in Eq. (2.17) incorporate the distributional assumptions for the elements of $\mathbf{x}$.

The quality of results obtained in a differential analysis is limited by the quality of the underlying Taylor series approximation. In particular, if y is a nonlinear function of the elements of $\mathbf{x}$, then the first-order Taylor series approximation in Eq. (2.9) may provide a poor representation of the relationships between y and the elements of $\mathbf{x}$. Better approximations to y can be obtained by using higher-order Taylor series. For example, a second-order approximation has the form

$$y(\mathbf{x}) \doteq y(\mathbf{x}_0) + \sum_{j=1}^{nX}[\partial f(\mathbf{x}_0)/\partial x_j][x_j - x_{j0}] + \frac{1}{2}\sum_{j=1}^{nX}\sum_{k=1}^{nX}[\partial^2 f(\mathbf{x}_0)/\partial x_j \partial x_k][(x_j - x_{j0})(x_k - x_{k0})]. \tag{2.18}$$

If the preceding approximation to $y(\mathbf{x})$ is used, the elements of $\mathbf{x}$ are uncorrelated, and fourth-order and higher-order terms are ignored in the derivation of $V(y)$, then the following estimates for the expected value and variance of y are obtained:

$$E(y) \doteq y(\mathbf{x}_0) + \frac{1}{2}\sum_{j=1}^{nX}[\partial^2 f(\mathbf{x}_0)/\partial x_j^2]V(x_j) \tag{2.19}$$

and

$$V(y) \doteq \sum_{j=1}^{nX}[\partial f(\mathbf{x}_0)/\partial x_j]^2 V(x_j) + \sum_{j=1}^{nX}[\partial f(\mathbf{x}_0)/\partial x_j][\partial^2 f(\mathbf{x}_0)/\partial x_j^2]\mu_3(x_j), \tag{2.20}$$

where $\mu_3(x_j)$ denotes the third central moment of x_j. As higher-order terms and correlations between the elements of $\mathbf{x}$ are included, the approximations to the expected value and variance for y rapidly become very complicated.[61-64]

Differential analysis has long played a prominent role in the propagation and analysis of uncertainty.[65-70] Usually, the most difficult part of a differential analysis is determining the necessary partial derivatives. As a result, much of the research related to differential analysis has been devoted to development of techniques for the determination of these derivatives, including adjoint techniques,[71-74] Green's function techniques,[75-78] and various numerical techniques.[79, 80] Automatic differentiation techniques are maturing and can now be applied to quite complex programs, which greatly facilitates the implementation of derivative-based analyses.[81-88]

2.3 Response Surface Methodology

Response surface methodology (RSM) is similar to Monte Carlo analysis except that an experimental design is used to select model input. A variety of possible designs exist, including factorial, fractional factorial, central composite, Plackett-Burman, and many more. Usually, the design selected depends on many factors, including properties of the model and the type of results desired from subsequent uncertainty and sensitivity analyses.

The experimental design results in a selection of points

$$\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{i,nX}], i = 1, 2, \ldots, nS, \quad (2.21)$$

from the S_{su}. However, the distributions in Eq. (1.2), and hence the probability space (S_{su}, $\mathcal{A}_{su}$, p_{su}), do not play a direct role in the selection of the $\mathbf{x}_i$. Rather, these points are typically selected on the basis of the ranges of the individual x_j contained in $\mathbf{x}$ (e.g., a low, central and high value for each x_j). As a result, there is not a probabilistic weight that can be associated with each design point in Eq. (2.21) as there is with the sample elements in Eq. (2.1).

After the design points in Eq. (2.21) are selected, evaluation of f for these points creates a mapping between model input and model results of the form shown in Eq. (2.3). However, because probabilistic weights cannot be assigned to the design points, uncertainty results of the form indicated in Eqs. (2.4)–(2.6) cannot be obtained directly from these evaluations. Rather, as an intermediate step, a response surface of the form indicated in Eq. (2.8) is constructed; more complex constructions are also possible. Once constructed, this response surface can be used in a Monte Carlo simulation with the distributions in Eq. (1.2) to estimate the uncertainty in y. Or, as an alternative, expected values and variances can be determined with propagation procedures similar to those shown in Eqs. (2.10)–(2.12).

The response surface in Eq. (2.8) is analogous to the Taylor series in Eq. (2.9). Specifically, each is a linear approximation to the model $y = f(\mathbf{x})$ indicated in Eq. (1.3). As a result, sensitivity analysis in RSM can be carried out in the same manner as sensitivity analysis in differential analysis. Specifically, sensitivity measures of the type indicated in Eqs. (2.13)–(2.17) can be calculated for a regression model of the form indicated in Eq. (2.8) and derived from the mapping

$$[\mathbf{x}_i, y(\mathbf{x}_i)], i = 1, 2, \ldots, nS, \quad (2.22)$$

associated with the design points in Eq. (2.21). In the context of the regression model in Eq. (2.8), the normalized coefficients in Eqs. (2.15) and (2.17) are known as standardized regression coefficients.

An extensive literature exists on experimental designs for use in RSM,[89-101] and many examples of the use of RSM in uncertainty and sensitivity analysis exist.[102-108] In a related but somewhat different problem, RSM is widely used in optimization problems, with this area of application actually being the source from which RSM developed.[109-113] In addition, several books related to RSM are also available.[114-117]

2.4 Fourier Amplitude Sensitivity Test (FAST) and Sobol' Variance Decomposition

The variance $V(y)$ associated with the model $y = f(\mathbf{x})$ in Eq. (1.3) is formally defined by the integral in Eq. (1.7). Although different in computational details, analyses based on both the Fourier Amplitude Sensitivity Test (FAST)[118-120] and the Sobol' variance decomposition[121] involve a decomposition of $V(y)$ into components due to individual variables and interactions between individual variables. Specifically, $V(y)$ can be decomposed into the form

$$V(y) = \sum_{1 \le j \le nX} V_j + \sum_{1 \le j < k \le nX} V_{jk} + \ldots + V_{12\ldots nX} \quad (2.23)$$

under the assumption that the x_j are independent, where V_j is the part of $V(y)$ due solely to x_j, V_{jk} is the part of $V(y)$ due to the interaction of x_j and x_k, V_{jkl} is the part of $V(y)$ due to the interaction of x_j, x_k and x_l, and so on up to $V_{12\ldots nX}$, which is the part of $V(y)$ due to the interaction of $x_1, x_2, \ldots, x_{nX}$.

Once the decomposition in Eq. (2.23) is available, various sensitivity measures such as

$$s_j = V_j / V(y) \quad (2.24)$$

$$s_{jk} = V_{jk} / V(y) \quad (2.25)$$

$$s_{jT} = \left(V_j + \sum_{\substack{l \le k < l \le nX \\ k \text{ or } l = j}} V_{kl} + \ldots + V_{12\ldots nX} \right) / V(y) \quad (2.26)$$

can be defined, where s_j is the fraction of $V(y)$ due solely to x_j, s_{jk} is the fraction of $V(y)$ due to the interaction of x_j and x_k, and s_{jT} is the fraction of $V(y)$ due to x_j or the interaction of x_j with other variables.

In the FAST approach, the multidimensional integrals in Eqs. (1.7) and (1.8) that define $V(y)$ and $E(y)$ are converted to the one-dimensional integrals through the construction of an appropriate space-filling curve

$$\mathbf{c}(s) = [G_1(\sin \omega_1 s), G_2(\sin \omega_2 s), \ldots, G_{nX}(\sin \omega_{nX} s)] \tag{2.27}$$

in $\mathcal{S}_{su}$, where G_j and ω_j are suitably defined functions and integers, respectively. Then,

$$E(y) \doteq \frac{1}{2\pi}\int_{-\pi}^{\pi} f[\mathbf{c}(s)]\, ds \tag{2.28}$$

and

$$V(y) \doteq \frac{1}{2\pi}\int_{-\pi}^{\pi} f^2[\mathbf{c}(s)]\, ds - E^2(y). \tag{2.29}$$

In general, some type of numerical procedure (e.g., Monte Carlo) is required to evaluate the integrals in Eqs. (2.28) and (2.29).

The following relationship can be established by using properties of the Fourier series representation for f:

$$V(y) \doteq \sum_{k=1}^{\infty}\left(A_k^2 + B_k^2\right), \tag{2.30}$$

where

$$A_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f[\mathbf{c}(s)] \cos(ks)\, ds$$

$$B_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f[\mathbf{c}(s)] \sin(ks)\, ds.$$

Further, V_j can be approximated by

$$V_j \doteq \sum_{k=1}^{\infty}\left(A_{k\omega_j}^2 + B_{k\omega_j}^2\right), \tag{2.31}$$

where ω_j is the integer associated with G_j in Eq. (2.27) in the conversions from multidimensional integrals to one-dimensional integrals in Eqs. (2.28) and (2.29). Thus, the approximation

$$s_j = V_j / V(y) \doteq \sum_{k=1}^{\infty}\left(A_{k\omega_j}^2 + B_{k\omega_j}^2\right) \Big/ \sum_{k=1}^{\infty}\left(A_k^2 + B_k^2\right) \tag{2.32}$$

follows from Eqs. (2.30) and (2.31).

In analyses based on the Sobol' variance decomposition, $E(y)$ and $V(y)$ are typically approximated by Monte Carlo techniques as indicated in Eqs. (2.5) and (2.6). Further, the individual terms, V_j, V_{jk}, V_{jkl}, ..., $V_{12\ldots nX}$ in the decomposition of $V(y)$ in Eq. (2.23) are defined by multiple integrals involving the elements x_j of $\mathbf{x}$. For example,

$$V_j = \int_{\mathcal{S}_j}\left[\int_{\prod_{l\in I(-j)}\mathcal{S}_l} f(\mathbf{x}) \prod_{l\in I(-j)} d_l(x_l)\, dx_l\right]^2 d_j(x_j)\, dx_j - E^2(y) \tag{2.33}$$

$$V_{jk} = \int_{\mathcal{S}_j}\int_{\mathcal{S}_k}\left[\int_{\prod_{l\in I(-j,-k)}\mathcal{S}_l} f(\mathbf{x}) \prod_{l\in I(-j,-k)} d_l(x_l)\, dx_l\right]^2 d_k(x_k)\, d_j(x_j)\, dx_k dx_j - V_j - V_k - E^2(y), \tag{2.34}$$

where, as indicated earlier, the x_j are assumed to be independent, $(\mathcal{S}_j, \mathcal{B}_j, p_j)$ is the probability space characterizing the uncertainty in x_j, d_j is the density function associated with $(\mathcal{S}_j, \mathcal{B}_j, p_j)$, $I(-j)$ and $I(-j,-k)$ denote the subsets of $I = \{1, 2, \ldots, nX\}$ that result from the deletion of $\{j\}$ and $\{j, k\}$, respectively, and the use of the product symbol (i.e., $\prod$) in conjunction with sets implies the concatenation of the elements of these sets. The probability space $(\mathcal{S}_{su}, \mathcal{B}_{su}, p_{su})$ associated with $\mathbf{x}$ is related to the probability spaces $(\mathcal{S}_j, \mathcal{B}_j, p_j)$ associated with the x_j by $\mathcal{S}_{su} = \prod_{j\in I}\mathcal{S}_j$, $\mathcal{B}_{su} = \prod_{j\in I}\mathcal{B}_j$, $p_{su} = \prod_{j\in I} p_j$ and $d_{su} = \prod_{j\in I} d_j$.

The integrals in Eqs. (2.33) and (2.34) are quite complex and in practice must be evaluated with some type of numerical procedure (e.g., Monte Carlo,[121] the Winding Stairs sampling scheme,[122-124] or simplifying approximations to f[125]). Once the necessary integrals, and hence V_j and V_{jk}, are evaluated, s_j and s_{jk} can be determined as indicated in Eqs. (2.24) and (2.25).

The determination of V_{jkl}, V_{jklm}, ..., $V_{12\ldots nX}$ with either the FAST approach or Sobol' indices is very de-

manding computationally and typically is not done. However, relatively efficient procedures exist to evaluate the total effect sensitivity measure with both the FAST approach[126] and the Sobol' variance decomposition.[127]

Additional information on the FAST approach and Sobol' variance decomposition is available in a number of publications.[118-121, 125-133] Further, a conceptually equivalent approach based on analysis of variance has also been developed[134-137] and has the desirable feature of allowing correlations between the elements of $\mathbf{x}$.[135-137]

2.5 Fast Probability Integration

Fast probability integration (FPI) is based on the use of analytic procedures to evaluate distribution functions.[138, 139] Specifically, the following approximation procedure is used:

$$\begin{aligned} prob(y > Y) &= \int_{\mathcal{S}_{su}} \delta_Y [f(\mathbf{x})] d_{su}(\mathbf{x})\, dV_{su} \\ &= \int_{\mathcal{S}_{su,n}} \delta_Y [f_n(\mathbf{u})] d_{su,n}(\mathbf{u})\, dV_{su,n} \\ &\doteq erfc\left(\beta/\sqrt{2}\right)/2, \end{aligned} \tag{2.35}$$

where (i) ($\mathcal{S}_{su,n}$, $\mathcal{A}_{su,n}$, $p_{su,n}$) represents the probability space that results when the elements x_j of the vectors $\mathbf{x}$ associated with ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}) are transformed to elements u_j of $\mathbf{u} \in \mathcal{S}_{su,n}$ that are mutually independent, standardized to mean zero and standard deviation one, and normally distributed, (ii) f_n denotes the reformulation of f that uses $\mathbf{u}$ rather than $\mathbf{x}$ as its argument, and (iii) β is related to the most probable point (MPP) for which $f_n(\mathbf{u}) = Y$ as described below and *erfc* is the complementary error function (i.e., $erfc(x) = (2/\sqrt{\pi})\int_x^\infty \exp(-t^2)\, dt$).

The equality

$$f_n(\mathbf{u}) = Y \tag{2.36}$$

defines a surface in $\mathcal{S}_{su,n}$ (see Fig. 1, Ref. 138). The MPP $\mathbf{u}_0 = [u_{10}, u_{20}, \ldots, u_{nX,0}]$ is the point on this surface that is closest to the origin in $\mathcal{S}_{su,n}$. In turn, β is given by

$$\beta = \|\mathbf{u}_0\| = \left[u_{10}^2 + u_{20}^2 + \ldots + u_{nX,0}^2\right]^{1/2} \tag{2.37}$$

and equals the distance from $\mathbf{u}_0$ to the origin. The outcome of this approach is that $prob(y > Y)$ is being approximated by the probability of the part of $\mathcal{S}_{su,n}$ that is cut off by a hyperplane that passes through the MPP $\mathbf{u}_0$ and is tangent to the surface defined by Eq. (2.36).

There are two major components to the implementation of an analysis based on FPI. First, the distributions indicated in Eq. (1.2) must be transformed to independent, normal distributions with mean zero and standard deviation one. Second, the MPP $\mathbf{u}_0$ associated with each probability $prob(y > Y)$ under consideration must be determined. This determination is typically based on search procedures using the partial derivatives of f_n with respect to the individual elements of $\mathbf{u}$. In addition, more sophisticated approximations to the surface at the MPP $\mathbf{u}_0$ than a hyperplane, and hence more sophisticated approximations to $prob(y > Y)$, can be developed. Although FPI is primarily used for uncertainty analysis, it can support some types of sensitivity analysis (Sect. 2.4, Ref. 138).

Additional information on FPI and related techniques is available from a number of sources.[138-147]

2.6 Comparison of Techniques

All techniques have positive and negative features, and no single technique is optimum for all situations. In the following, the positive and negative features of the individual techniques are briefly reviewed.

Monte Carlo techniques are based on the use of a probabilistic procedure to select model input and result in a mapping between analysis inputs and analysis outcomes that is then used to produce uncertainty and sensitivity analysis results. Desirable features of Monte Carlo analysis include (i) extensive sampling from the ranges of the uncertain variables, (ii) uncertainty results that are obtained without the use of surrogate models (e.g., Taylor series in differential analysis and response surfaces in RSM), (iii) extensive modifications of, or manipulations with, the original model are not required (i.e., as is the case for the other techniques), (iv) the extensive sampling from the individual variables facilitates the identification of nonlinearities, thresholds and discontinuities, (v) a variety of sensitivity analysis procedures are available, and (vi) the approach is conceptually simple, widely used, and easy to explain. The major drawback is computational cost. This is especially the case if long-running models are under consideration or probabilities very close to zero or one must be estimated.

Differential analysis is based on developing a Taylor series approximation to the model under consideration. Desirable properties of differential analysis include (i) the effects of small perturbations away from the base-case value at which the Taylor series is developed are revealed, (ii) uncertainty and sensitivity analyses based on variance propagation are straightforward once the Taylor series is developed, (iii) techniques (e.g., adjoint, Green's function, specialized compilers) exist to facilitate the calculation of derivatives, and (iv) the approach has been widely studied and applied. There are two primary drawbacks: (i) differential analysis is inherently local, and (ii) a differential analysis can be difficult to implement and can require large amounts of human and/or computational time.

Response surface methodology (RSM) is based on using an experimental design to select model input and then developing a response surface replacement for the original model that is used in subsequent uncertainty and sensitivity analyses. Desirable properties of RSM include (i) complete control over the structure of the model input through the experimental design selected for use, (ii) near optimum choice for a model whose predictions are known to be a linear or quadratic function of the input variables, (iii) uncertainty and sensitivity analyses are straightforward once the necessary response surface replacement has been developed, and (iv) experimental designs for use in RSM have been widely studied. Drawbacks to RSM include (i) difficulty of developing an appropriate experimental design, (ii) use of a limited number of values for each input variable, (iii) possible need for a large number of design points, (iv) difficulties in detecting thresholds, discontinuities and nonlinearities, (v) difficulty in including correlations and restrictions between input variables, and (vi) difficulty in constructing an appropriate response surface approximation to the model under consideration.

The FAST approach and Sobol' variance decomposition are based on a direct decomposition of variance into the parts contributed by individual variables. Desirable properties of the FAST approach and Sobol' variance decomposition include (i) full range of each input variable is explored, (ii) estimation of expected value and variance is by direct calculation rather than by use of a surrogate model, (iii) fractional contribution of each variable to total variance is determined, (iv) effects of variable interactions can be determined, (v) sensitivity analysis is not predicated on a search for linear or monotonic relationships, and (vi) modifications to the original model are not required. Drawbacks include (i) the mathematics is complicated and difficult to explain, (ii) the approaches are not widely known and applied, (iii) evaluating the required integrals can be both complex and computationally demanding, and (iv) correlations cannot be imposed on the input variables.

Fast probability integration is based on the use of analytic procedures to evaluate distribution functions. The desirable feature of fast probability integration is that it allows the estimation of the tails of a distribution without the estimation of the full distribution. This has the potential to require less computation than the use of Monte Carlo procedures to estimate the same tail probabilities. Less desirable features are that (i) the underlying mathematics is complicated and difficult to explain, (ii) the calculation of the partial derivatives required in the approach can be computationally demanding, and (iii) the approach is not appropriate for the calculation of full distributions or the consideration of distributions for a large number of different variables. Further, the approach is primarily one of uncertainty analysis and lacks associated sensitivity analysis procedures.

This review considers the use of Monte Carlo techniques in general and Latin hypercube sampling in particular in analyses that involve the propagation of uncertainty through complex systems. Although a variety of techniques exist for the propagation of uncertainty as previously indicated, Monte Carlo techniques provide the most effective approach to the propagation and analysis of uncertainty in many situations for various combinations of the following reasons: (i) large uncertainties are often present and a sampling-based approach provides a full coverage of the range of each uncertain variable, (ii) modification of the model is not required, (iii) direct estimates of distribution functions are provided, (iv) analyses are conceptually simple and logistically easy to implement, (v) analysis procedures can be developed that allow the propagation of results through systems of linked models, and (vi) a variety of sensitivity analysis procedures are available. Latin hypercube sampling is often the preferred sampling procedure in Monte Carlo analyses due to the efficient manner in which it stratifies across the range of each sampled variable.

3. Random, Stratified and Latin Hypercube Sampling

3.1 Description of Sampling Techniques

In Monte Carlo analysis, some type of sampling procedure must be used to generate the sample in Eq. (2.1). The simplest procedure is random sampling. With random sampling from uncorrelated variables, each sample element is generated independently of all other sample elements, and the probability that this element will come from a particular subset of $\mathcal{S}_{su}$ (i.e., $\mathcal{E} \in \mathcal{S}_{su}$) is equal to the probability of that subset (i.e., $p_{su}(\mathcal{E})$).

The nature of a random sample will be illustrated for $\mathbf{x} = [U, V]$, U assigned a uniform distribution on [0, 10], V assigned a triangular distribution and a mode of 8 on [0, 10], and $nS = 5$. The sample is generated by independently sampling five random numbers $RU(1)$, $RU(2)$, ..., $RU(5)$ from a uniform distribution on [0, 1] and then using the CDF for U to obtain five values $U(1)$, $U(2)$, ..., $U(5)$ for U (Fig. 3.1a). Similarly,

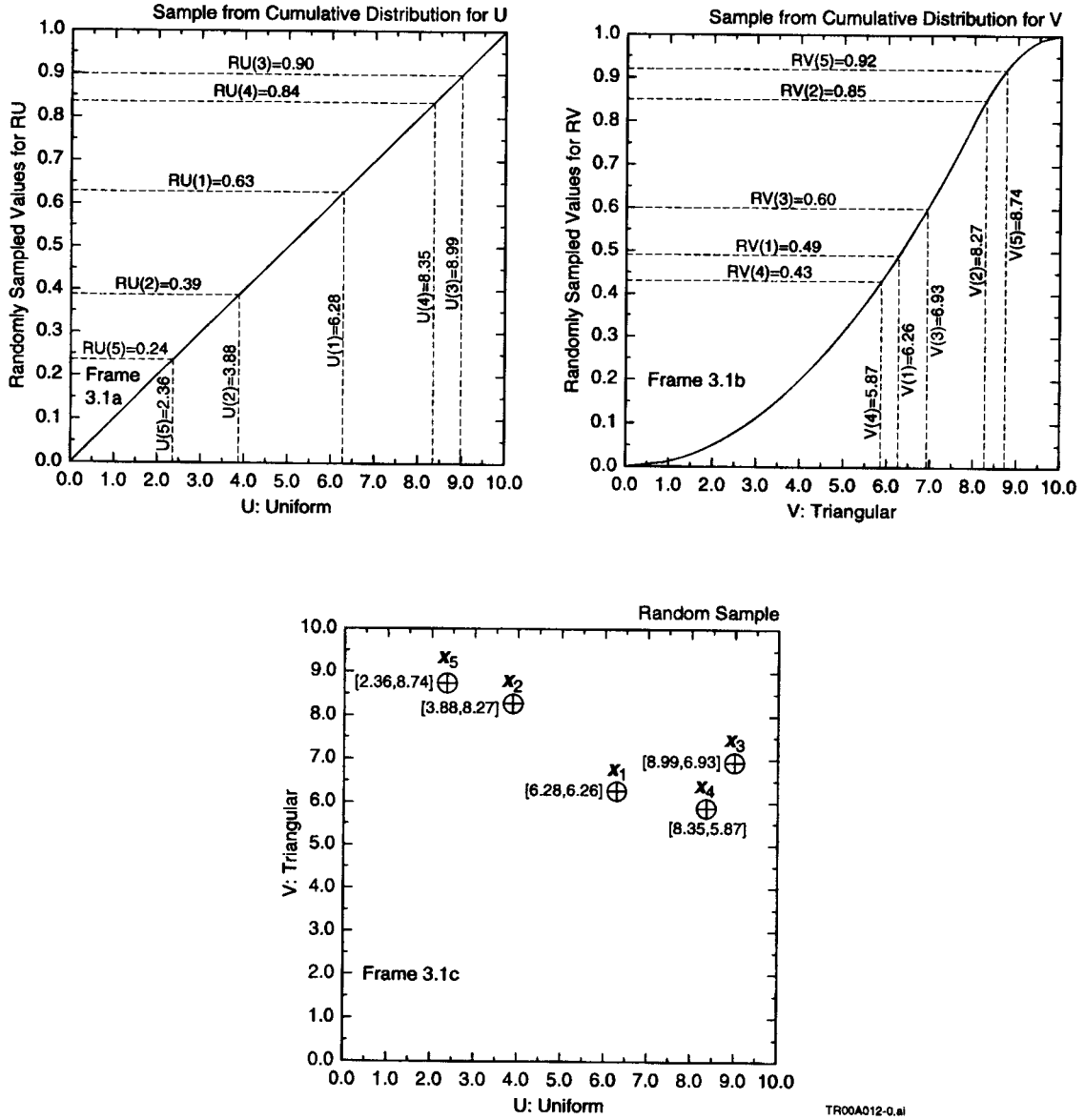

Fig. 3.1. Generation of a random sample of size $nS = 5$ from $\mathbf{x} = [U, V]$ with U uniform on [0, 10] and V triangular on [0, 10] with a mode of 8.

random sampling is again used to obtain an additional five independent random numbers $RV(1)$, $RV(2)$, ..., $RV(5)$ from a uniform distribution on [0, 1], and the CDF for V is used to obtain five values $V(1)$, $V(2)$, ..., $V(5)$ for V (Fig. 3.1b). Then,

$$\mathbf{x}_i = [U(i), V(i)], i = 1, 2, ..., 5, \quad (3.1)$$

constitutes a random sample of size $nS = 5$ generated in consistency with the distributions assigned to U and V (Fig. 3.1c). The generation of a random sample

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, ..., x_{i,nX}\right], i = 1, 2, ..., nS, \quad (3.2)$$

when $\mathbf{x}$ has dimension $nX > 2$ is carried out in an analogous manner.

The generation of a random sample in multiple dimensions ultimately depends on being able to generate uniformly distributed random numbers from the interval [0, 1]. The generation of such random numbers has been widely studied and discussed.[57, 148-150] As an aside, such numbers are often called pseudorandom numbers because they are generated by reproducible algorithmic processes rather than in a truly random manner. For this presentation, the capability to generate random numbers is taken for granted and discussed no further.

With random sampling, there is no assurance that a sample element will be generated from any particular subset of the sample space $\mathcal{S}_{su}$. In particular, important subsets of $\mathcal{S}_{su}$ with low probability but high consequences are likely to be missed. Stratified sampling, or importance sampling as it is also sometimes called, provides a way to mitigate this problem by specifying subsets of $\mathcal{S}_{su}$ from which sample elements will be selected. Specifically, $\mathcal{S}_{su}$ is exhaustively subdivided into a collection $\mathcal{E}_1, \mathcal{E}_2, ..., \mathcal{E}_{nI}$ of disjoint subsets (i.e., $\cup_{k=1}^{nI} \mathcal{E}_k = \mathcal{S}_{su}$ and $\mathcal{E}_p \cap \mathcal{E}_q = \emptyset$ for $p \neq q$) (Fig. 3.2). The $\mathcal{E}_k$ constitute the strata associated with the sampling procedure. Then, the corresponding sample (i.e., the stratified or importance sample)

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, ..., x_{i,nX}\right], i = 1, 2, ..., nS = \sum_{k=1}^{nI} nI_k, \quad (3.3)$$

is obtained by randomly sampling nI_k sample elements from strata $\mathcal{E}_k$. The preceding sampling is carried out conditional on the restriction of $\mathbf{x}$ to $\mathcal{E}_k$. Further, if $\mathbf{x}_i \in \mathcal{E}_k$, then the corresponding weight w_i for use in probabilistic calculations is given by $w_i = p_{su}(\mathcal{E}_k)/nI_k$. In most applications, $nI_k = 1$, and so the sample size nS is equal to the number of strata and $w_i = p_{su}(\mathcal{E}_k)$ for $\mathbf{x}_i \in \mathcal{E}_k$.

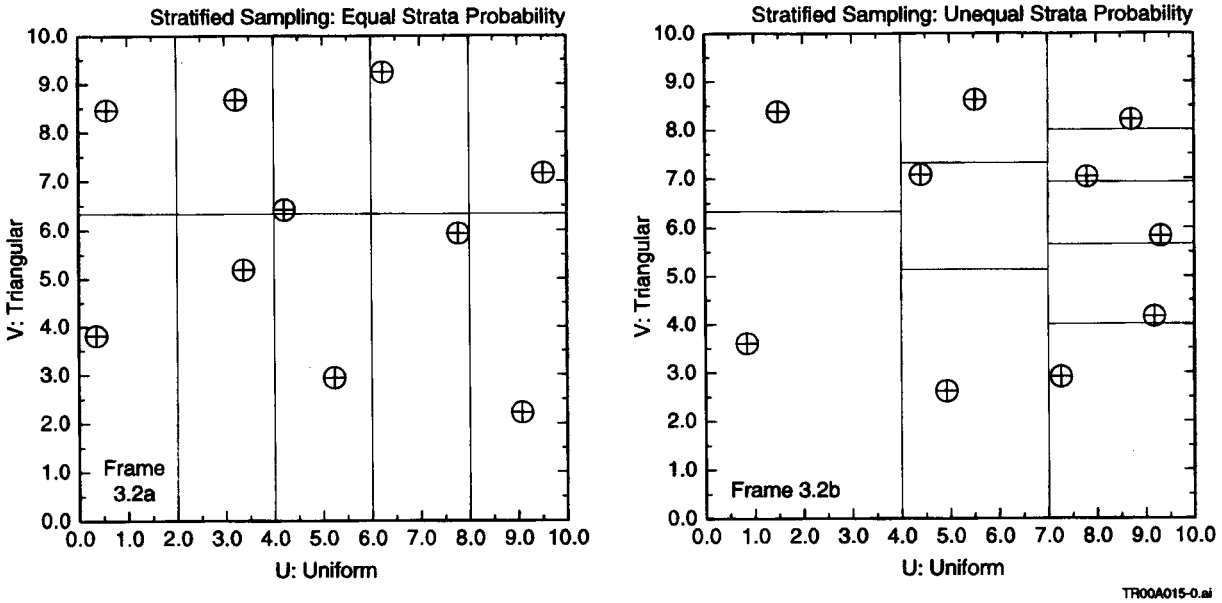

Fig. 3.2. Generation of a stratified sample of size $nS = 10$ with one random sample per strata (i.e., $nI_k = 1$) from $\mathbf{x} = [U, V]$ with U uniform on [0, 10] and V triangular on [0, 10] with a mode of 8: (a) Equal strata probability (i.e., $p_{su}(\mathcal{E}_k) = 0.1$), and (b) Unequal strata probability (i.e., $p_{su}(\mathcal{E}_k) =$ 0.2, 0.2, 0.1, 0.1, 0.1, 0.06, 0.06, 0.06, 0.06, 0.06).

Stratified sampling has the advantage of forcing the inclusion of specified subsets of $\mathcal{S}_{su}$ while maintaining the probabilistic character of random sampling. Indeed, it can be argued that stratified sampling is always the best procedure to use when enough information is available for its appropriate implementation. A major problem associated with stratified sampling is the necessity of defining the strata $\mathcal{E}_1$, $\mathcal{E}_2$, ..., $\mathcal{E}_{nI}$ and also calculating their probabilities. Both of these requirements are avoided when random sampling is used. When the dimensionality of $\mathcal{S}_{su}$ is high, the determination of strata and strata probabilities becomes a major undertaking. The event tree and fault procedures that underlie many large analyses can be viewed as algorithms to determine the strata and strata probabilities for use in a stratified sampling procedure. These determinations are further complicated when many analysis outcomes are under consideration (i.e., when $\mathbf{y}$ in Eq. (1.1) is of high dimension); in particular, strata definitions that are appropriate for one analysis outcome may be inappropriate for other analysis outcomes. A compounding problem is that all the analysis outcomes that will be studied in the course of an analysis may not even be known at the beginning of the analysis.

Latin hypercube sampling can be viewed as a compromise procedure that incorporates many of the desirable features of random sampling and stratified sampling and also produces more stable analysis outcomes than random sampling. Like random and stratified sampling, Latin hypercube sampling is a probabilistic procedure in the sense that a weight (i.e., $w_i = 1/nS$) can be associated with each sample element that can be used in probabilistic calculations (i.e., in the estimation of the integrals in Eqs. (1.4) - (1.8)). Like random sampling, the implementation of Latin hypercube sampling is easier than the implementation of stratified sampling because it is not necessary to determine strata and strata probabilities. However, Latin hypercube sampling does have the property of densely stratifying across the range of each element of $\mathbf{x}$, which is a property closer to those possessed by stratified sampling. Thus, Latin hypercube sampling displays properties between random sampling, which involves no stratification, and stratified sampling, which stratifies on $\mathcal{S}_{su}$.

Latin hypercube sampling operates in the following manner to generate a sample of size nS from $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ in consistency with the distributions D_1, D_2, ..., D_{nX} indicated in Eq. (1.2) (i.e., in consistency with the probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$). The range of each variable (i.e., the x_j) is exhaustively divided into nS disjoint intervals of equal probability and one value is selected at random from each interval. The nS values thus obtained for x_1 are paired at random without replacement with the nS values obtained for x_2. These nS pairs are combined in a random manner without replacement with the nS values of x_3 to form nS triples. This process is continued until a set of nS nX-tuples is formed. These nX-tuples are of the form

$$\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{i,nX}], \quad i = 1, 2, \ldots, nS, \tag{3.4}$$

and constitute the Latin hypercube sample (LHS). The individual x_j must be independent for the preceding construction procedure to work; a method for generating Latin hypercube and random samples from correlated variables has been developed by Iman and Conover[151] and will be discussed in Sect. 5.1. Latin hypercube sampling is an extension of quota sampling[152] and can be viewed as an n-dimensional randomized generalization of Latin square sampling (Ref. 153, pp. 206-209).

The generation of an LHS is illustrated for $\mathbf{x} = [U, V]$ and $nS = 5$ (Fig. 3.3). The ranges of U and V are subdivided into five intervals of equal probability, with this subdivision represented by the lines that originate at 0.2, 0.4, 0.6 and 0.8 on the ordinates of Figs. 3.3a and 3.3b, extend horizontally to the CDFs, and then drop vertically to the abscissas to produce the 5 indicated intervals. Random values $U(1)$, $U(2)$, ..., $U(5)$ and $V(1)$, $V(2)$, ..., $V(5)$ are then sampled from these intervals. The sampling of these random values is implemented by (i) sampling $RU(1)$ and $RV(1)$ from a uniform distribution on [0, 0.2], $RU(2)$ and $RV(2)$ from a uniform distribution on [0.2, 0.4], and so on, and then (ii) using the CDFs to identify (i.e., sample) the corresponding U and V values, with this identification represented by the dashed lines that originate on the ordinates of Figs. 3.3a and 3.3b, extend horizontally to the CDFs, and then drop vertically to the abscissas to produce $U(1)$, $U(2)$, ..., $U(5)$ and $V(1)$, $V(2)$, ..., $V(5)$. The generation of the LHS is then completed by randomly pairing (without replacement) the resulting values for U and V. As this pairing is not unique, many possible LHSs can result, with the LHS in Fig. 3.3c resulting from the pairings $[U(1), V(5)]$, $[U(2), V(1)]$, $[U(3), V(2)]$, $[U(4), V(3)]$, $[U(5), V(4)]$ and the LHS in Fig. 3.3d resulting from the pairings $[U(1), V(3)]$, $[U(2), V(2)]$, $[U(3), V(3)]$, $[U(4), V(5)]$, $[U(5), V(1)]$.

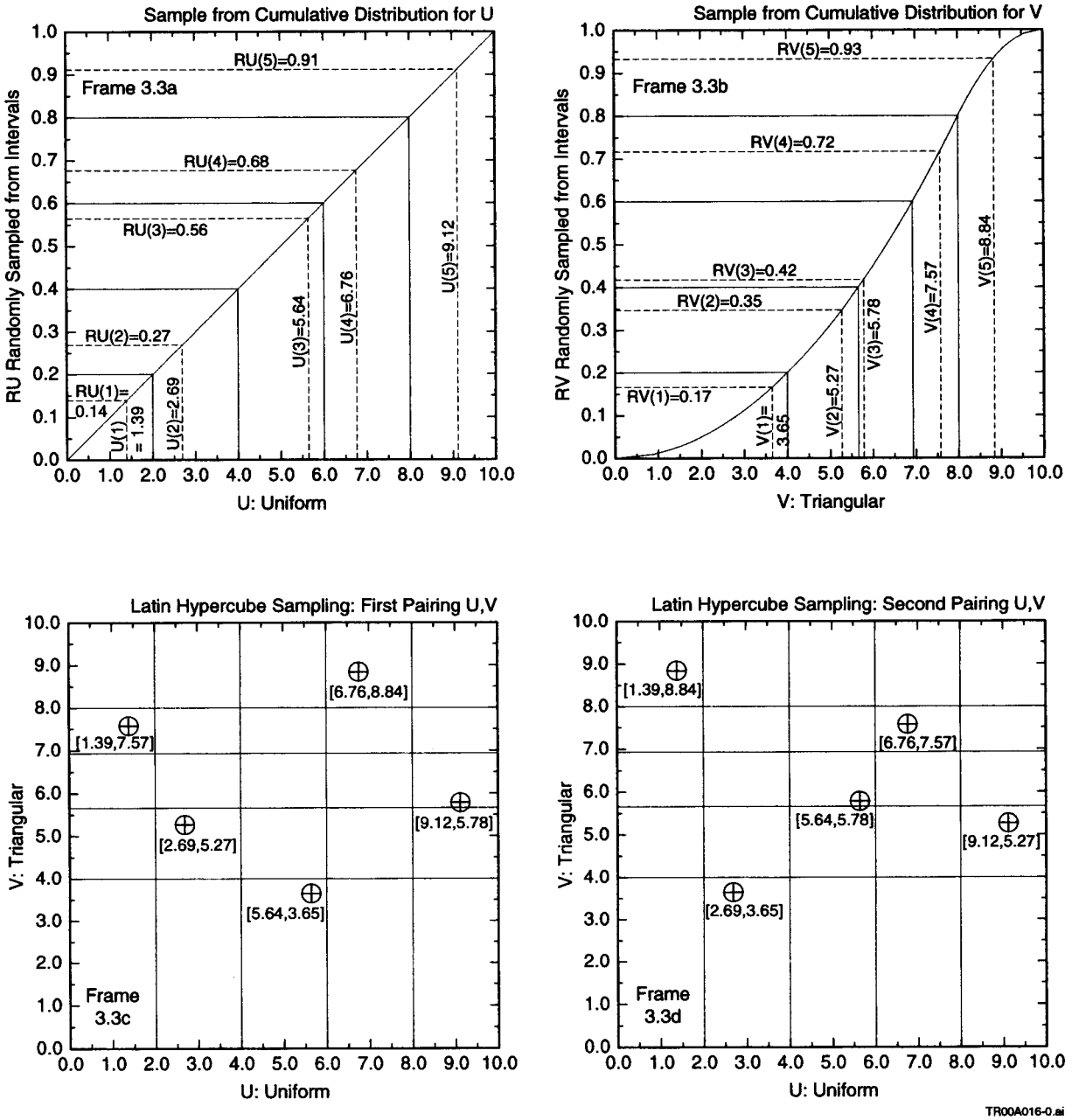

Fig. 3.3. Example of Latin hypercube sampling to generate a sample of size $nS = 5$ from $\mathbf{x} = [U, V]$ with U uniform on [0, 10] and V triangular on [0, 10] with a mode of 8.

The generation of an LHS for $nS > 2$ proceeds in a manner similar to that shown in Fig. 3.3 for $nV = 2$. The sampling of the individual variables for $nS > 2$ takes place in the same manner as shown in Figs. 3.3a and 3.3b. However, the nX variables define an nX-dimensional solid rather than a 2-dimensional rectangle in the plane. Thus, Figs. 3.3c and 3.3d would involve a partitioning of an nX-dimensional solid rather than a rectangle.

3.2 Properties of Sampling Techniques

Random sampling, stratified sampling and Latin hypercube sampling are now discussed and compared. This discussion is derived from the study by McKay et al.[31] For notational convenience, a single element y of the vector $\mathbf{y}$ in Eq. (1.1) is considered.

The following estimator is widely used in conjunction with random sampling:

$$T(y_1, y_2, \ldots, y_{nS}) = (1/nS)\sum_{i=1}^{nS} g(y_i), \tag{3.5}$$

where $y_i = f(\mathbf{x}_i)$ for the random sample appearing in Eq. (3.2) and g is an arbitrary function. If $g(y) = y$, then T represents the sample mean, which is used to estimate the expected value $E(y)$ of y. If $g(y) = y^r$, then T represents an estimate for the r^{th} sample moment, which is used in obtaining an estimate for the corresponding population moment. If $g(y) = 1$ for $y \le Y$ and $g(y) = 0$ otherwise, then T is an estimate of the quantile on the distribution function of y associated with Y.

Let Υ denote the expected value for the population of Ts that results from repeated calculations with independent random samples of size nS from $\mathbf{x}$. McKay et al.[31] show that both stratified sampling and Latin hypercube sampling yield unbiased estimates for Υ, which is also the case for random sampling. That is, the expected value of repeated calculations of T with either sampling method is Υ.

For notational convenience, let T_R, T_S and T_L represent estimates of Υ (i.e., values of T calculated as shown in Eq. (3.5)) obtained with a random sample of size nS, a stratified sample of size nS with all strata of equal probability and one random selection per strata, and an LHS of size nS, respectively. Then, as shown by McKay et al.,[31]

$$Var(T_S) \le Var(T_R), \tag{3.6}$$

where Var represents the variance of T_S and T_R under repeated estimations. No direct means of comparing the variance of T_L and T_R appears to be known. However, the following result has been established by McKay et al.[31]

Theorem 3.1. If $y = f(x_1, x_2, \ldots, x_{nX})$ is monotonic in each of the x_j and $g(y)$ is a monotonic function of y, then

$$Var(T_L) \le Var(T_R). \tag{3.7}$$

As indicated earlier, uncertainty analysis generally involves estimating the mean, variance and distribution function for the particular dependent variable under consideration. Estimates for these quantities with random sampling, stratified sampling, and Latin hypercube sampling are now considered. For each sampling method, the form for the estimator of the expected value of y is given by

$$\bar{y} = \hat{E}(y) = (1/nS)\sum_{i=1}^{nS} y_i, \tag{3.8}$$

where $y_i = f(\mathbf{x}_i)$. To obtain this representation for the stratified sample, it is assumed that $\mathbf{x}_i$ comes from stratum $\mathcal{E}_i$, $p_{su}(\mathcal{E}_i) = 1/nS$, and $nI_i = 1$. The symbols $\bar{y}_R, \bar{y}_S$ and $\bar{y}_L$ are used to represent the value obtained in Eq. (3.8) with random sampling, stratified sampling, and Latin hypercube sampling, respectively. Each of $\bar{y}_R, \bar{y}_S$ and $\bar{y}_L$ is an unbiased estimator of $E(y)$.

The goodness of an unbiased estimator can be measured by its variance. As shown in McKay et al.,[31]

$$Var(\bar{y}_R) = (1/nS)Var(y), \tag{3.9}$$

$$Var(\bar{y}_S) = Var(\bar{y}_R) - \left(1/nS^2\right)\sum_{i=1}^{nS}(\mu_i - \mu)^2, \tag{3.10}$$

and

$$Var(\bar{y}_L) = Var(\bar{y}_R) + \frac{nS-1}{nS^{nX+1}(nS-1)^{nX}}\sum_{\mathcal{R}}(\mu_r - \mu)(\mu_s - \mu), \tag{3.11}$$

where

$$\mu = E(y), \tag{3.12}$$

$\mu_i = E(y \mid \mathbf{x} \in \mathcal{E}_i)$ in Eq. (3.10) for the stratified sample, (3.13)

$\mu_r = E(y \mid \mathbf{x} \in \text{cell } r)$ in Eq. (3.11) for the LHS, (3.14)

and $\mathcal{R}$ in Eq. (3.11) denotes the restricted space of all pairs (μ_r, μ_s) for which the associated cells have no coordinates in common. The cells being referred to in conjunction with Latin hypercube sampling in Eq. (3.11) are the nS^{nX} possible combinations of intervals of equal probability used in the construction of the sample. Each cell can be labeled by a set of coordinates

$$\mathbf{m}_r = \left[m_{r1}, m_{r2}, \ldots, m_{r,nX}\right], \tag{3.15}$$

where m_{rj} is the interval number for variable x_j associated with cell r, $r = 1, 2, \ldots, nS^{nX}$. The statement that cells r and s have no coordinate in common means that $m_{rj} \neq m_{sj}$ for $j = 1, 2, \ldots, nX$.

Comparison of Eqs. (3.9) and (3.10) shows that

$$Var(\bar{y}_S) \leq Var(\bar{y}_R). \tag{3.16}$$

The relationship between $Var(\bar{y}_R)$ and $Var(\bar{y}_L)$ is not easily ascertained by comparing Eqs. (3.9) and (3.11). However, the previously stated theorem by McKay et al.[31] (Theorem 3.1) implies that

$$Var(\bar{y}_L) \leq Var(\bar{y}_R) \tag{3.17}$$

when $y = f(x_1, x_2, \ldots, x_{nX})$ is monotonic in each of the x_j. In the example presented in McKay et al.,[31] the sampling variability in $\bar{y}_L$ (i.e., $Var(\bar{y}_L)$) was considerably less than that for $\bar{y}_R$ and $\bar{y}_S$.

For each sampling method, the form for the estimator of the variance of y is given by

$$S^2 = (1/nS)\sum_{i=1}^{nS}(y_i - \bar{y})^2, \tag{3.18}$$

and its expectation is given by

$$E(S^2) = Var(y) - Var(\bar{y}), \tag{3.19}$$

where $\bar{y}$ is $\bar{y}_R$, $\bar{y}_S$ or $\bar{y}_L$, depending on which sampling technique is in use. For convenience, S_R^2, S_S^2 and S_L^2 are used to represent the values obtained in Eq. (3.18) for random sampling, stratified sampling (equal probability strata), and Latin hypercube sampling.

For the random sample, $nS\,S_R^2/(nS-1)$ is an unbiased estimator of the variance of y. The bias in the case of stratified sampling is unknown. However, it follows from Eqs. (3.9), (3.16) and (3.19) that

$$\left[(nS-1)/nS\right]Var(y) \leq E\left(S_S^2\right) \leq Var(y). \tag{3.20}$$

The bias in S_L^2 is also unknown. However, in a derivation analogous to the one used for Eq. (3.20), it follows from Eqs. (3.9), (3.17) and (3.19) that

$$\left[(nS-1)/nS\right]Var(y) \leq E\left(S_L^2\right) \leq Var(y) \tag{3.21}$$

when $y = f(x_1, x_2, \ldots, x_{nX})$ is monotonic in each of the x_j. In the example given in McKay et al.,[31] S_L^2 was found to have little bias and considerably less sampling variability than either random or stratified sampling.

For each sampling method, the form for the estimator of the distribution function of y is given by

$$G(y) = (1/nS)\sum_{i=1}^{nS} u(y - y_i), \tag{3.22}$$

where $u(z) = 1$ if $z \geq 0$ and $u(z) = 0$ otherwise. More specifically, $G(y)$ is the estimator for the quantile on the distribution function associated with y. The locus of points $(y, G(y))$ is the empirical distribution function associated with $y_1, y_2, \ldots, y_{nS}$. Since Eq. (3.22) is of the form shown in Eq. (3.5), the expected value of $G(y)$ is the same under all three sampling plans. Under random sampling, $G(y)$ is an unbiased estimator for the distribution function of y, and so stratified and Latin hypercube sampling also provide unbiased estimates.

As shown in McKay et al.,[31] the variances for the estimators in Eq. (3.22) are given by

$$Var[G_R(y)] = (1/nS)D(y)[1 - D(y)], \tag{3.23}$$

$$Var[G_S(y)] = Var[G_R(y)] - \left(1/nS^2\right)\sum_{i=1}^{nS}[D_i(y) - D(y)]^2 \tag{3.24}$$

and

$$Var[G_L(y)] = Var[G_R(y)] + \frac{nS-1}{nS^{nX+1}(nS-1)^{nX}} \sum_{\mathcal{R}}[D_r(y) - D(y)][D_s(y) - D(y)], \tag{3.25}$$

where G_R, G_S and G_L represent the estimator in Eq. (3.24) with random, stratified and Latin hypercube sampling, respectively, D represents the true distribution function for y, D_i and D_r represent the distribution function for y conditional on $\mathbf{x}$ belonging to stratum i or cell r as appropriate (see Eqs. (3.13)) and (3.14)), and $\mathcal{R}$ represents the same restricted space that it did in Eq. (3.11).

The equality in Eq. (3.24) implies that

$$Var[G_S(y)] \le Var[G_R(y)]. \tag{3.26}$$

Thus, the variance in estimating $D(y)$ with stratified sampling is less than that with random sampling. The relationship between $Var[G_L(y)]$ and $Var[G_R(y)]$ is not readily seen by comparing Eqs. (3.23) and (3.25). In the example given in McKay et al.,[31] the sampling variability in $G_L(y)$ (i.e., $Var[G_L(y)]$) was found to be considerably less than that in $G_R(y)$ and $G_S(y)$.

The comparisons involving random sampling, stratified sampling and Latin hypercube sampling discussed so far have all been for samples of a fixed size nS. Stein[154] has derived asymptotic comparisons of the variability of estimates T_R and T_L of T obtained with random sampling and Latin hypercube sampling, respectively, under the assumption that the x_js are independent. In particular, Stein found that the inequality

$$Var\left[T_L(y_1, y_2, \ldots, y_{nS})\right] < Var\left[T_R(y_1, y_2, \ldots, y_{nS})\right] \tag{3.27}$$

can be expected to hold for sufficiently large sample sizes nS for most models.

A more explicit statement of Stein's result requires some additional notation. Let $\mathcal{S}_{su,j}$, $j = 1, 2, \ldots, nX$, represent the sample space for x_j, and let $d_{su,j}$ represent the corresponding density function, with both $\mathcal{S}_{su,j}$ and $d_{su,j}$ deriving from the distribution D_j indicated in Eq. (1.2). Further, let $I = \{1, 2, \ldots, nX\}$, $I(-j) = I - \{j\}$, $d_{su}(\mathbf{x}) = \prod_{j \in I} d_{su,j}(x_j)$, and $d_{su,-j}(\mathbf{x}) = \prod_{k \in I(-j)} d_{su,k}(x_k)$. The representation of $d_{su}(\mathbf{x})$ and $d_{su,-j}(\mathbf{x})$ as products involving $d_{su,j}(x_j)$ is possible because the x_js are assumed to be independent.

Stein's result is based on the following decomposition of $g[f(\tilde{\mathbf{x}})]$:

$$g\left[f(\tilde{\mathbf{x}})\right] = \mu + \sum_{j=1}^{nX}\alpha_j(\tilde{\mathbf{x}}) + r(\tilde{\mathbf{x}}), \tag{3.28}$$

where

$\tilde{\mathbf{x}} = [\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_{nX}]$ is an arbitrary element of $\mathcal{S}_{su}$,

$$\mu = \int_{\mathcal{S}_{su}} g[f(\mathbf{x})]d_{su}(\mathbf{x})dV_{su},$$

$$\mathcal{S}_{su,-j}(x) = \{\mathbf{x} \mid \mathbf{x} \in \mathcal{S}_{su} \text{ and } x_j = x\},$$

$$\alpha_j(\tilde{\mathbf{x}}) = \int_{\mathcal{S}_{su,-j}(\tilde{x}_j)}\{g[f(\mathbf{x})] - \mu\}d_{su,-j}(\mathbf{x})dV_{su,-j},$$

$dV_{su,-j}$ represents an increment of volume from $\mathcal{S}_{su,-j}(\tilde{x}_j)$ and $r(\tilde{\mathbf{x}})$ is formally defined by

$$r(\tilde{\mathbf{x}}) = g\left[f(\tilde{\mathbf{x}})\right] - \mu - \sum_{j=1}^{nX}\alpha_j(\tilde{\mathbf{x}}). \tag{3.29}$$

The function $\alpha_j(\tilde{\mathbf{x}})$ characterizes the "main effect" of the element $\tilde{x}_j$ of $\tilde{\mathbf{x}}$, and the function $r(\tilde{\mathbf{x}})$ characterizes the nonadditive component of $g[f(\tilde{\mathbf{x}})]$. As an aside, this decomposition also underlies the procedures introduced in Sect. 2.4. The following result is proved by Stein (Ref. 154, Corollary 1, p. 145):

Theorem 3.2. If $\int_{\mathcal{S}_{su}} g^2[f(\mathbf{x})]d_{su}(\mathbf{x})dV_{su}$ is finite, then

$$Var\left[T_L(y_1, y_2, \ldots, y_{nS})\right] = \int_{\mathcal{S}_{su}} r^2(\mathbf{x})d_{su}(\mathbf{x})dV_{su}/nS + o\left(nS^{-1}\right), \tag{3.30}$$

where the notation $F(nS^{-1}) = o(nS^{-1})$ indicates that $F(nS^{-1})/nS^{-1} \to 0$ as $nS \to \infty$ (Ref. 30, p. xv).

The corresponding variance associated with random sampling is given by

$$Var\left[T_R(y_1, y_2, \ldots, y_{nS})\right] = \int_{S_{su}} \left\{g[f(\mathbf{x})] - \mu\right\}^2 d_{su}(\mathbf{x}) dV_{su} / nS = \int_{S_{su}} r^2(\mathbf{x}) d_{su}(\mathbf{x}) dV_{su} / nS + \sum_{j=1}^{nX} \alpha_j^2(\mathbf{x}) d_{su}(\mathbf{x}) dV_{su} / nS, \quad (3.31)$$

with the second equality following from Eq. (3.28) and the equalities

$$0 = \int_{S_{su,j}} \alpha_j(\mathbf{x}) d_{su,j}(x_j) dx_j \quad (3.32)$$

for $j = 1, 2, \ldots, nX$ and

$$0 = \int_{S_{su,-j}} (x_j) r(\mathbf{x}) d_{su,-j}(\mathbf{x}) dV_{su,-j} \quad (3.33)$$

for $x_j \in S_{su,j}$ and $j = 1, 2, \ldots, nX$. Thus, above some sample size, Latin hypercube sampling results in estimates for T with lower variance than random sampling unless all the main effects $\alpha_j(\mathbf{x})$, $j = 1, 2, \ldots, nX$, are zero.

For sufficiently large sample sizes, $T_L - \Upsilon$ has a distribution that is approximately normal, where Υ is the expected value of T_L. Specifically, the following result has been established by Owen:[155]

Theorem 3.3. If $g[f(\mathbf{x})]$ is bounded, then $nS^{1/2}(T_L - \Upsilon)$ converges in distribution to a normal distribution with mean zero and variance

$$\int_{S_{su}} r^2(\mathbf{x}) d_{su}(\mathbf{x}) dV_{su}$$

as nS increases (see Ref. 156, Sect. 1.4, for formal definition of convergence in distribution).

In practice, most models satisfy the boundedness condition imposed on $g[f(\mathbf{x})]$. Thus, in concept, the preceding result can be used to place confidence intervals on results obtained with Latin hypercube sampling. In practice, determining how large nS must be for approximate normality to hold can be difficult.

Additional results on variance reduction associated with Latin hypercube sampling and further references are given in several recent papers.[157, 158] Also, a number of references related to the theoretical development of Latin hypercube sampling are given at the end of Sect. 5.1.

3.3 Historical Development of Latin Hypercube Sampling

The introduction of Latin hypercube sampling can be traced to concerns in the reactor safety community over the treatment of uncertainty in analyses related to the safety of nuclear power plants. In particular, the Reactor Safety Study[159] was published by U.S. Nuclear Regulatory Commission (NRC) in 1975 and widely praised for its advancement of the state of probabilistic risk assessment (PRA).[160] However, it was also criticized for inadequately representing the uncertainty in its results.[160] This led to an active interest on the part of the NRC and its contractors in the propagation of uncertainty through models for complex systems.

In this environment, Latin hypercube sampling was conceived of by W.J. Conover (the original, unpublished manuscript documenting this work is reproduced in App. A) and formally published in conjunction with colleagues at Los Alamos Scientific Laboratory.[31] The first applications of Latin hypercube sampling were in the analysis of loss of coolant accidents (LOCAs) in the context of reactor safety.[161, 162] R. L. Iman, a student of Conover's and a staff member at Sandia National Laboratories, recognized the potential of Latin hypercube sampling and became an early and active proponent of its use. Among his contributions was to write the first widely distributed program for Latin hypercube sampling.[163, 164] A brief description of the early development of Latin hypercube sampling was prepared by Iman in 1980 (this unpublished description is reproduced in App. B).

Much of the early use of Latin hypercube sampling was in programs related to radioactive waste disposal carried out at Sandia National Laboratories for the NRC.[165-167] In addition, the NRC also supported work on Latin hypercube sampling and associated sensitivity analysis techniques as part of its MELCOR project to develop a new suite of models for use in performing reactor safety studies.[168-170]

In the mid 1980s, the NRC decided to reassess the results obtained in the Reactor Safety Study, with particular attention to be paid to the assessment and propagation of uncertainty. This study, often referred to as NUREG-1150 after its report number, was a very large analysis and probably the largest integrated analysis of

any system carried out in the 1980s.[171, 172] As part of the NUREG-1150 analyses, Latin hypercube sampling was used in the propagation of uncertainty through PRAs for 5 nuclear power plants.[173-177] In addition to the extensive technical report literature documenting these PRAs, summaries are also available in the journal literature.[172, 178-182] Subsequent to NUREG-1150, Latin hypercube sampling was used in a very extensive PRA for the LaSalle nuclear power station.[183-186]

After the NUREG-1150 analyses, the next large project to make use of Latin hypercube sampling involved performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP), which was under development by the U.S. Department of Energy (DOE) for the geologic disposal of transuranic radioactive waste.[187, 188] Latin hypercube sampling was used in several PAs for the WIPP, including the PA that supported the DOE's successful compliance certification application (CCA) to the U.S. Environmental Protection Agency (EPA) for the WIPP.[189, 190] With its certification, the WIPP became the first operational facility in the United States for the geologic disposal of radioactive waste. As an aside, EPA staff members charged with writing regulations for the geologic disposal of radioactive waste were acquainted with, and influenced by, uncertainty analyses performed with Latin hypercube sampling, with the result that the final regulations developed for the WIPP mandated an uncertainty propagation of the type for which Latin hypercube sampling is well suited.[191-194]

At present, the largest project that is making use of Latin hypercube sampling is the Yucca Mountain Project (YMP) to develop a deep geologic disposal facility for high level radioactive waste at Yucca Mountain, Nevada.[195-197] This project is both large and controversial. It is also a very important project that has been much in the news recently and is likely to get even more attention in the near future for various reasons. Another large project that is currently using Latin hypercube sampling is the System Assessment Capability (SAC) program for the Hanford Site.[198, 199]

The preceding background discussion has concentrated on the large analyses that have used Latin hypercube sampling. However, Latin hypercube sampling has also been used in smaller analyses in a variety of fields (e.g., Refs. 33-39, 41-44, 200-214). A recent check (Sept. 9, 2001) of SciSearch shows 330 citations to the original article on Latin hypercube sampling,[31] with the number of citations steadily increasing with time. Further, this check does not indicate the extensive use of Latin hypercube sampling in analyses documented in the technical report literature. Thus, the use of Latin hypercube sampling is extensive and growing. As an indication of the interest in Latin hypercube sampling, the original article was recently declared a *Technometrics* classic in experimental design.[215]

The growing use of Latin hypercube sampling and other techniques for the propagation and analysis of uncertainty derives from the recognition that it is not enough just to report the results of an analysis. For the analysis to be useful in a decision making context, it also necessary to assess and report how much confidence should be placed in the results of the analysis (e.g., see the recommendations given in quotes reproduced in Ref. 7).

4. Comparison of Random and Latin Hypercube Sampling

Because of its efficient stratification properties, Latin hypercube sampling is primarily intended for use with long-running models. When a model can be evaluated quickly, there is little reason to use Latin hypercube sampling. However, due to their computational complexity and expense, long-running models do not constitute convenient vehicles for comparing random and Latin hypercube sampling. For this reason, the present section will use two relatively simple functions (i.e., models) to compare random and Latin hypercube sampling. No comparisons with stratified sampling are made because the stratification used in a real analysis will always depend on the goals of the analysis and the properties of the model(s) used in the analysis. In particular, the efficacy of stratified sampling derives from an informed selection of strata of unequal probability.

4.1 Monotonic Function

The function

$$f_1(U,V) = U + V + UV + U^2 + V^2 + U \min\{\exp(3V), 10\} \tag{4.1}$$

is monotonic for positive values of its arguments U, V and thus reasonably well behaved. For the purpose of comparing random and Latin hypercube sampling, U and V are assumed to be uncorrelated and uniformly disturbed on [1.0, 1.5] and [0, 1], respectively.

Both random and Latin hypercube sampling can be used to estimate the distribution of f that derives from the distributions assigned to U and V. To illustrate the robustness (i.e., stability) of results obtained with the two sampling procedures, 10 samples of size 25, 50 and 100 are generated for each procedure and the associated CDFs for f_1 constructed. The CDFs constructed for Latin hypercube sampling show less variability from sample to sample than the CDFs constructed for random sampling (Fig. 4.1). Thus, Latin hypercube sampling is producing a more stable estimate for the CDF than is being produced by random sampling, which is consistent with the result in Theorem 3.1.

4.2 Nonmonotonic Function

Unlike the function f_1 in Eq. (4.1), the following function is monotonic for positive values of one argument (i.e., U) and nonmonotonic for positive values of the other argument (i.e., V):

$$f_2(U,V) = U + V + UV + U^2 + V^2 + Ug(V) \tag{4.2}$$

where

$$h(V) = (V - 11/43)^{-1} + (V - 22/43)^{-1} + (V - 33/43)^{-1}$$

$$g(V) = h(V) \quad \text{if } |h(V)| < 10$$

$$= 10 \quad \text{if } h(V) \geq 10$$

$$= -10 \quad \text{if } h(V) \leq -10.$$

For the purpose of comparing random and Latin hypercube sampling, U and V are again assumed to be uncorrelated and uniformly distributed on [1.0, 1.5] and [0, 1], respectively. Consideration of samples of size 25, 50 and 100 illustrates that Latin hypercube sampling produces more stable CDF estimates than produced by random sampling (Fig. 4.2).

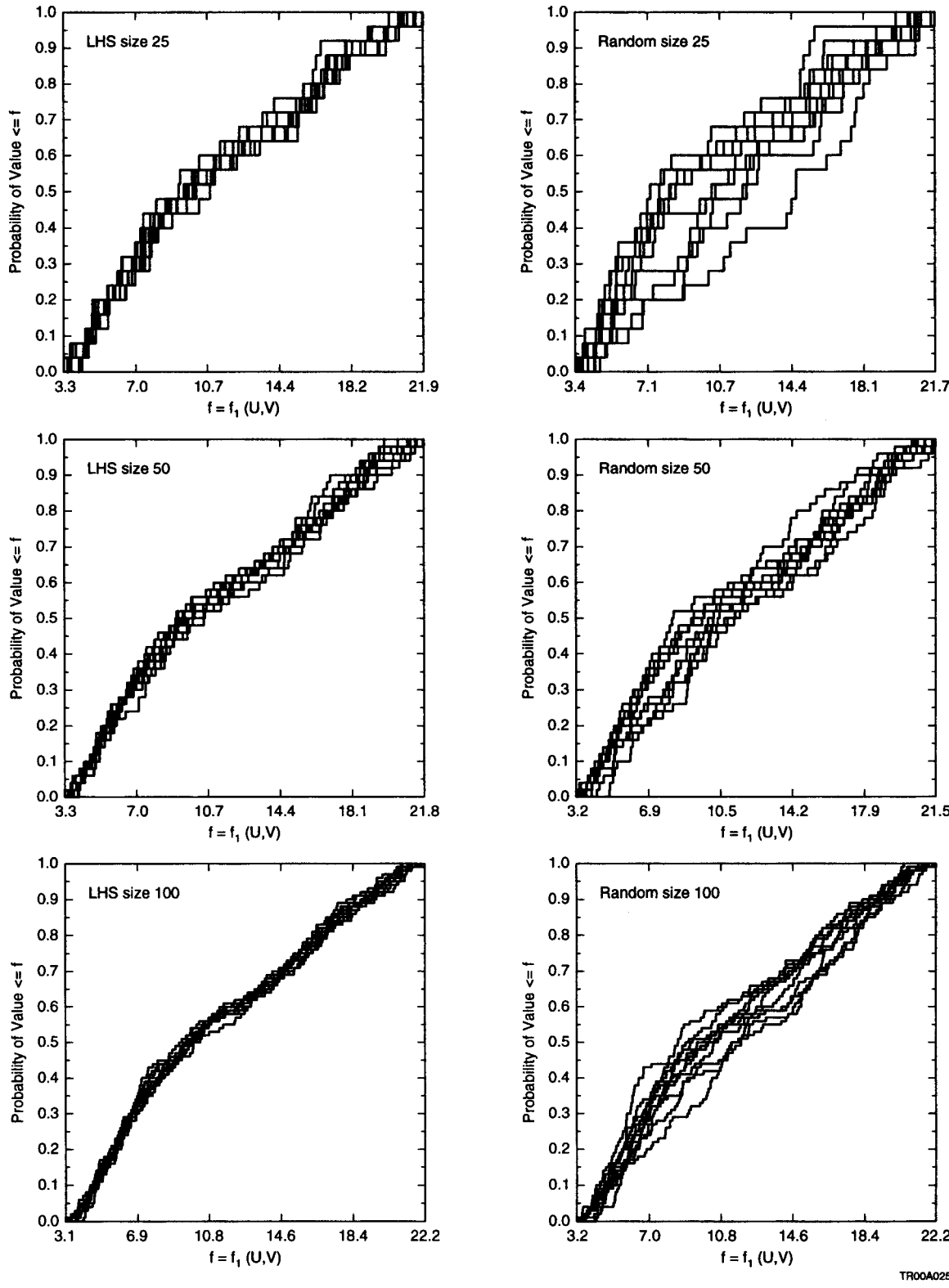

Fig. 4.1. Comparison of estimated CDFs for monotonic function $f_1(U, V)$ in Eq. (4.1) obtained with 10 replicated random and Latin hypercube samples of size 25, 50 and 100.

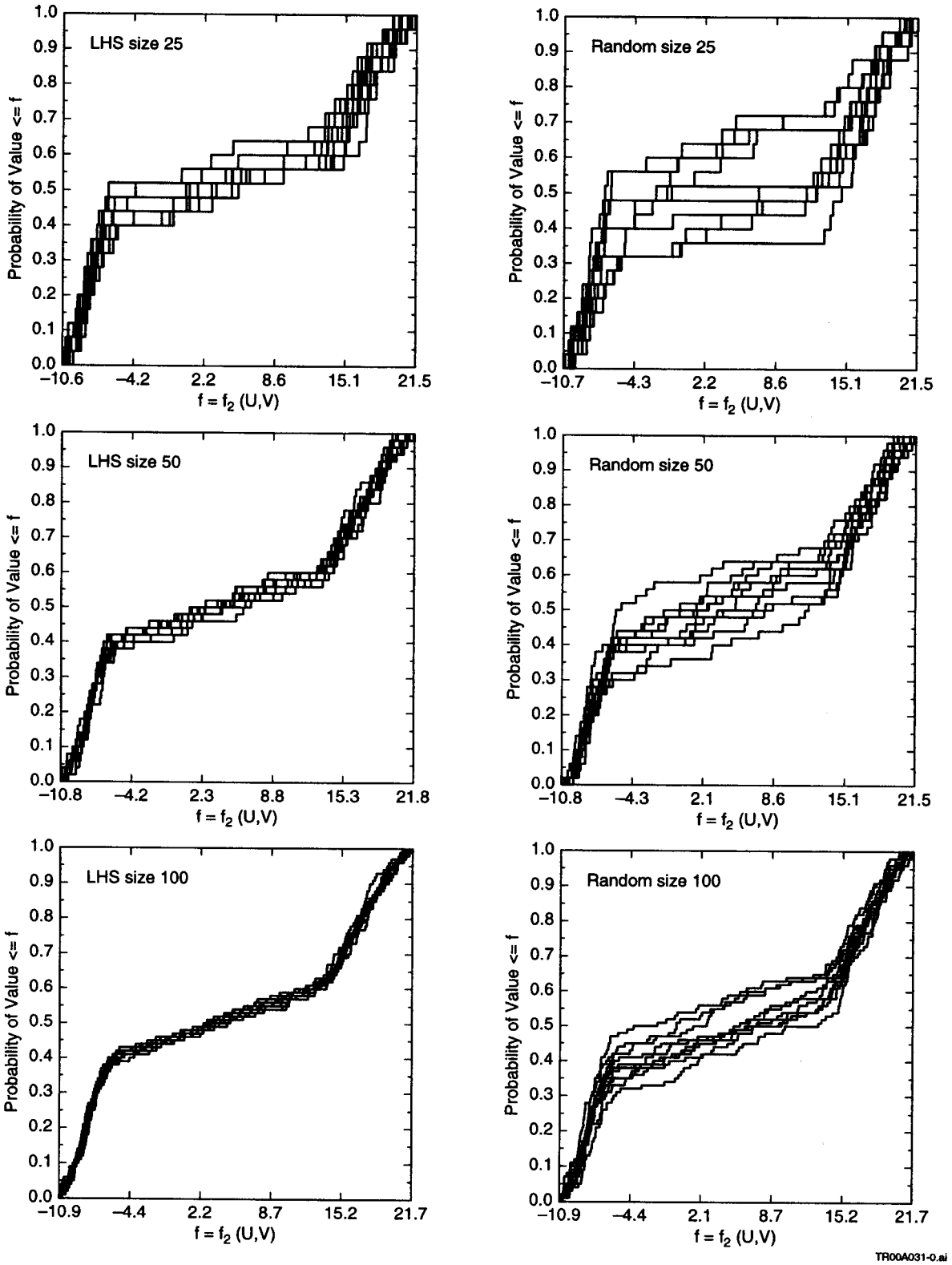

Fig. 4.2. Comparison of estimated CDFs for nonmonotonic function $f_2(U, V)$ in Eq. (4.2) obtained with 10 replicated random and Latin hypercube samples of size 25, 50 and 100.

5. Operations Involving Latin Hypercube Sampling

5.1 Correlation Control

As indicated in Eq. (1.2), the uncertainty in the inputs $x_1, x_2, \ldots, x_{nX}$ to an analysis can be represented by distributions $D_1, D_2, \ldots, D_{nX}$. If appropriate, correlations can also be specified between variables and form part of the definition of the corresponding probability space $(S_{su}, \mathcal{A}_{su}, p_{su})$. Given that $D_1, D_2, \ldots, D_{nX}$ are characterizing subjective uncertainty, correlations involving $x_1, x_2, \ldots, x_{nX}$ must in some sense derive from a belief that a particular value for one variable implies something about the possible values for one or more other variables (e.g., a low value for x_1 implies a high value for x_2, or a high value for x_3 implies a high value for x_5 and a low value for x_6), with the actual relationship being less strong than a strict functional dependence.

Two widely used possibilities exist for defining correlations between variables: the Pearson correlation coefficient (CC) and the Spearman rank correlation coefficient (RCC). For samples of the form in Eqs. (3.2) and (3.4), the CC between two variables, say x_j and x_k, is defined by

$$r_{x_j x_k} = \frac{\sum_{i=1}^{nS}(x_{ij}-\bar{x}_j)(x_{ik}-\bar{x}_k)}{\left[\sum_{i=1}^{nS}(x_{ij}-\bar{x}_j)^2\right]^{1/2}\left[\sum_{i=1}^{nS}(x_{ik}-\bar{x}_k)^2\right]^{1/2}}, \quad (5.1)$$

where

$$\bar{x}_j = \sum_{i=1}^{nS} x_{ij}/nS, \quad \bar{x}_k = \sum_{i=1}^{nS} x_{ik}/nS.$$

The CC takes on values between −1 and 1 and provides a measure of the strength of the linear relationship between two variables, with variables tending to increase and decrease together for positive and negative CCs, respectively, and with gradations in the absolute value of the CC between 0 and 1 corresponding to a trend from no linear relationship to an exact linear relationship.

The RCC is defined similarly to the CC but with rank-transformed data. Specifically, the smallest value of a variable is given a rank of 1; the next largest value is given a rank of 2; and so on up to the largest value, which is given a rank equal to the sample size nS. In the event of ties, average ranks are assigned. The RCC is then calculated in the same manner as the CC except for the use of rank-transformed data. Specifically,

$$R_{x_j x_k} = \frac{\sum_{i=1}^{nS}\left[R(x_{ij})-\bar{R}(x_j)\right]\left[R(x_{ik})-\bar{R}(x_k)\right]}{\left\{\sum_{i=1}^{nS}\left[R(x_{ij})-\bar{R}(x_j)\right]^2\right\}^{1/2}\left\{\sum_{i=1}^{nS}\left[R(x_{ik})-\bar{R}(x_k)\right]^2\right\}^{1/2}}, \quad (5.2)$$

where $R(x_{ij})$ and $R(x_{ik})$ denote the rank-transformed values of x_{ij} and x_{ik}, respectively, and $\bar{R}(x_j) = \bar{R}(x_k) = (nS+1)/2$. Like the CC, the RCC takes on values between −1 and 1 but provides a measure of the strength of the monotonic relationship between two variables.

In the authors' opinion, most individuals intuitively think in terms of RCCs rather than CCs when correlations are used in association with assessments of subjective uncertainty. In particular, what is usually possessed is some idea of the extent to which large and small values for one variable should be associated with large and small values for another variable. This is exactly the type of information that is quantitatively captured by RCCs. Therefore, this section will discuss the imposition of a rank correlation structure on random and LHSs.

An effective technique for imposing rank correlations has been proposed by Iman and Conover.[151] This technique has several desirable properties including (i) distribution independence in the sense that it can be applied to all types of distributions, (ii) simplicity in that no unusual mathematical techniques are required in its implementation, (iii) the stratification associated with Latin hypercube sampling is preserved, (iv) the marginal distributions for the individual sample variables are preserved, and (v) complex correlation structures involving many variables can be imposed on a sample.

The following discussion provides an overview of the Iman/Conover procedure for inducing a desired rank correlation structure on either a random or an LHS and is adapted from Sect. 3.2 of Helton.[216] The procedure begins with a sample of size m from the n input variables under consideration. This sample can be represented by the $m \times n$ matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix} \tag{5.3}$$

where x_{ij} is the value for variable j in sample element i. Thus, the rows of **X** correspond to sample elements, and the columns of **X** contain the sampled values for individual variables.

The procedure is based on rearranging the values in the individual columns of **X** so that a desired rank correlation structure results between the individual variables. For convenience, let the desired correlation structure be represented by the $n \times n$ matrix

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix} \tag{5.4}$$

where c_{kl} is the desired rank correlation between variables x_k and x_l.

Although the procedure is based on rearranging the values in the individual columns of **X** to obtain a new matrix **X*** that has a rank correlation structure close to that described by **C**, it is not possible to work directly with **X**. Rather, it is necessary to define a new matrix

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1n} \\ s_{21} & s_{22} & \cdots & s_{2n} \\ \vdots & \vdots & & \vdots \\ s_{m1} & s_{m2} & \cdots & s_{mn} \end{bmatrix} \tag{5.5}$$

that has the same dimensions as **X**, but is otherwise independent of **X**. Each column of **S** contains a random permutation of the m van der Waerden scores $\Phi^{-1}(i/m + 1)$, $i = 1, 2, \ldots, m$, where Φ^{-1} is the inverse of the standard normal distribution (Ref. 217, p. 317). The matrix **S** is then rearranged to obtain the correlation structure defined by **C**. This rearrangement is based on the Cholesky factorization of **C** (Ref. 218, p. 89). That is, a lower triangular matrix P is constructed such that

$$\mathbf{C} = \mathbf{P}\mathbf{P}^T. \tag{5.6}$$

This construction is possible because **C** is a symmetric, positive-definite matrix (Ref. 218, p. 88).

If the correlation matrix associated with **S** is the $n \times n$ identity matrix (i.e., if the correlations between the values in different columns of **S** are zero), then the correlation matrix for

$$\mathbf{S}^* = \mathbf{S}\mathbf{P}^T \tag{5.7}$$

is **C** (Ref. 219, p. 25). At this point, the success of the procedure depends on the following two conditions: (i) that the correlation matrix associated with **S** be close to the $n \times n$ identity matrix, and (ii) that the correlation matrix for **S*** be approximately equal to the rank correlation matrix for **S***. If these two conditions hold, then the desired matrix **X*** can be obtained by simply rearranging the values in the individual columns of **X** in the same rank order as the values in the individual columns of **S***. This is the first time that the variable values contained in **X** enter into the correlation process. When **X*** is constructed in this manner, it will have the same rank correlation matrix as **S***. Thus, the rank correlation matrix for **X*** will approximate **C** to the same extent that the rank correlation matrix for **S*** does.

The condition that the correlation matrix associated with **S** be close to the identity matrix is now considered. For convenience, the correlation matrix for **S** will be represented by **E**. Unfortunately, **E** will not always be the identity matrix. However, it is possible to make a correction for this. The starting point for this correction is the Cholesky factorization for **E**:

$$\mathbf{E} = \mathbf{Q}\mathbf{Q}^T. \tag{5.8}$$

This factorization exists because **E** is a symmetric, positive-definite matrix. The matrix **S*** defined by

$$\mathbf{S}^* = \mathbf{S}(\mathbf{Q}^{-1})^T\mathbf{P}^T \tag{5.9}$$

has **C** as its correlation matrix. In essence, multiplication of **S** by $(\mathbf{Q}^{-1})^T$ transforms **S** into a matrix whose associated correlation matrix is the $n \times n$ identity matrix; then, multiplication by $\mathbf{P}^T$ produces a matrix whose associated correlation matrix is **C**. As it is not possible to be sure that **E** will be an identity matrix, the matrix **S*** used in the procedure to produce correlated input should be defined in the corrected form shown in Eq. (5.9) rather than in the uncorrected form shown in Eq. (5.7).

The condition that the correlation matrix for **S*** be approximately equal to the rank correlation matrix for **S*** depends on the choice of the scores used in the definition of **S**. On the basis of empirical investigations, Iman and Conover[151] found that van der Waerden

scores provided an effective means of defining **S**, and these scores are incorporated into the rank correlation procedure in the widely used LHS program.[164] Other possibilities for defining these scores exist, but have not been extensively investigated. The user should examine the rank correlation matrix associated with $\mathbf{S}^*$ to ensure that it is close to the target correlation matrix **C**. If this is not the case, the construction procedure used to obtain $\mathbf{S}^*$ can be repeated until a suitable approximation to **C** is obtained. Results given in Iman and Conover[151] indicate that the use of van der Waerden scores leads to rank correlation matrices for $\mathbf{S}^*$ that are close to the target matrix **C**.

As a single example, the effects of imposing rank correlations of 0.00, 0.25, 0.50, 0.75, 0.90 and 0.99 on a pair of variables are shown in Fig. 5.1. The results of various rank-correlation assumptions with a variety of marginal distributions are illustrated by Iman and Davenport.[220, 221]

The control of orthogonality and the induction of correlations within LHSs are areas of much research interest, and a number of results exist in this area in addition to the original Iman and Conover rank correlation techniques discussed in this section.[222-240]

5.2 Reweighting of Samples

Once a sampling-based uncertainty study has been performed, it is sometimes necessary to assess the effects that arise from changed definitions for the distributions $D_1, D_2, \ldots, D_{nX}$ in Eq. (1.2). If the model under consideration is expensive to evaluate, it is desirable to perform this assessment without reevaluating (i.e., rerunning) the model. When the distributions but not the ranges of the variables change, this assessment can be carried out with a reweighting technique developed by Iman and Conover.[241]

Latin hypercube sampling as described in Sect. 3.1 is based on dividing the range of each variable into nS intervals of equal probability, where nS is the sample size. The Iman/Conover reweighting technique is based on a generalization of Latin hypercube sampling that involves the division of variable ranges into intervals of unequal probability.

For this generalization of an LHS size nS from the variables $x_1, x_2, \ldots, x_{nX}$, the range of each variable x_j is divided into nS mutually exclusive intervals I_{ij}, $i = 1, 2, \ldots, nS$, and one value x_{ij}, $i = 1, 2, \ldots, nS$, of x_j is randomly selected from each interval I_{ij}. The preceding variable values (i.e., x_{ij}, $i = 1, 2, \ldots, nS, j = 1, 2, \ldots, nX$) are now used as described in Sect. 3.1 to generate an LHS. Specifically, the nS values for x_1 are randomly paired without replacement with the nS values for x_2. The resultant nS pairs are randomly combined without replacement with the nS values for x_3 to produce nS triples. This process is continued until nS nX-tuples are produced, with these nX-tuples constituting the LHS

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, \ldots, x_{i,nX} \right], \; i = 1, 2, \ldots, nS. \tag{5.10}$$

The preceding division of the ranges of the variables into the intervals I_{ij} produces a corresponding division of $\mathcal{S}_{su}$ into nS^{nX} cells. Specifically, each cell is of the form

$$C_{\mathbf{n}} = I_{k1} \times I_{l2} \times \cdots \times I_{m,nX}, \tag{5.11}$$

where $\mathbf{n} = [k, l, \ldots, m]$ is a vector of nX integers between 1 and nS that designates one of the nS^{nX} mutually exclusive cells into which $\mathcal{S}_{su}$ has been partitioned. Further, the probability $prob(C_{\mathbf{n}})$ of $C_{\mathbf{n}}$ can be calculated from the definition of $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. For example,

$$prob(C_{\mathbf{n}}) = prob(I_{k1})\, prob(I_{l2}) \cdots prob(I_{m,nX}) \tag{5.12}$$

if the x_js are independent.

Theorem 5.1. If $\mathbf{x}_i$, $i = 1, 2, \ldots, nS$, is an LHS of the form indicated in Eq. (5.10), $C_{\mathbf{n}_i}$, $i = 1, 2, \ldots, nS$, designates the cell in Eq. (5.11) that contains $\mathbf{x}_i$, $\mathbf{f}$ is the function in Eq. (1.1), and g is an arbitrary function, then

$$T = \sum_{i=1}^{nS} nS^{nX-1}\, prob\left(C_{\mathbf{n}_i}\right) g[\mathbf{f}(\mathbf{x}_i)] \tag{5.13}$$

is an unbiased estimator of the expected value of $g[\mathbf{f}(\mathbf{x})]$ (Theorem 1, p. 1760, Ref. 241).

The preceding result reduces to the unbiasedness of the estimator in Eq. (3.5) when Latin hypercube sampling with equal probability intervals is used (i.e., $prob(C_{\mathbf{n}_i}) = 1/nS^{nX}$) and $\mathbf{f}(\mathbf{x}_i)$ is real valued (i.e., $y_i = \mathbf{f}(\mathbf{x}_i)$). The importance of Theorem 5.1 is that it allows a recalculation of expected values, moments and distribution functions that result from changed distribution assumptions without a rerunning of the model under consideration. Specifically, the same values for $g[\mathbf{f}(\mathbf{x}_i)]$ are used in conjunction with new values for $prob(C_{\mathbf{n}_i})$

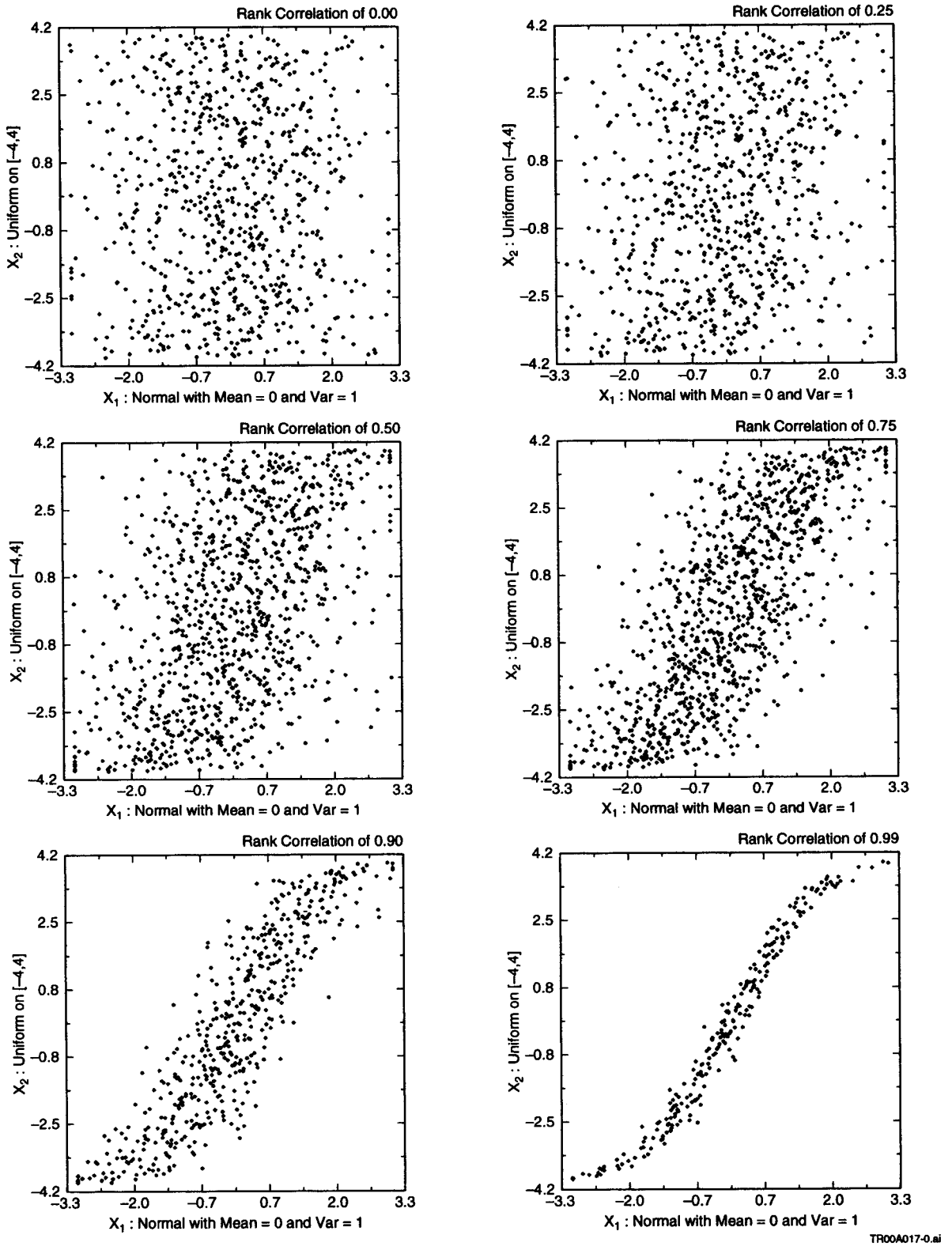

Fig. 5.1. Examples of rank correlations of 0.00, 0.25, 0.50, 0.75, 0.90 and 0.99 imposed with the Iman/Conover restricted pairing technique for an LHS of size $nS = 1000$.

calculated for the changed distributions for the elements of **x**. A related result is given by Beckman and McKay.[242]

5.3 Replication of Samples

A brief overview of the variability in statistics obtained with Latin hypercube sampling is given in Sect. 3.2. The variability results when the same quantity is repeatedly estimated with independently generated samples of the same size. In essence, this variability is a measure of the numerical error in using a sampling-based (i.e., Monte Carlo) procedure in the estimation of an integral. Unfortunately, the theoretical results indicated in Sect. 3.2 do not lead in any convenient way to error estimates in real analyses.

In practice, a replicated sampling procedure proposed by R.L. Iman[243] provides a more effective approach to estimating the potential sampling error in quantities derived from Latin hypercube sampling. With this procedure, the LHS in Eq. (3.4) is repeatedly generated with different random seeds. These samples are used to produce a sequence of values T_r, $r = 1, 2, \ldots, nR$, for the statistic T in Eq. (3.5), where nR is the number of replicated samples. Then,

$$\bar{T} = \sum_{r=1}^{nR} T_r / nR \tag{5.14}$$

and

$$SE(\bar{T}) = \left[\sum_{r=1}^{nR} (T_r - \bar{T})^2 / nR(nR-1) \right]^{1/2} \tag{5.15}$$

provide an additional estimate for T and an estimate of the standard error for this estimate of T. The t-distribution with $nR-1$ degrees of freedom can be used to obtain a confidence interval for the estimate for $\bar{T}$. Specifically, the $1 - \alpha$ confidence interval is given by $\bar{T} \pm t_{1-\alpha/2} SE(\bar{T})$, where $t_{1-\alpha/2}$ is the $1 - \alpha/2$ quantile of the t-distribution with $nR - 1$ degrees of freedom (e.g., $t_{1-\alpha/2} = 2.262$ for $\alpha = 0.05$ and $nR = 10$; Ref. 217, Table A25).

As an example, 0.95 confidence intervals for the cumulative probabilities associated with individual values in the range of the function f_1 defined in Eq. (4.1) are shown in Fig. 5.2, with the 10 replicated LHSs producing narrower confidence intervals than the 10 random samples. The confidence intervals in Fig. 5.2 were calculated for individual values on the abscissa and then connected to obtain the confidence-interval curves (i.e., the curves of upper and lower bounds). Thus, the confidence intervals apply to individual cumulative probabilities rather than to an entire CDF.

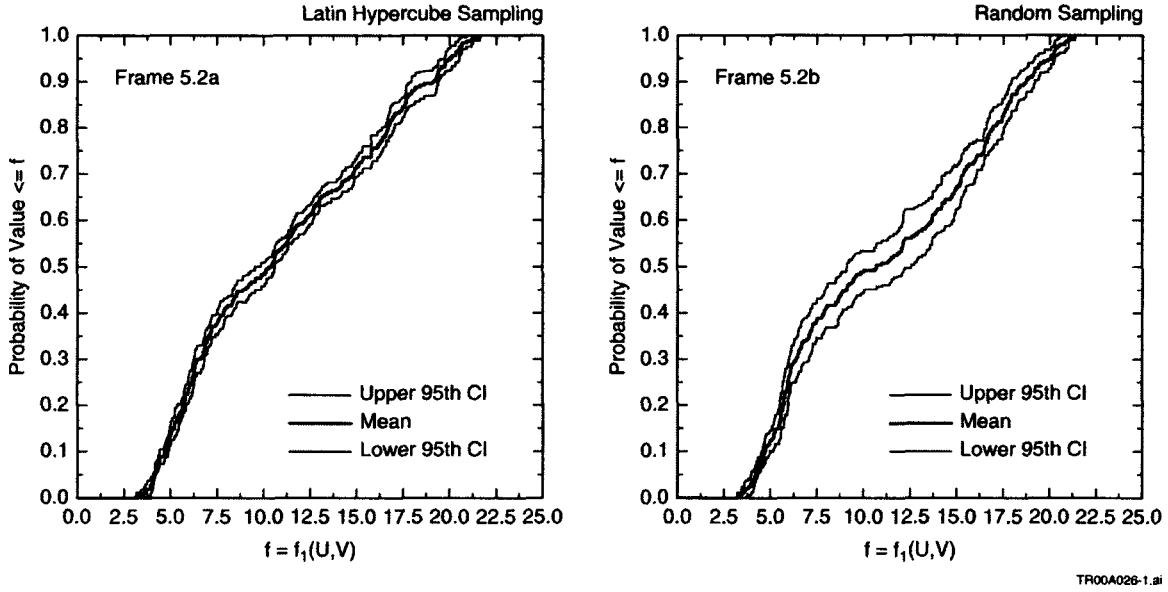

Fig. 5.2. Upper and lower bounds on 0.95 confidence intervals (CIs) for cumulative probabilities associated with function $f_1(U, V)$ in Eq. (4.1) obtained from $nR = 10$ samples of size $nS = 25$ each (see Fig. 4.1 for CDFs): (a) Latin hypercube sampling, and (b) random sampling.

6. Example Uncertainty and Sensitivity Analysis

An example uncertainty and sensitivity analysis involving a model for two-phase fluid flow follows. The analysis problem is briefly described (Sect. 6.1), and then techniques for the presentation of uncertainty analysis results are described and illustrated (Sect. 6.2). The section then concludes with illustrations of various sensitivity analysis procedures, including examination of scatterplots (Sect. 6.3), regression-based techniques (Sect. 6.4), and searches for nonrandom patterns (Sect. 6.5).

6.1 Analysis Problem

The following examples use results from an uncertainty and sensitivity analysis of a large model for two-phase fluid flow (Ref. 244, Chapts. 7, 8; Refs. 245-247) carried out in support of the 1996 CCA for the WIPP, which is being developed by the DOE for the geologic (i.e., deep underground) disposal of transuranic radioactive waste.[189, 248] The indicated model involves the numerical solution of a system of nonlinear partial differential equations and is implemented by the BRAGFLO program (Sect. 4.2, Ref. 244; Ref. 245).

The 1996 WIPP PA considered $nX = 57$ uncertain inputs (Table 6.1), of which 31 were used in the two-phase flow analysis and 26 were used in other parts of the PA (see Sect. 7). The distributions assigned to these variables (Fig. 6.1) are intended to characterize subjective uncertainty, correspond to the distributions in Eq. (1.2), and define the probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$.

Latin hypercube sampling was used to generate $nR = 3$ replicated samples of size $nS = 100$ each (Sect. 5.3) for a total of 300 sample elements. For convenience, these replicates are referred to as R1, R2 and R3, respectively. The Iman/Conover restricted pairing technique (Sect. 5.1) was used to induce specified rank correlations for three pairs of variables (Table 6.1) and to keep correlations between all other variables close to zero (Table 6.2).

As is typical of most studies of real systems, the original analysis involved a large number of dependent variables, of which only 11 will be used for illustration in this section (Table 6.3). The variables in Table 6.3 were calculated for three distinct sets of conditions designated by E0, E1 and E2 in the 1996 WIPP PA, where E0 corresponds to undisturbed conditions (i.e., no human disruption of the repository), E1 corresponds to a single drilling intrusion through the repository that penetrates an area of pressurized brine in a geologic formation beneath the repository, and E2 corresponds to a single drilling intrusion through the repository that does not penetrate pressurized brine.

6.2 Uncertainty Analysis

In this example, the model predictions are functions rather than single numbers as indicated in conjunction with Fig. 1.1. The distributions of curves in Fig. 6.2 constitute one way of displaying the uncertainty in these functions that results from uncertainty in model input. However, the model predictions at individual times are real valued and thus can be displayed as CDFs or CCDFs. A popular presentation format[250] is to display estimates for the CDF, the corresponding density function, and the mean in a single plot (Fig. 6.3).

For distributions of curves such as those in Fig. 6.2, summaries can be obtained by plotting mean and percentile values of the dependent variable for individual values on the abscissa (Fig. 6.4). Conceptually, a vertical line is drawn through a point on the abscissa and the curves above this point. If a sample of size nS is involved, this results in selecting nS values for the dependent variable (i.e., the nS values above the point on the abscissa). These values can then be used to estimate a mean, a median, and various percentiles. Connecting these estimates for a sequence of values on the abscissa produces summary plots of the form shown in Fig. 6.4.

The purpose of replicating the LHS in this example was to obtain an indication of the stability of the resultant distribution estimates with an LHS of size 100. In this analysis, these estimates were quite stable (e.g., Fig. 6.5). Similar stability has also been observed in other studies.[32, 170, 251, 252]

Presentation of multiple plots of the form illustrated in Fig. 6.3 can be cumbersome when a large number of predicted variables is involved. When these variables have the same units, box plots provide a way to present a compact summary of multiple distributions (Fig. 6.6). In this summary, the endpoints of the boxes are formed by the lower and upper quartiles of the data, that is, $x_{0.25}$ and $x_{0.75}$. The vertical line within the box represents the median, $x_{0.50}$. The mean is identified by the large dot. The bar on the right of the box extends to the minimum of $x_{0.75} + 1.5\ (x_{0.75} - x_{0.25})$ and the maximum value. In a similar manner, the bar on the left of the box extends to the maximum of $x_{0.25} - 1.5\ (x_{0.75} - x_{0.25})$ and the minimum value. The observations falling outside of these bars are shown in crosses. The

Table 6.1. Example Elements of $\mathbf{x}_{SU}$ in the 1996 WIPP PA (see Table 5.1, Ref. 244, Table 1, Ref. 249 and App. PAR, Ref. 189 for complete listings of the $nV = 57$ elements of $\mathbf{x}_{SU}$ and sources of additional information)

ANHBCEXP—Brooks-Corey pore distribution parameter for anhydrite (dimensionless). Distribution: Student's with 5 degrees of freedom. Range: 0.491 to 0.842. Mean, Median: 0.644.

ANHBCVGP—Pointer variable for selection of relative permeability model for use in anhydrite. Used in BRAGFLO. See *ANHBCEXP*. Distribution: Discrete with 60% 0, 40% 1. Value of 0 implies Brooks-Corey model; value of 1 implies van Genuchten-Parker model.

ANHCOMP—Bulk compressibility of anhydrite (Pa^{-1}). Distribution: Student's with 3 degrees of freedom. Range: 1.09×10^{-11} to 2.75×10^{-10} Pa^{-1}. Mean, Median: 8.26×10^{-11} Pa^{-1}. Correlation: –0.99 rank correlation with *ANHPRM*.

ANHPRM—Logarithm of intrinsic anhydrite permeability (m^2). Distribution: Student's with 5 degrees of freedom (see Figure 6.1a). Range: –21.0 to –17.1 (i.e., permeability range is 1×10^{-21} to $1 \times 10^{-17.1}$ m^2). Mean, Median: –18.9. Correlation: –0.99 rank correlation with *ANHCOMP*.

BHPRM—Logarithm of intrinsic borehole permeability (m^2). Distribution: Uniform. Range: –14 to –11 (i.e., permeability range is 1×10^{-14} to 1×10^{-11} m^2). Mean, median: –12.5.

BPCOMP—Logarithm of bulk compressibility of brine pocket (Pa^{-1}). Distribution: Triangular. Range: –11.3 to –8.00 (i.e., bulk compressibility range is $1 \times 10^{-11.3}$ to 1×10^{-8} Pa^{-1}). Mean, mode: –9.80, –10.0. Correlation: –0.75 rank correlation with *BPPRM*.

BPPRM—Logarithm of intrinsic brine pocket permeability (m^2). Distribution: Triangular. Range: –14.7 to –9.80 (i.e., permeability range is $1 \times 10^{-14.7}$ to $1 \times 10^{-9.80}$ m^2). Mean, mode: –12.1, –11.8. Correlation: –0.75 with *BPCOMP*.

HALCOMP—Bulk compressibility of halite (Pa^{-1}). Distribution: Uniform. Range: 2.94×10^{-12} to 1.92×10^{-10} Pa^{-1}. Mean, median: 9.75×10^{-11} Pa^{-1}, 9.75×10^{-11} Pa^{-1}. Correlation: –0.99 rank correlation with *HALPRM*.

HALPOR—Halite porosity (dimensionless). Used in BRAGFLO. Distribution: Piecewise uniform (see Fig. 6.1b). Range: 1.0×10^{-3} to 3×10^{-2}. Mean, median: 1.28×10^{-2}, 1.00×10^{-2}.

HALPRM—Logarithm of halite permeability (m^2). Distribution: Uniform. Range: –24 to –21 (i.e., permeability range is 1×10^{-24} to 1×10^{-21} m^2). Mean, median: –22.5, –22.5. Correlation: –0.99 rank correlation with *HALCOMP*.

SALPRES—Initial brine pressure, without the repository being present, at a reference point located in the center of the combined shafts at the elevation of the midpoint of MB 139 (Pa). Distribution: Uniform. Range: 1.104×10^7 to 1.389×10^7 Pa. Mean, median: 1.247×10^7 Pa, 1.247×10^7 Pa.

SHRBRSAT—Residual brine saturation in shaft (dimensionless). Distribution: Uniform. Range: 0 to 0.4. Mean, median: 0.2, 0.2.

SHRGSSAT—Residual gas saturation in shaft (dimensionless). Distribution: Uniform. Range: 0 to 0.4. Mean, median: 0.2, 0.2.

WASTWICK—Increase in brine saturation of waste due to capillary forces (dimensionless). Distribution: Uniform. Range: 0 to 1. Mean, median: 0.5, 0.5.

Table 6.1. Example Elements of $\mathbf{x}_{su}$ in the 1996 WIPP PA (see Table 5.1, Ref. 244, Table 1, Ref. 249 and App. PAR, Ref. 189 for complete listings of the $nV = 57$ elements of $\mathbf{x}_{su}$ and sources of additional information) (continued)

WGRCOR—Corrosion rate for steel under inundated conditions in the absence of CO_2 (m/s). Distribution: Uniform. Range: 0 to 1.58×10^{-14} m/s. Mean, median: 7.94×10^{-15} m/s, 7.94×10^{-15} m/s.

WGRMICI—Microbial degradation rate for cellulose under inundated conditions (mol/kg s). Distribution: Uniform. Range: 3.17×10^{-10} to 9.51×10^{-9} mol/kg s. Mean, median: 4.92×10^{-9} mol/kg s, 4.92×10^{-9} mol/kg s. Variable 3 in LHS.

WMICDFLG—Pointer variable for microbial degradation of cellulose. Distribution: Discrete, with 50% 0, 25% 1, 25% 2.

WMICDFLG = 0, 1, 2 implies no microbial degradation of cellulose, microbial degradation of only cellulose, microbial degradation of cellulose, plastic and rubber.

WPRTDIAM—Waste particle diameter (m). Distribution: Loguniform. Range: 4.0×10^{-5} to 2.0×10^{-1} m. Mean, median: 2.35×10^{-2} m, 2.80×10^{-2} m.

WRGSSAT—Residual gas saturation in waste (dimensionless). Distribution: Uniform. Range: 0 to 0.15. Mean, median: 0.075, 0.075.

WTAUFAIL—Shear strength of waste (Pa). Distribution: Uniform. Range: 0.05 to 10 Pa. Mean, median: 5.03 Pa, 5.03 Pa.

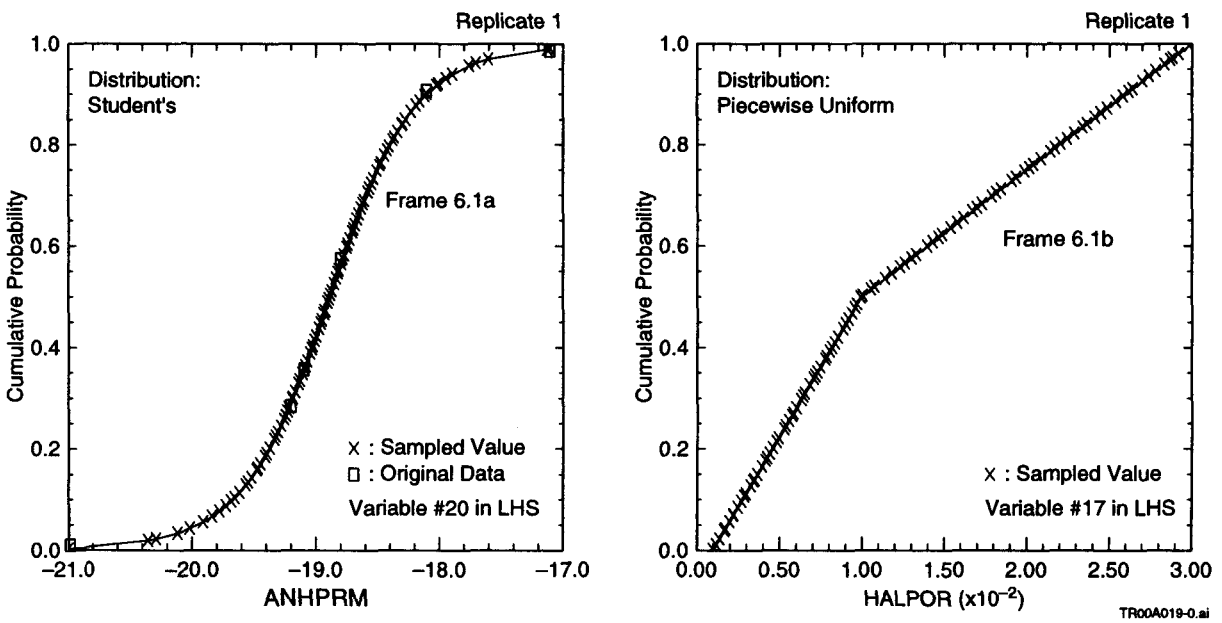

Fig. 6.1. Distributions used to characterize subjective uncertainty in *ANHPRM* and *HALPOR* in 1996 WIPP PA (see Appendix, Ref. 244), for distributions assigned to all uncertain variables included in 1996 WIPP PA).

Table 6.2. Example Rank Correlations in the LHS that Constitutes Replicate R1 in the 1996 WIPP PA

WGRCOR	1.0000							
WMICDFLG	0.0198	1.0000						
HALCOMP	0.0011	0.0235	1.0000					
HALPRM	–0.0068	–0.0212	–0.9879	1.0000				
ANHCOMP	0.0080	0.0336	–0.0123	–0.0025	1.0000			
ANHPRM	0.0049	–0.0183	0.0037	0.0113	–0.9827	1.0000		
BPCOMP	0.0242	0.1071	–0.0121	0.0057	–0.0184	0.0078	1.0000	
BPPRM	–0.0514	–0.0342	0.0035	0.0097	0.0283	–0.0202	–0.7401	1.0000
	WGRCOR	*WMICDFLG*	*HALCOMP*	*HALPRM*	*ANHCOMP*	*ANHPRM*	*BPCOMP*	*BPPRM*

Table 6.3. Predicted Variables (i.e., elements of **y** in Eq. (1.1)) Used to Illustrate Uncertainty and Sensitivity Analysis Results for Two-Phase Fluid Flow Model (see Table 7.1.1, Ref. 244, for additional information)

BRAALIC:	Cumulative brine flow (m^3) from anhydrite marker beds into disturbed rock zone (DRZ) surrounding repository (i.e., *BRAABNIC* + *BRAABSIC* + *BRM38NIC* + *BRM38SIC* + *BRM39NIC* + *BRM39SIC*)
BRAABNIC:	Cumulative brine flow (m^3) out of anhydrite marker beds A and B into north end of DRZ
BRAABSIC:	Same as *BRAABNIC* but into south end of DRZ
BRM38NIC:	Cumulative brine flow (m^3) out of anhydrite marker bed 138 into north end of DRZ
BRM38SIC:	Same as *BRM38NIC* but into south end of DRZ
BRM39NIC:	Cumulative brine flow (m^3) out of anhydrite marker bed 139 into north end of DRZ
BRM39SIC:	Same as *BRM39NIC* but into south end of DRZ
BRNREPTC:	Cumulative brine flow (m^3) into repository from all sources
GAS_MOLE:	Cumulative gas production (mole) in repository due to corrosion of iron and microbial degradation of cellulose
PORVOL_T:	Total pore volume (m^3) in repository
WAS_SATB:	Brine saturation (dimensionless) in lower waste panel (i.e., the southern waste panel, which in the numerical implementation of the analysis is the waste panel that is penetrated by a drilling for the E1 and E2 scenarios)

flattened shape of box plots makes it possible to summarize multiple distributions in a small area and also facilitates comparisons of these distributions.

6.3 Examination of Scatterplots

The simplest sensitivity analysis procedure is an examination of the scatterplots associated with individual sampled variables and the particular model prediction under consideration (see Eq. (2.7)). If a variable has a substantial effect on the model prediction, then this will result in a discernible pattern in the corresponding scatterplot (Fig. 6.7); in contrast, little or no pattern will appear in the scatterplot in the absence of an effect. Further, the examination of multiple scatterplots can reveal interactions in the effects of variables. For example, large values of *WAS_SATB* tend to be associated with large values of *BHPRM* (Fig. 6.7a); however, given the occurrence of a large value for *BHPRM*, the resultant value for *WAS_SATB* is determined primarily by *WRGSSAT* (Fig. 6.7b). Latin hypercube sampling is a particularly effective procedure for the generation of scatterplots due to its full stratification across the range of each sampled variable.

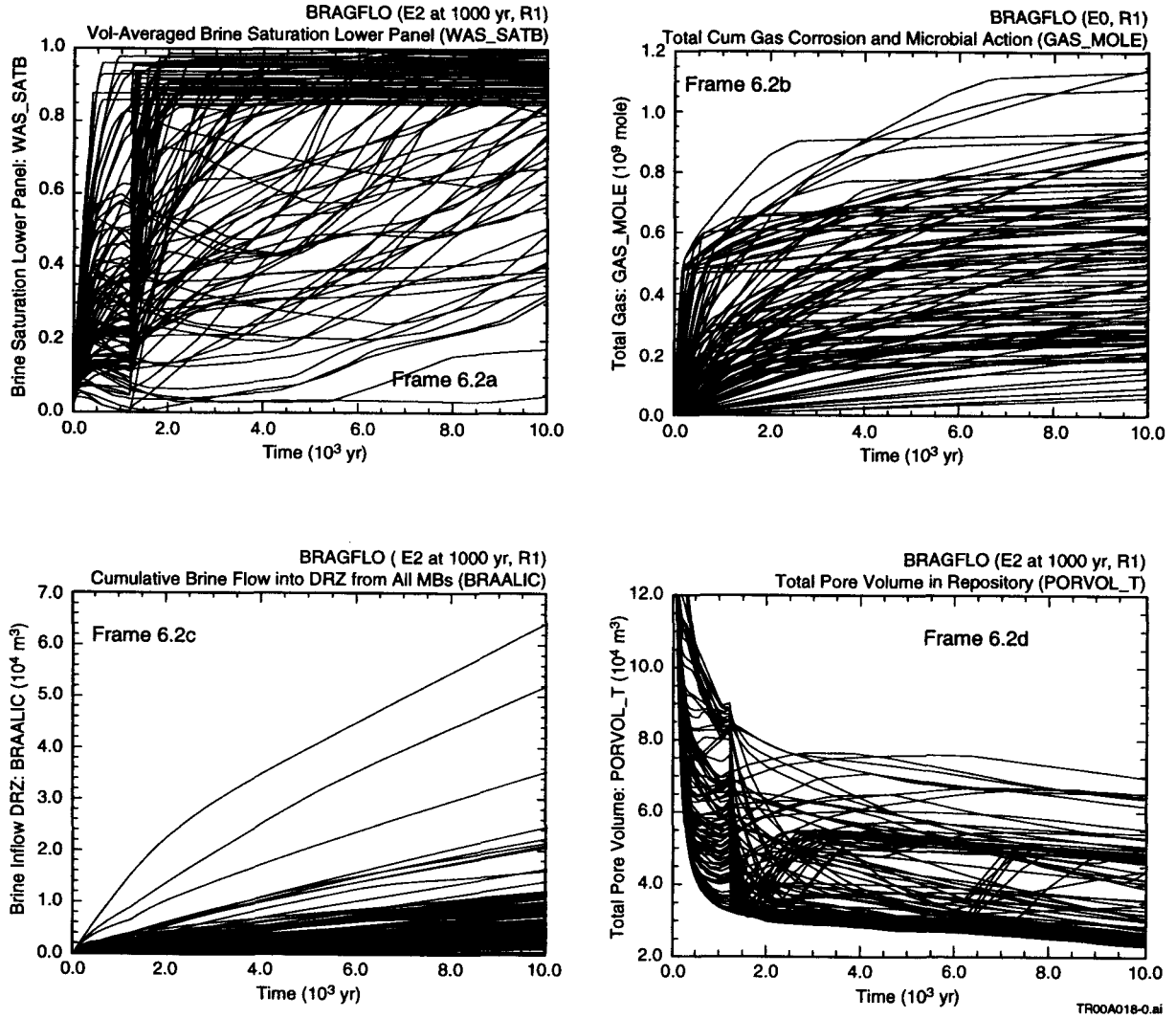

Fig. 6.2. Time-dependent results used to illustrate sensitivity analysis techniques: (a) saturation in lower waste panel with an E2 intrusion at 1000 yr (*E2: WAS_SATB*), (b) total cumulative gas generation due to corrosion and microbial degradation of cellulose under undisturbed (i.e., E0) conditions (*E0: GAS_MOLE*), (c) cumulative brine flow into disturbed rock zone (DRZ) surrounding repository with an E2 intrusion at 1000 yr (*E2: BRAALIC*); and (d) total pore volume in repository with an E2 intrusion at 1000 yr (*E2: PORVOL_T*).

6.4 Regression-Based Techniques

A more sophisticated approach to sensitivity analysis is to use formal search procedures to identify specific patterns in the mapping in Eq. (2.3). For example, regression-based techniques are often effective in identifying linear relationships and relationships that can be made linear by a suitable transformation (Ref. 216, Sect. 3.5). Stepwise regression analysis provides an efficient and informative way to carry out a regression-based sensitivity analysis, with variable importance being indicated by the order in which variables are selected in the stepwise procedure, the changes in R^2 values that occur as individual variables are added to the regression model, and the size of the standardized regression coefficients (SRCs) for the variables included in the regression model. When the relationships between the sampled and predicted variables are nonlinear but monotonic, the rank transformation[253] is often effective in linearizing the underlying relationships and thus facilitating the use of regression-based techniques.

As an example, stepwise regression analyses for y = *E0:GAS_MOLE* and y = *E2:BRAALIC* with raw and rank-transformed data are presented in Table 6.4. For *E0:GAS_MOLE*, similar results are obtained with raw

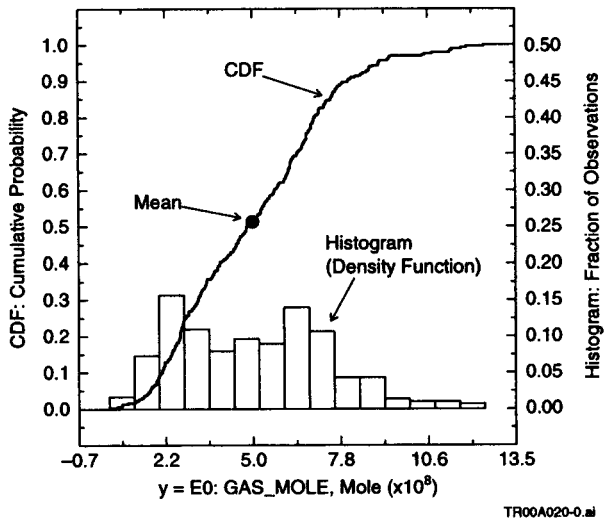

Fig. 6.3. Presentation of estimated CDF, mean, and density function for y = *E0:GAS_MOLE* at 10,000 yr.

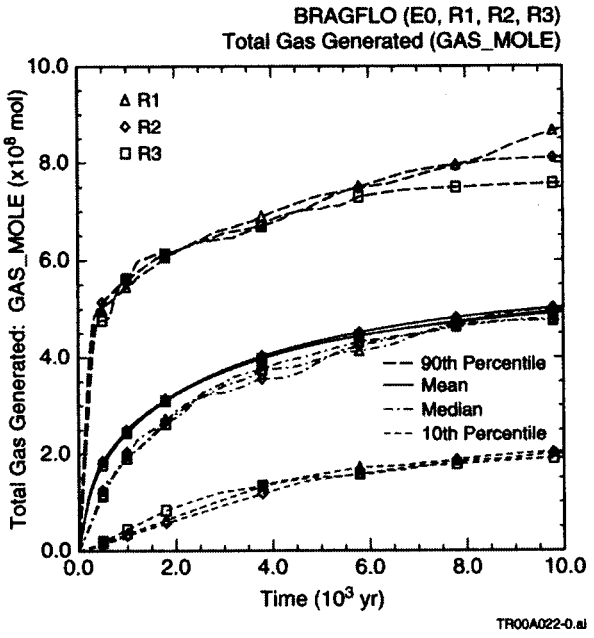

Fig. 6.5. Individual mean and percentile curves for y = *E0:GAS_MOLE* for replicates R1, R2 and R3.

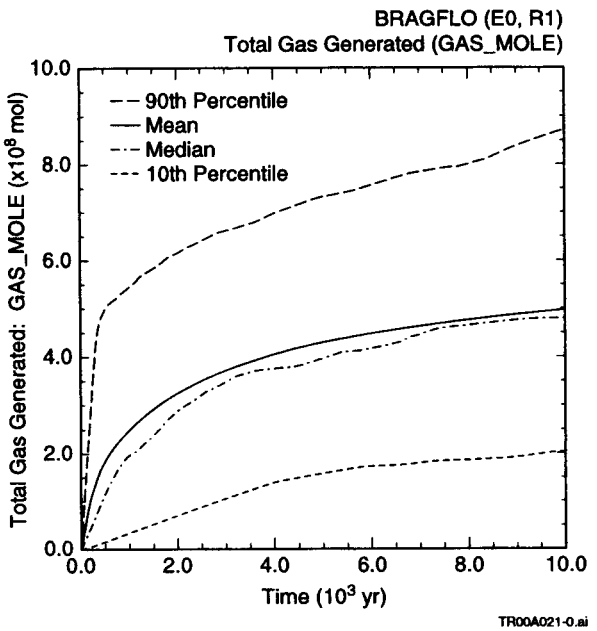

Fig. 6.4. Mean and percentile curves for y = *E0:GAS_MOLE* for replicate R1.

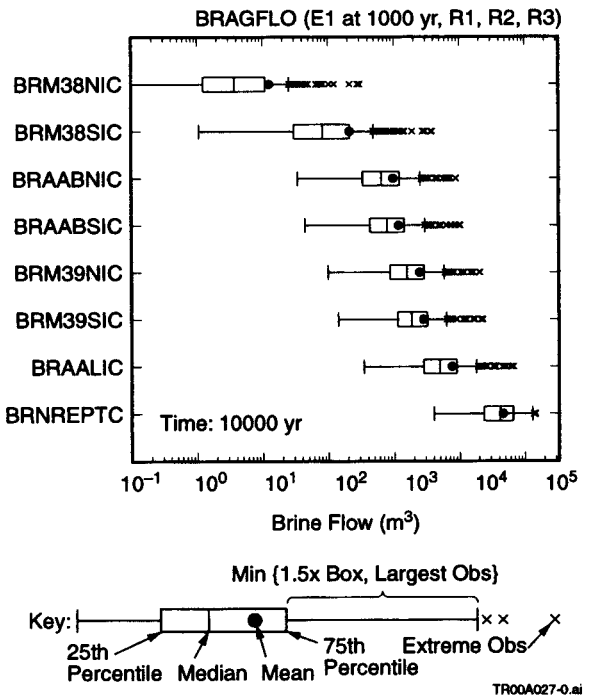

Fig. 6.6. Use of box plots to summarize cumulative brine flows over 10,000 yr in the vicinity of the repository for an E1 intrusion at 1000 yr into lower waste panel (see Table 6.3 for a description of individual variables).

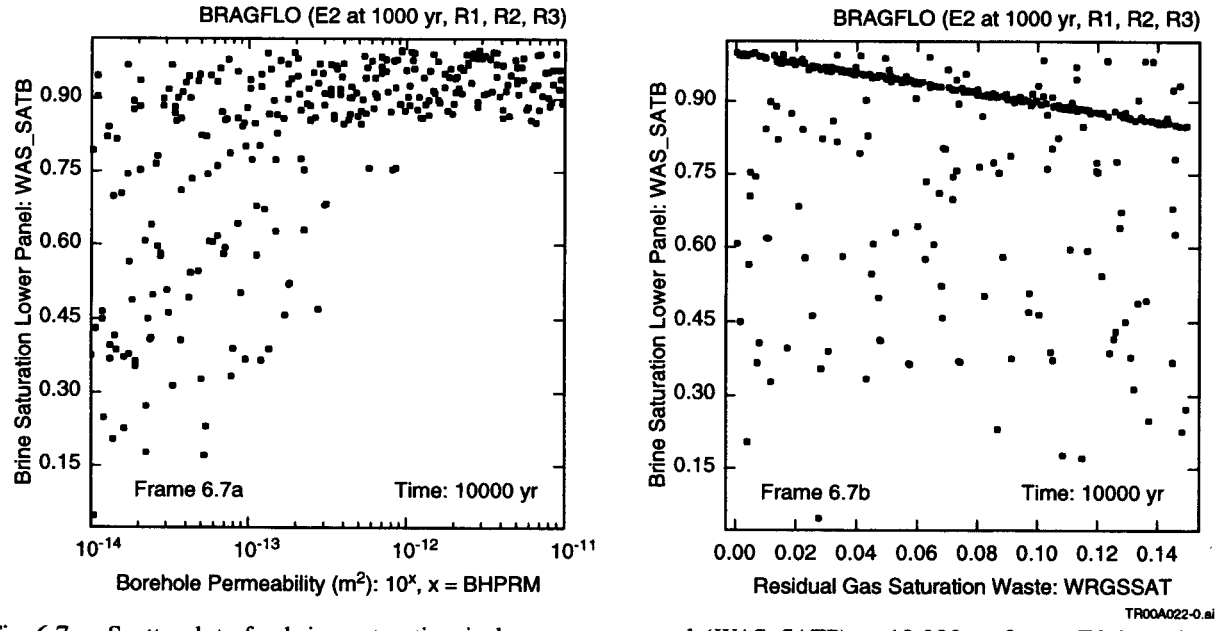

Fig. 6.7. Scatterplots for brine saturation in lower waste panel (*WAS_SATB*) at 10,000 yr for an E2 intrusion at 1000 yr into lower waste panel versus *BHPRM* and *WRGSSAT*.

and rank-transformed data (i.e., the same variables are selected in both analyses and the final regression models have R^2 values of 0.85 and 0.82, respectively). For *E2:BRAALIC*, the use of rank-transformed data considerably improves the resolution of the analysis and produces a final regression model with six variables and an R^2 value of 0.90; in contrast, the use of raw data produces a final regression model with three variables and an R^2 value of 0.62.

An alternative to regression analysis is to calculate correlation coefficients (CCs) or partial correlation coefficients (PCCs) between sampled and predicted variables (Ref. 216, Sect. 3.5). As with regression analysis, these coefficients can be calculated with raw or rank-transformed data, with the latter case producing rank correlation coefficients (RCCs) and partial rank correlation coefficients (PRCCs). When the variables within the sample are independent (i.e., orthogonal), CCs and SRCs are equal, as is also the case for RCCs and standardized rank regression coefficients (SRRCs). Similar, but not entirely equivalent, measures of variable importance are given by SRCs and PCCs. Specifically, SRCs characterize the effect on the output variable that results from perturbing an input variable by a fixed fraction of its standard deviation, and PCCs characterize the strength of the linear relationship between an input and output variable after a correction has been made for the linear effects of the other input variables. Similar interpretations apply to SRRCs and PRCCs for rank-transformed variables. Although SRCs and PCCs are not equal, use of their absolute values to order variable importance produces identical importance orderings when the values for the individual variables within the sample are independent, as is also the case for SRRCs and PRCCs.

As in Fig. 6.2, model predictions are often time dependent. When this is the case, presenting stepwise regression analyses at multiple times in the format used in Table 6.4 can become quite unwieldy. In such situations, a more compact alternative is to present plots of time-dependent coefficients (Fig. 6.8). In particular, the coefficients are calculated at multiple times and then the coefficients for individual variables are connected to obtain the curves in Fig. 6.8. This presentation format is relatively compact and also displays how variable importance changes with time.

6.5 Searches for Nonrandom Patterns

Regression-based techniques are not always successful in identifying the relationships between sampled variables and model predictions. As an example, the regression analyses with raw and rank-transformed data in Table 6.5 perform poorly, with the final regression models having R^2 values of 0.33 and 0.20. Given the low R^2 values, there is little reason to believe that the variable orderings are meaningful or even that all the influential variables have been identified.

Table 6.4. Stepwise Regression Analyses with Raw and Rank-Transformed Data with Pooled Results from Replicates R1, R2 and R3 (i.e., for a total of 300 observations) for Output Variables *E0:GAS_MOLE* and *E2:BRAALIC* at 10,000 yr

	Raw Data: y = *E0:GAS_MOLE*			Rank-Transformed Data: y = *E0:GAS_MOLE*		
Step[a]	Variable[b]	SRC[c]	R^{2d}	Variable[b]	SRRC[e]	R^{2d}
1	*WMICDFLG*	0.65	0.41	*WMICDFLG*	0.62	0.39
2	*HALPOR*	0.59	0.76	*HALPOR*	0.57	0.72
3	*WGRCOR*	0.27	0.84	*WGRCOR*	0.28	0.80
4	*WASTWICK*	0.07	0.84	*ANHPRM*	0.08	0.81
5	*ANHPRM*	0.07	0.85	*WASTWICK*	0.07	0.81
6	*SHRGSSAT*	0.07	0.85	*SHRGSSAT*	0.07	0.82

	Raw Data: y = *E2:BRAALIC*			Rank-Transformed Data: y = *E2:BRAALIC*		
Step	Variable	SRC	R^2	Variable	SRRC	R^2
1	*ANHPRM*	0.77	0.59	*ANHPRM*	0.91	0.83
2	*WMICDFLG*	–0.14	0.61	*WMICDFLG*	–0.15	0.85
3	*SALPRES*	0.09	0.62	*BHPRM*	0.13	0.87
4				*HALPRM*	0.12	0.88
5				*SALPRES*	0.10	0.89
6				*WGRCOR*	–0.05	0.90

[a] Steps in stepwise regression analysis.
[b] Variables listed in order of selection in regression analysis with *ANHCOMP* and *HALCOMP* excluded from entry into regression model because of –0.99 rank correlation within the pairs (*ANHPRM, ANHCOMP*) and (*HALPRM, HALCOMP*).
[c] Standardized regression coefficients (SRCs) in final regression model.
[d] Cumulative R^2 value with entry of each variable into regression model.
[e] Standardized rank regression coefficients (SRRCs) in final regression model.

When regression-based approaches to sensitivity analysis do not yield satisfactory insights, important variables can be searched for by attempting to identify patterns in the mapping in Eq. (2.3) with techniques that are not predicated on searches for linear or monotonic relationships. Possibilities include use of (i) the F-statistic to identify changes in the mean value of y across the range of individual x_js, (ii) the χ^2-statistic to identify changes in the median value of y across the range of individual x_js, (iii) the Kruskal-Wallis statistic to identify changes in the distribution of y across the range of individual x_js, and (iv) the χ^2-statistic to identify nonrandom joint distributions involving y and individual x_js.[254] For convenience, the preceding will be referred to as tests for (i) common means (CMNs), (ii) common medians (CMDs), (iii) common locations (CLs), and (iv) statistical independence (SI), respectively.

The preceding statistics are based on dividing the values of x_j in Eq. (2.7) into intervals (Fig. 6.9). Typically, these intervals contain equal numbers of values for x_j (i.e., the intervals are of equal probability); however, this is not always the case (e.g., when x_j has a finite number of values of unequal probability). The calculation of the F-statistic for CMNs and the Kruskal-Wallis statistic for CLs involves only the division of x_j into intervals. The F-statistic and the Kruskal-Wallis statistic are then used to indicate if the y values associated with these intervals appear to have different means and distributions, respectively. The χ^2-statistic for CMDs involves a further partitioning of the y values into values above and below the median for all y in Eq. (2.7) (i.e., the horizontal line in Fig. 6.9a), with the corresponding significance test used to indicate if the y values associated with the individual intervals defined for x_j appear to have medians that are different from the median for all values of y. The χ^2-statistic for SI involves a partitioning of the y values in Eq. (2.7) into intervals of equal probability analogous to the partitioning of the values of x_j (i.e., the horizontal lines in Fig. 6.9b), with the corresponding significance test used to indicate if the distribution of the points (x_{ij}, y_i) over the cells in Fig. 6.9b appears to be different from what

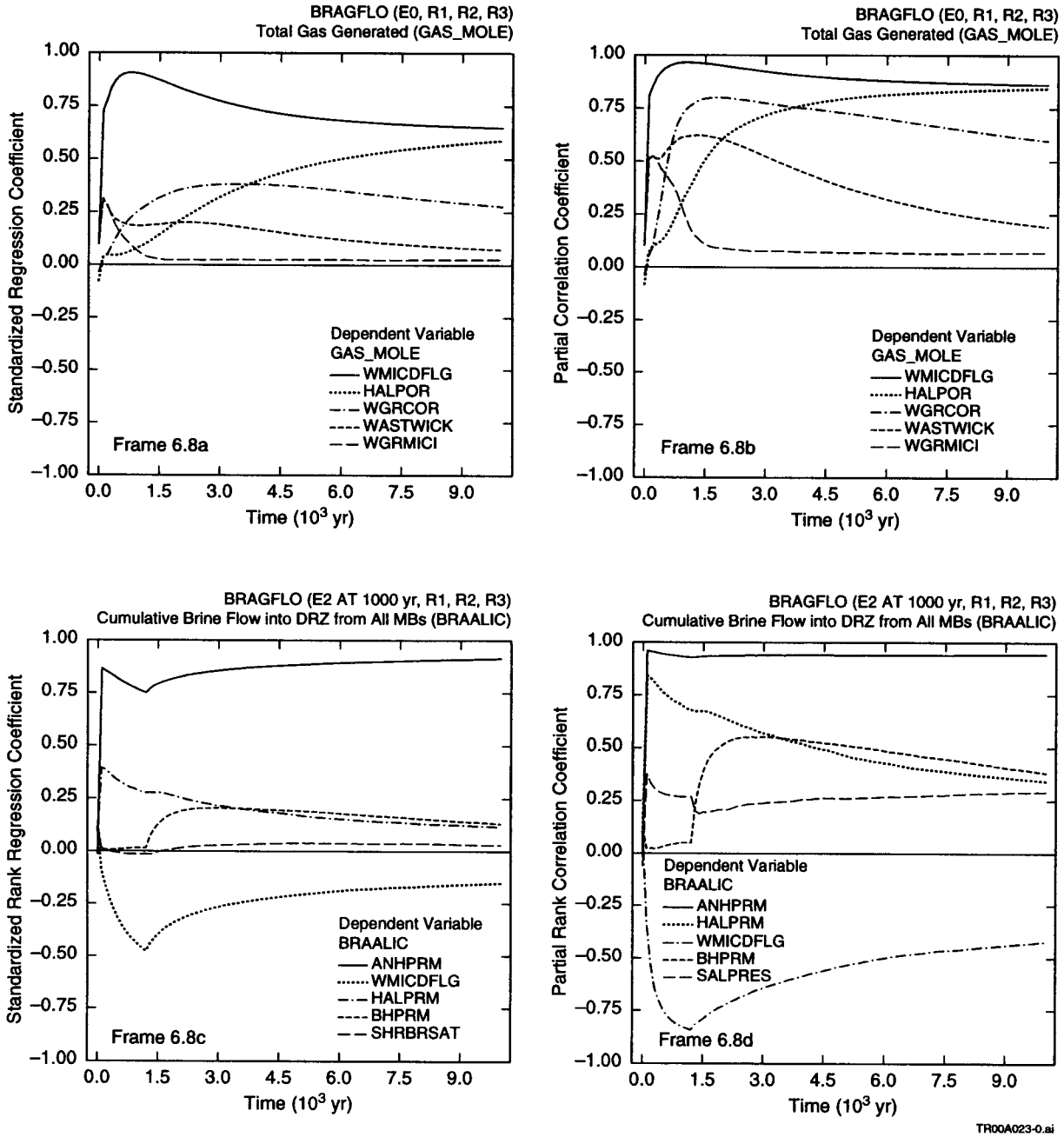

Fig. 6.8. Time-dependent coefficients: (a, b) SRCs and PCCs for cumulative gas generation under undisturbed (i.e., E0) conditions (y = *E0:GAS_MOLE*; see Fig. 6.2b), and (c, d) SRRCs and PRCCs for cumulative brine flow into DRZ with an E2 intrusion at 1000 yr (y = *E2:BRAALIC*; see Fig. 6.2c).

Table 6.5. Stepwise Regression Analyses with Raw and Rank-Transformed Data with Pooled Results for Replicates R1, R2 and R3 (i.e., for a total of 300 observations) for Output Variable *E2:PORVOL_T* at 10,000 yr

	Raw Data: y = *E2:PORVOL_T*			Rank-Transformed Data: y = *E2:PORVOL_T*		
Step[a]	Variable[b]	SRC[c]	R^{2d}	Variable[b]	SRRC[e]	R^{2d}
1	*HALPRM*	0.37	0.15	*HALPRM*	0.35	0.13
2	*BHPRM*	0.33	0.25	*ANHPRM*	0.23	0.18
3	*ANHPRM*	0.24	0.31	*HALPOR*	0.13	0.20
4	*HALPOR*	0.15	0.33			

[a] Steps in stepwise regression analysis.

[b] Variables listed in order of selection in regression analysis with *ANHCOMP* and *HALCOMP* excluded from entry into regression model because of –0.99 rank correlation within the pairs (*ANHPRM, ANHCOMP*) and (*HALPRM, HALCOMP*).

[c] Standardized regression coefficients (SRCs) in final regression model.

[d] Cumulative R^2 value with entry of each variable into regression model.

[e] Standardized rank regression coefficients (SRRCs) in final regression model.

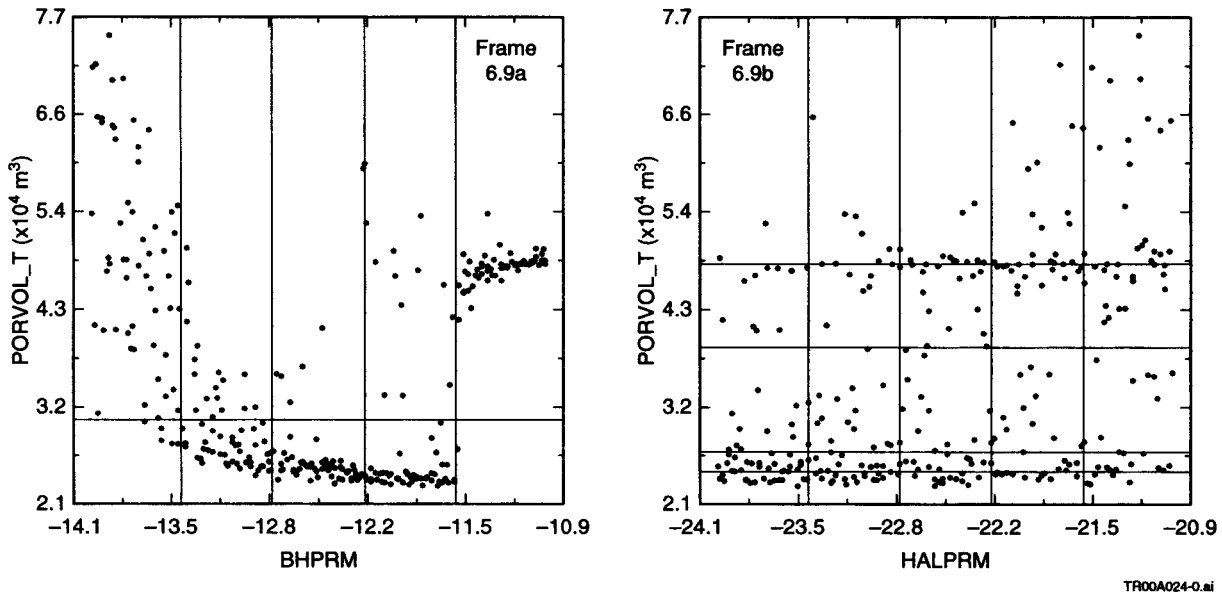

Fig. 6.9. Partitionings of (x_{ij}, y_i), $i = 1, 2, \ldots, nS = 300$: (a) division of x_j = *BHPRM* into intervals of equal probability and y = *E2:PORVOL_T* into values above and below the median, and (b) division of x_j = *HALPRM* and y =*E2:PORVOL_T* into intervals of equal probability.

would be expected if there was no relationship between x_j and y. For each statistic, a p-value can be calculated which corresponds to the probability of observing a stronger pattern than the one actually observed if there is no relationship between x_j and y. An ordering of p-values then provides a ranking of variable importance (i.e., the smaller the p-value, the stronger the effect of x_j on y appears to be). More detail on these and other related procedures is given in Kleijnen and Helton.[254, 255]

As an example, analyses for y = *E2:PORVOL_T* with the tests for CMNs, CMDs, CLs and SI are presented in Table 6.6. For perspective, tests based on p-values for CCs and RCCs are also presented in Table 6.6, with the p-values indicating the probability of ob-

serving larger, in absolute value, CCs and RCCs due to chance variation in the absence of any relationship between x_j and y.[254] The ordering of variable importance with CMNs, CMDs, CLs and SI is different from the orderings obtained with CCs and RCCs. In particular, the tests for CMNs, CMDs, CLs and SI are identifying the nonlinear and nonmonotonic relationship involving *BHPRM* that is being missed with the tests based on CCs and RCCs. If desired, the top-down correlation technique introduced by Iman and Conover could be used to provide a formal assessment of the agreement between the results for the different sensitivity analysis procedures in Table 6.6.[254, 256]

Variance decomposition procedures provide another way to identify nonlinear and nonmonotonic relationships and are typically implemented with Monte Carlo procedures (Sect. 2.4). In addition, many procedures have been proposed by the ecological community for identifying nonrandom patterns that may have a use in sampling-based sensitivity analysis (e.g., Refs. 257-270). Finally, the two-dimensional Kolmogorov-Smirnov test has the potential to be a useful tool for the identification of nonrandom patterns in sampling-based sensitivity analysis (e.g., Refs. 271-274). Further information on sampling-based procedures for uncertainty and sensitivity analysis is available in a number of reviews (e.g., Refs. 32, 38, 216, 254, 275-281).

Table 6.6. Sensitivity Results Based on CMNs, CMDs, CLs, SI, CCs and RCCs for *y = E2:PORVOL_T*

	CMN		CMD		CL		SI		CC		RCC	
Variable	Rank	*p*-Val	Rank	*p*-Val	Rank	*p*-Val	Rank	*p*-Val	Rank	*p*-Val	Rank	*p*-Val
BHPRM	1.0	0.0000	1.0	0.0000	1.0	0.0000	1.0	0.0000	10.0	0.3295	4.0	0.0926
HALPRM	2.0	0.0000	2.0	0.0000	2.0	0.0000	2.0	0.0001	1.0	0.0000	1.0	0.0000
ANHPRM	3.0	0.0005	3.0	0.0007	3.0	0.0000	4.0	0.0082	2.0	0.0000	2.0	0.0000
HALPOR	4.0	0.0341	6.0	0.0700	5.0	0.1072	5.0	0.1137	3.0	0.0097	3.0	0.0225
ANHBCEXP	5.0	0.0496	5.0	0.0595	4.0	0.0655	18.5	0.5739	9.0	0.1938	9.0	0.2535
ANHBCVGP	6.0	0.0899	16.0	0.4884	6.0	0.1248	13.0	0.2942	4.0	0.0894	5.0	0.1248
SHRBRSAT	9.0	0.1923	7.0	0.0823	8.0	0.1464	7.0	0.1850	21.0	0.6859	15.0	0.4559
BPPRM	10.0	0.2010	4.0	0.0477	7.0	0.1350	18.5	0.5739	22.0	0.7069	14.0	0.4329
WGRCOR	19.0	0.5386	17.0	0.5249	10.0	0.2320	3.0	0.0003	14.0	0.4688	18.0	0.6601

7. Uncertainty in Analyses for Complex Systems (adapted from Ref. 275, Chapt. 10)

7.1 Stochastic and Subjective Uncertainty

Many large analyses maintain a separation between two categorizations of uncertainty: (i) stochastic uncertainty, which arises because the system under study can behave in many different ways (e.g., many different accidents are possible at a nuclear power station), and (ii) subjective uncertainty, which arises from a lack of knowledge about quantities assumed to have fixed values in a particular analysis (e.g., a reactor containment building might be assumed to have a fixed failure strength, with the exact value of this strength being unknown). Thus, stochastic uncertainty in a property of the system under study, and subjective uncertainty is a property of the analysis and the associated analysts. Alternative terminology includes the use of aleatory, variability, irreducible and type A as alternatives to the designation stochastic and the use of epistemic, state of knowledge, reducible and type B as alternatives to the designation subjective. The categorization and treatment of stochastic and subjective uncertainty in analyses for complex systems has been widely discussed from a variety of perspectives. [7, 8, 282-294] Further, the use of probability to characterize both subjective and stochastic uncertainty can be traced back to the beginnings of the formal development of probability in the late seventeenth century.[295-297]

The distributions in Eq. (1.2) were assumed to characterize subjective uncertainty, and the probability space associated with these distributions was represented by ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}), with the subscript "*su*" used as a designation for "subjective." Analyses that involve stochastic and subjective uncertainty have two underlying probability spaces: a probability space ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) for stochastic uncertainty, and a probability space ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}) for subjective uncertainty. In the preceding, the subscript "*st*" is used as a designator for "stochastic."

An example of a large analysis that maintained a separation between stochastic and subjective uncertainty is the NRC's reassessment of the risk from commercial nuclear reactors in the United States (i.e., NUREG-1150), where stochastic uncertainty arose from the many possible accidents that could occur at the power plants under study and subjective uncertainty arose from the many uncertain quantities required in the estimation of the probabilities and consequences of these accidents.[171, 172, 182] Numerous other examples also exist (e.g., Refs. 183-186, 298-307).

7.2 Performance Assessment for the WIPP

This presentation will use the PA carried out in support of the DOE's 1996 CCA for the WIPP as an example of an analysis involving both stochastic and subjective uncertainty.[189, 190, 248] Parts of this analysis involving the model for two-phase flow implemented in the BRAGFLO program have already been introduced and used to illustrate uncertainty and sensitivity analysis in the presence of subjective uncertainty (Sect. 6.1). Although the analyses with BRAGFLO were an important part of the 1996 WIPP PA, they constitute only one component of a large analysis. The following provides a high-level overview of sampling-based uncertainty and sensitivity analysis in the 1996 WIPP PA. The need to treat both stochastic and subjective uncertainty in the 1996 WIPP PA arose from regulations promulgated by the EPA and briefly summarized in the next paragraph.

The following is the central requirement in the EPA's regulation for the WIPP, 40 CFR 191, Subpart B, and the primary determinant of the conceptual and computational structure of the 1996 WIPP PA (p. 38086, Ref. 191):

> § 191.13 Containment requirements:
>
> (a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon performance assessments, that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall: (1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A);[a] and (2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the

[a] Radionuclide releases normalized to amount of radioactive material placed in the disposal facility; see Ref. 191 or Ref. 193 for a description of the normalization process.

quantities calculated according to Table 1 (Appendix A).

(b) Performance assessments need not provide complete assurance that the requirements of 191.13(a) will be met. Because of the long time period involved and the nature of the events and processes of interest, there will inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future performance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much shorter time frames. Instead, what is required is a reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a) will be achieved.

The EPA also promulgated 40 CFR 194,[192] where the following elaboration on the intent of 40 CFR 191.13 is given (pp. 5242-5243, Ref. 192):

§ 194.34 Results of performance assessments.

(a) The results of performance assessments shall be assembled into "complementary, cumulative distribution functions" (CCDFs) that represent the probability of exceeding various levels of cumulative release caused by all significant processes and events. (b) Probability distributions for uncertain disposal system parameter values used in performance assessments shall be developed and documented in any compliance application. (c) Computational techniques, which draw random samples from across the entire range of the probability distributions developed pursuant to paragraph (b) of this section, shall be used in generating CCDFs and shall be documented in any compliance application. (d) The number of CCDFs generated shall be large enough such that, at cumulative releases of 1 and 10, the maximum CCDF generated exceeds the 99th percentile of the population of CCDFs with at least a 0.95 probability. (e) Any compliance application shall display the full range of CCDFs generated. (f) Any compliance application shall provide information which demonstrates that there is at least a 95 percent level of statistical confidence that the mean of the population of CCDFs meets the containment requirements of § 191.13 of this chapter.

In addition to the requirements in 40 CFR 191.13 and 40 CFR 194.34 just quoted, 40 CFR 191 and 40 CFR 194 contain many additional requirements for the certification of the WIPP for the disposal of TRU waste.[308] However, it is the indicated requirements that determine the overall structure of the 1996 WIPP PA.

Together, 191.13(a) and 194.34(a) lead to a CCDF and boundary line[309-311] as illustrated in Fig. 7.1, with the CCDF for releases to the accessible environment required to fall below the boundary line. The CCDF derives from disruptions that could occur in the future and is thus characterizing the effects of stochastic uncertainty. In contrast, 194.34(b) and (c) require the characterization and propagation of the effects of subjective uncertainty. Ultimately, this uncertainty will lead to a distribution of CCDFs of the form illustrated in Fig. 7.1, with this distribution deriving from subjective uncertainty.

The probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ for subjective uncertainty used in the 1996 WIPP PA has already been introduced in Sect. 6.1, with Table 6.1 listing examples of the 57 uncertain variables associated with the elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$. Specifically, $\mathbf{x}_{su}$ is a vector of the form

$$\mathbf{x}_{su} = [x_1, x_2, \ldots, x_{57}] \tag{7.1}$$

in the 1996 WIPP PA. The probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ was defined by specifying distributions for the elements of $\mathbf{x}_{su}$ as indicated in Eq. (1.2) and illustrated in Fig. 6.1.

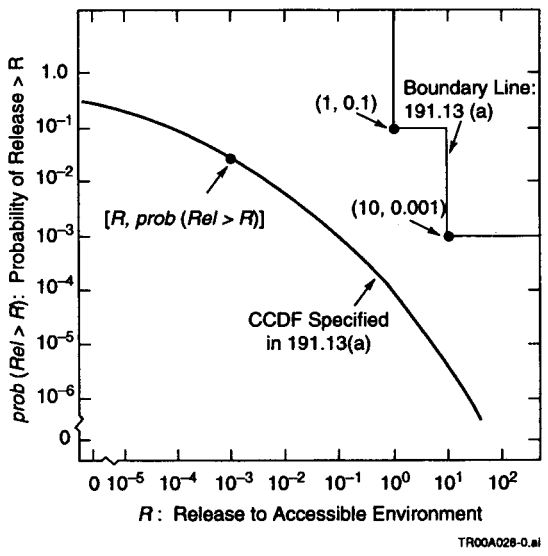

Fig. 7.1. Boundary line and associated CCDF specified in 40 CFR 191, Subpart B (Fig. 2, Ref. 312).

In the 1996 WIPP PA, the probability space ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) for stochastic uncertainty derives from the many different disruptions that could occur at the WIPP over the 10,000 yr regulatory time frame imposed on it. In particular, regulatory guidance[308] and extensive review of potential features, events and processes (FEPs) that could affect the WIPP[313] led to the elements $\mathbf{x}_{st}$ of the sample space $\mathcal{S}_{st}$ being defined as vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, l_1, e_1, b_1, p_1, \mathbf{a}_1}_{1^{st}\text{ intrusion}}, \underbrace{t_2, l_2, e_2, b_2, p_2, \mathbf{a}_2}_{2^{nd}\text{ intrusion}}, \ldots, \underbrace{t_n, l_n, e_n, b_n, p_n, \mathbf{a}_n}_{n^{th}\text{ intrusion}}, t_{min}], \tag{7.2}$$

where n is the number of exploratory drilling intrusions for natural resources (i.e., oil or gas) that occur in the immediate vicinity of the repository, t_i is the time (yr) of the i^{th} intrusion, l_i designates the location of the i^{th} intrusion, e_i designates the penetration of an excavated or nonexcavated area by the i^{th} intrusion, b_i designates whether or not the i^{th} intrusion penetrates pressurized brine in the Castile Formation, p_i designates the plugging procedure used with the i^{th} intrusion (i.e., continuous plug, two discrete plugs, three discrete plugs), $\mathbf{a}_i$ designates the type of waste penetrated by the i^{th} intrusion (i.e., no waste, contact-handled waste, and remotely handled waste, with $\mathbf{a}_i$ represented as a vector because a single drilling intrusion can penetrate several "waste streams" that have different properties), and t_{min} is the time at which potash mining occurs within the land withdrawal boundary. The definition of ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) was then completed by assigning a distribution to each element of $\mathbf{x}_{st}$.[314]

The FEPs review process also led to the identification of processes and associated models for use in the estimation of consequences (e.g., normalized radionuclide releases to the accessible environment in the context of the EPA regulations) for elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$ (Fig. 7.2, Table 7.1). Symbolically, this estimation process can be represented by

$$\begin{aligned} f(\mathbf{x}_{st}) = {} & f_C(\mathbf{x}_{st}) + f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \\ & + f_{DBR}\{\mathbf{x}_{st}, f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})], f_B(\mathbf{x}_{st})\} \\ & + f_{MB}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] + f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \\ & + f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \\ & + f_{S-T}\{\mathbf{x}_{st,0}, f_{S-F}(\mathbf{x}_{st,0}), f_{N-P}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]\}, \end{aligned} \tag{7.3}$$

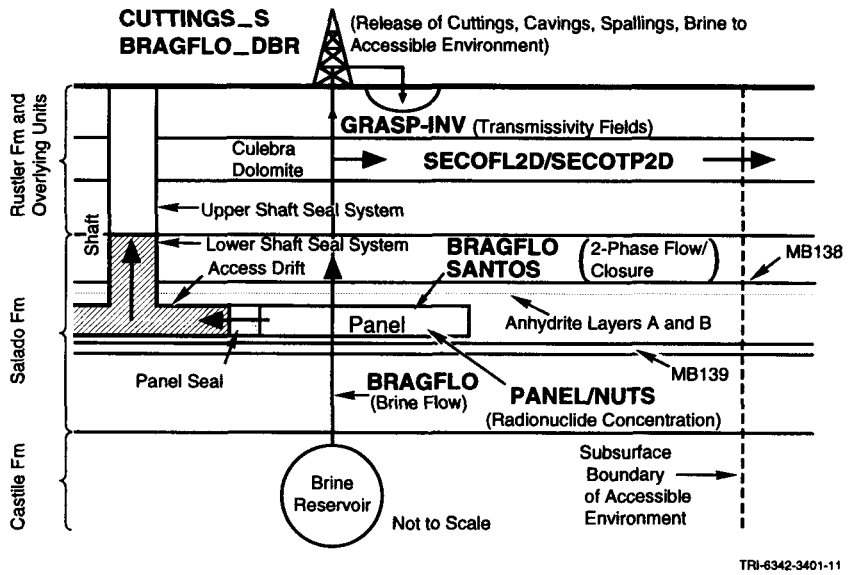

Fig. 7.2. Computer programs (models) used in 1996 WIPP PA (Fig. 5, Ref. 312).

Table 7.1. Summary of Computer Models Used in the 1996 WIPP PA (Table 1, Ref. 312).

BRAGFLO: Calculates multiphase flow of gas and brine through a porous, heterogeneous reservoir. Uses finite difference procedures to solve system of nonlinear partial differential equations that describes the mass conservation of gas and brine along with appropriate constraint equations, initial conditions and boundary conditions. Additional information: Sect. 4.2, Ref. 244; Ref. 245.

BRAGFLO_DBR: Special configuration of BRAGFLO model used in calculation of dissolved radionuclide releases to the surface (i.e., direct brine releases) at the time of a drilling intrusion. Uses initial value conditions obtained from calculations performed with BRAGFLO and CUTTINGS_S. Additional information: Sect. 4.7, Ref. 244; Ref. 315.

CUTTINGS_S: Calculates the quantity of radioactive material brought to the surface in cuttings and cavings and also in spallings generated by an exploratory borehole that penetrates a waste panel, where cuttings designates material removed by the drillbit, cavings designates material eroded into the borehole due to shear stresses resulting from the circular flow of the drilling fluid (i.e., mud), and spallings designates material carried to the borehole at the time of an intrusion due to the flow of gas from the repository to the borehole. Spallings calculation uses initial value conditions obtained from calculations performed with BRAGFLO. Additional information: Sects. 4.5, 4.6, Ref. 244; Ref. 316.

GRASP-INV: Generates transmissivity fields (estimates of transmissivity values) conditioned on measured transmissivity values and calibrated to steady-state and transient pressure data at well locations using an adjoint sensitivity and pilot-point technique. Additional information: Refs. 317, 318.

NUTS: Solves system of partial differential equations for radionuclide transport in vicinity of repository. Uses brine volumes and flows calculated by BRAGFLO as input. Additional information: Sect. 4.3, Ref. 244; Ref. 319.

PANEL: Calculates rate of discharge and cumulative discharge of radionuclides from a waste panel through an intruding borehole. Discharge is a function of fluid flow rate, elemental solubility and radionuclide inventory. Uses brine volumes and flows calculated by BRAGFLO as input. Based on solution of system of linear ordinary differential equations. Additional information: Sect. 4.4, Ref. 244; Ref. 319.

SANTOS: Solves quasistatic, large deformation, inelastic response of two-dimensional solids with finite element techniques. Used to determine porosity of waste as a function of time and cumulative gas generation, which is an input to calculations performed with BRAGFLO. Additional information: Sect. 4.2.3, Ref. 244; Refs. 320, 321.

SECOFL2D: Calculates single-phase Darcy flow for groundwater flow in two dimensions. The formulation is based on a single partial differential equation for hydraulic head using fully implicit time differencing. Uses transmissivity fields generated by GRASP-INV. Additional information: Sect. 4.8, Ref. 244; Ref. 322.

SECOTP2D: Simulates transport of radionuclides in fractured porous media. Solves two partial differential equations: one provides two-dimensional representation for convective and diffusive radionuclide transport in fractures and the other provides one-dimensional representation for diffusion of radionuclides into rock matrix surrounding the fractures. Uses flow fields calculated by SECOFL2D. Additional information: Sect. 4.9, Ref. 244; Ref. 322.

where $f(\mathbf{x}_{st})$ ~ normalized radionuclide release to the accessible environment associated with $\mathbf{x}_{st}$ and, in general, many additional consequences, $\mathbf{x}_{st}$ ~ particular future under consideration, $\mathbf{x}_{st,0}$ ~ future involving no drilling intrusions but a mining event at the same time t_{min} as in $\mathbf{x}_{st}$, $f_C(\mathbf{x}_{st})$ ~ cuttings and cavings release to accessible environment for $\mathbf{x}_{st}$ calculated with CUTTINGS_S, $f_B(\mathbf{x}_{st})$ ~ results calculated for $\mathbf{x}_{st}$ with BRAGFLO (in practice, $f_B(\mathbf{x}_{st})$ is a vector containing a large amount of information including time-dependent pressures and saturations for gas and brine), $f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ spallings release to accessible environment for $\mathbf{x}_{st}$ calculated with the spallings model contained in CUTTINGS_S, $f_{DBR}\{\mathbf{x}_{st}, f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})], f_B(\mathbf{x}_{st})\}$ ~ direct brine release to accessible environment for $\mathbf{x}_{st}$ calculated with a modified version of BRAGFLO designated BRAGFLO_DBR, $f_{MB}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release through anhydrite marker beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS, $f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release through Dewey Lake Red Beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS, $f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release to land surface due to brine flow up a plugged borehole for $\mathbf{x}_{st}$ calculated with NUTS or PANEL as appropriate, $f_{S-F}(\mathbf{x}_{st,0})$ ~ flow field calculated for $\mathbf{x}_{st,0}$ with SECOFL2D, $f_{N-F}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release to Culebra for $\mathbf{x}_{st}$ calculated with NUTS or PANEL as appropriate, and $f_{S-T}(\mathbf{x}_{st,0}, f_{S-F}\{\mathbf{x}_{st,0}), f_{N-P}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]\}$ ~ groundwater transport release through Culebra to accessible environment calculated with SECOTP2D ($\mathbf{x}_{st,0}$ is used as an argument to f_{S-T} because drilling intrusions are assumed to cause no perturbations to the flow field in the Culebra).

The probability space $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ for stochastic uncertainty and the function f indicated in Eq. (7.3) lead to the required CCDF for normalized releases to the accessible environment (Fig. 7.1). In particular, this CCDF can be represented as an integral involving $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and f (Fig. 7.3). If $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and f could be unambiguously defined, then the CCDF in Fig. 7.3 could be determined with certainty and compared against the specified boundary line. Unfortunately, such certainty does not exist in the 1996 WIPP PA, which leads to the probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ for subjective uncertainty.

When the elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$ are included, the function f in Eq. (7.3) has the form $f(\mathbf{x}_{st}, \mathbf{x}_{su})$. In turn, the expression defining the CCDF in Fig. 7.3 becomes

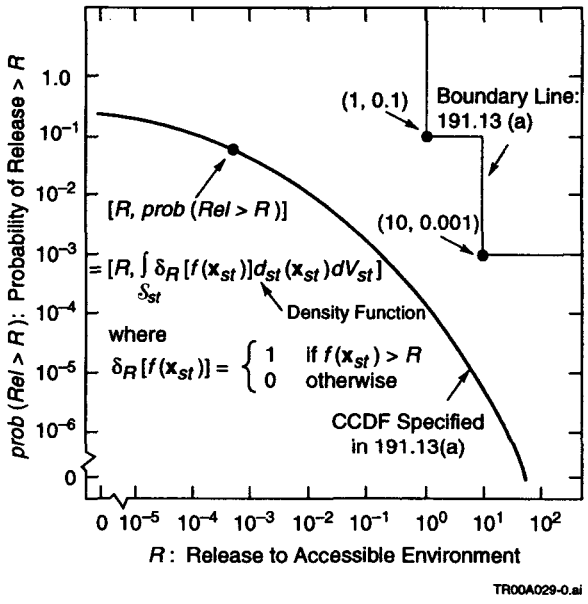

Fig. 7.3. Definition of CCDF specified in 40 CFR 191, Subpart B as an integral involving the probability space $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ for stochastic uncertainty and a function f defined on $\mathcal{S}_{st}$ (Fig. 4, Ref. 312).

$$prob(Rel > R \mid \mathbf{x}_{su}) = \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su})\right] d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su}) dV_{st}, \quad (7.4)$$

where $\delta_R[f(\mathbf{x}_{st}, \mathbf{x}_{su})] = 1$ if $f(\mathbf{x}_{st}, \mathbf{x}_{su}) > R$ and 0 if $f(\mathbf{x}_{st}, \mathbf{x}_{su}) \leq R$. Uncertainty in $\mathbf{x}_{su}$ as characterized by $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ then leads to a distribution of CCDFs, with one CCDF resulting for each $\mathbf{x}_{su}$ in $\mathcal{S}_{su}$ (Fig. 7.4).

7.3 Implementation of 1996 WIPP PA

The guidance in 194.34(a) was implemented by developing the probability space $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$, the function $f(\mathbf{x}_{st}, \mathbf{x}_{su})$, and a Monte Carlo procedure based on simple random sampling (Sect. 5.1) for the approximation of the integral, and hence the associated CCDF, in Eq. (7.4). Conditional on an element $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$, the Monte Carlo approximation procedure has the form

$$prob(Rel > R \mid \mathbf{x}_{su}) \doteq \sum_{i=1}^{nS} \delta_R\left[f(\mathbf{x}_{st,i}, \mathbf{x}_{su})\right] / nS, \quad (7.5)$$

where $\mathbf{x}_{st,i}$, $i = 1,2,\ldots,nS = 10{,}000$, is a random sample from $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$. This approximation procedure re-

quired evaluating the models in Table 7.1 for a relatively small number of elements of $\mathcal{S}_{st}$ and then using these evaluations to the construct $f(\mathbf{x}_{st,i}, \mathbf{x}_{su})$ for the large number of sample elements (i.e., nS = 10,000) used in the summation in Eq. (7.5) (see Ref. 244 and Refs. 314-316, 319, 322, 323 for numerical details).

The guidance in 194.34(b) was implemented by developing the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. Latin hypercube sampling was selected as the sampling technique required in 194.34(c) because of the efficient manner in which it stratifies across the range of each sampled variable. For a Latin hypercube or random sample of size n, the requirement in 194.34(c) is equivalent to the inequality

$$1 - 0.99^n > 0.95, \tag{7.6}$$

which results in a minimum value of 298 for n. In consistency with the preceding result, the 1996 WIPP PA used an LHS of size 300 from the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ for subjective uncertainty. Actually, as discussed below, three replicated LHSs of size 100 each were used, which resulted in a total sample size of 300 (Sect. 6.1). Further, the requirement in 194.34(d) is met by simply providing plots that contain all the individual CCDFs produced in the analysis (i.e., one CCDF for each LHS element, which generates plots of the form indicated in Fig. 7.4).

The requirement in 194.34(f) involves the mean of the distribution of CCDFs, with this distribution resulting from subjective uncertainty (Fig. 7.4). In particular, each individual CCDF in Fig. 7.4 is conditional on an element $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$ and is defined by the points $[R, prob(Rel > R|\mathbf{x}_{su})]$, with $prob(Rel > R|\mathbf{x}_{su})$ given in Eq. (7.5). Similarly, the mean CCDF is defined by the points $[R, \overline{prob}(Rel > R)]$, where

$$\overline{prob}(Rel > R) = \text{mean probability of a release greater than size } R$$

$$= \int_{\mathcal{S}_{su}} prob(Rel > R \mid \mathbf{x}_{su}) d_{su}(\mathbf{x}_{su}) dV_{su}$$

$$= \int_{\mathcal{S}_{su}} \left\{ \int_{\mathcal{S}_{st}} \delta_R \left[f(\mathbf{x}_{st}, \mathbf{x}_{su}) \right] d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su}) dV_{st} \right\} d_{su}(\mathbf{x}_{su}) dV_{su} \tag{7.7}$$

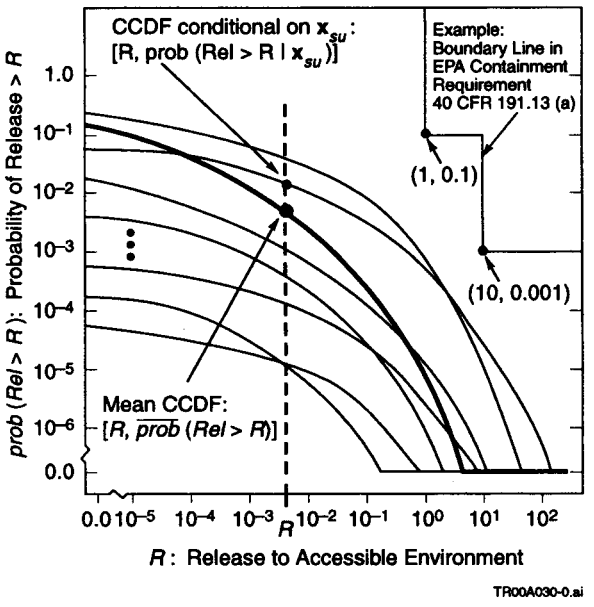

Fig. 7.4. Individual CCDFs conditional on elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$ (i.e., CCDFs represented by $[R, prob(Rel > R|\mathbf{x}_{su})]$; see Eq. (7.4)) and associated mean CCDF (i.e., CCDF represented by $[R, \overline{prob}(Rel > R)]$; see Eq. (7.7)).

and $d_{su}(\mathbf{x}_{su})$ is the density function associated with $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. The integral over $\mathcal{S}_{su}$ in the definition of $\overline{prob}(Rel > R)$ is too complex to be determined exactly. The EPA anticipated that a sampling-based integration procedure would be used to estimate this integral, with the requirement in 194.34(f) placing a condition on the accuracy of this procedure.

Given that Latin hypercube sampling is to be used to estimate the outer integral in Eq. (7.7), the confidence intervals required in 194.34(f) can be obtained with the replicated sampling technique proposed by Iman (Sect. 5.3). As discussed in Sect. 5.3, the LHS to be used is repeatedly generated with different random seeds. These samples lead to a sequence $\overline{prob}_r(Rel > R)$, r = 1, 2, ..., nR, of estimated mean exceedance probabilities, where $\overline{prob}_r(Rel > R)$ defines the mean CCDF obtained for sample r (i.e., $\overline{prob}_r(Rel > R)$ is the mean probability that a normalized release of size R will be exceeded; see Eq. (7.7)) and nR is the number of independent LHSs generated with different random seeds. Then,

$$\overline{\overline{prob}}(Rel > R) = \sum_{r=1}^{nR} \overline{prob}_r(Rel > R)/nR \qquad (7.8)$$

and

$$SE(R) = \left\{ \sum_{r=1}^{nR} \left[\overline{\overline{prob}}(Rel > R) - \overline{prob}_r(Rel > R) \right]^2 / nR(nR-1) \right\}^{1/2} \qquad (7.9)$$

provide an additional estimate of the mean CCDF and estimates of the standard errors associated with the individual mean exceedance probabilities. The t-distribution with $nR-1$ degrees of freedom can be used to place confidence intervals around the mean exceedance probabilities for individual R values (i.e., around $\overline{\overline{prob}}(Rel > R)$). Specifically, the $1-\alpha$ confidence interval is given by $\overline{\overline{prob}}(Rel > R) \pm t_{1-\alpha/2}\, SE(R)$, where $t_{1-\alpha/2}$ is the $1-\alpha/2$ quantile of the t-distribution with $nR-1$ degrees of freedom (e.g., $t_{1-\alpha/2} = 4.303$ for $\alpha = 0.05$ and $nR = 3$; Ref. 217, Table A25). The same procedure can also be used to place pointwise confidence intervals around percentile curves. The implementation of this procedure is the reason for the three replicated LHSs indicated in Sect. 6.1.

At the beginning of the computational implementation of the 1996 WIPP PA, only the 31 variables in $\mathbf{x}_{su}$ that are used as input to BRAGFLO had been fully specified (i.e., their distributions D_j had been unambiguously defined); the remaining variables that would be incorporated into the definition of $\mathbf{x}_{su}$ were still under development. To allow the calculations with BRAGFLO to proceed, the LHSs indicated in Sect. 6.1 were actually generated from $nX = 75$ variables, with the first 31 variables being the then specified inputs to BRAGFLO and the remaining 44 variables being assigned uniform distributions on [0, 1]. Later, when the additional variables were fully specified, the uniformly distributed variables were used to generate sampled values from them consistent with their assigned distributions. This procedure allowed the analysis to go forward while maintaining the integrity of the Latin hypercube sampling procedure for the overall analysis. As previously indicated, 26 additional variables were eventually defined, with the result that the elements $\mathbf{x}_{su}$ of S_{su} had an effective dimension of $nX = 57$.

7.4 Uncertainty and Sensitivity Analysis Results in 1996 WIPP PA

The CCDF used in comparisons with the EPA release limits (Figs. 7.1, 7.3) is the most important single result generated in the 1996 WIPP PA. This CCDF arises from stochastic uncertainty. However, because there is subjective uncertainty in quantities used in the generation of this CCDF, its value cannot be unambiguously known. The use of Latin hypercube sampling leads to an estimate of the uncertainty in the location of this CCDF (Fig. 7.5), with the individual CCDFs falling

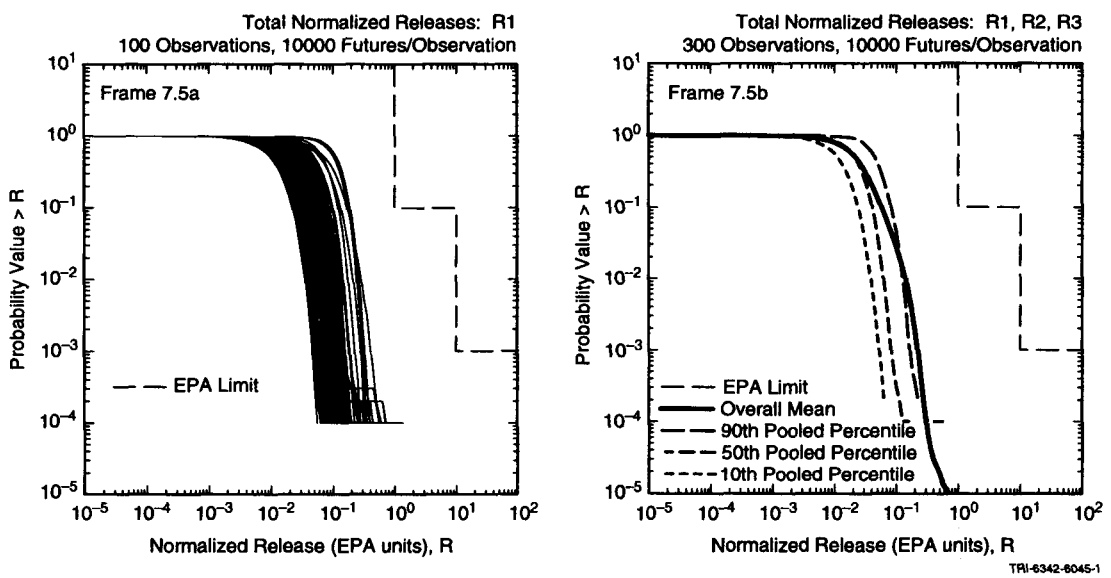

Fig. 7.5. Distribution of CCDFs for total normalized release to the accessible environment over 10,000 yr: (a) 100 individual CCDFs for replicate R1, and (b) mean and percentile curves estimated from 300 CCDFs obtained by pooling replicates R1, R2 and R3 (Figs. 6, 7, Ref. 312).

substantially to the left of the release limits. The left frame (Fig. 7.5a) shows the individual CCDFs obtained for replicate R1, and the right frame (Fig. 7.5b) shows the mean and selected percentile curves obtained from pooling the three replicates. The mean curve in Fig. 7.5b is formally defined in Eq. (7.7), and the construction procedures used to obtain the individual curves in Fig. 7.5b are described in conjunction with Fig. 6.4.

The replicated samples described in Sect. 6.1 were used to obtain an indication of the stability of results obtained with Latin hypercube sampling. For the total release CCDFs in Fig. 7.5, the results obtained for the three replicates (i.e., R1, R2, R3) were very stable, with little variation in the locations of the mean and percentile curves occurring across replicates (Fig. 7.6a). Indeed, the mean and percentile curves for the individual replicates overlie each other to the extent that they are almost indistinguishable. As a result, the procedure indicated in conjunction with Eqs. (7.8) and (7.9) provides a very tight confidence interval around the estimated mean CCDF (Fig. 7.6b).

The sampling-based approach to uncertainty analysis has created a pairing between the individual LHS elements and the individual CCDFs in Fig. 7.5a that can be explored with the previously discussed sensitivity analysis techniques (Sect. 6). One possibility for investigating the sources of the uncertainty that give rise to the distribution of CCDFs in Fig. 7.5a is to determine what is giving rise to the variation in exceedance probabilities for individual release values on the abscissa. This variation in exceedance probabilities can be investigated in exactly the same manner as the variation in cumulative gas generation (*GAS_MOLE*) and brine inflow (*BRAALIC*) at individual times was investigated for the curves in Fig. 6.2 and presented in Fig. 6.8. Specifically, PRCCs, SRRCs, or some other measure of sensitivity can be calculated for the exceedance probabilities associated with individual release values. This measure for different sampled variables can be plotted above the corresponding release values on the abscissa and then connected to obtain a representation for how sensitivity changes for changing values on the abscissa. For the CCDFs in Fig. 7.5a, this analysis approach shows that the exceedance probabilities for individual release values are primarily influenced by *WMICDFLG* and *WTAUFAIL*, with the exceedance probabilities tending to increase as *WMICDFLG* increases and tending to decrease as *WTAUFAIL* increases (Fig. 7.7).

Another possibility is to reduce the individual CCDFs to expected values over stochastic uncertainty and then to perform a sensitivity analysis on the resultant expected values. In the context of the CCDF representation in Eq. (7.4), this expected value can be formally defined by

$$E(R \mid \mathbf{x}_{su}) = \int_{\mathcal{S}_{st}} f(\mathbf{x}_{st}, \mathbf{x}_{su}) d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su}) dV_{st}. \quad (7.10)$$

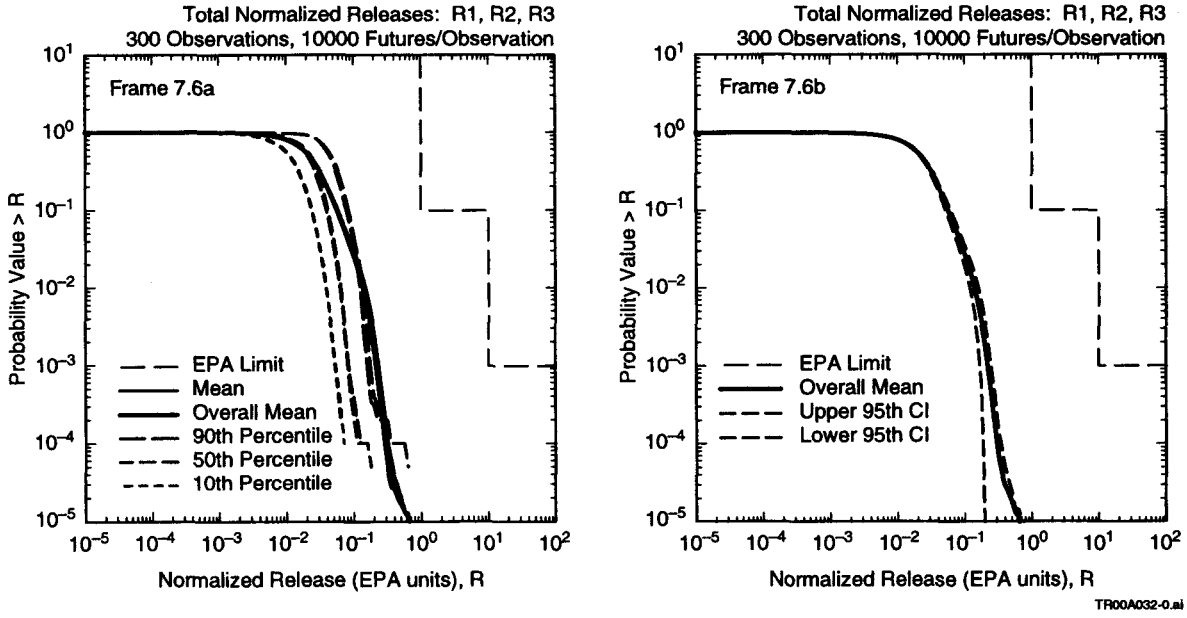

Fig. 7.6. Stability of estimated distribution of CCDFs for normalized release to the accessible environment: (a) mean and quantile curves for individual replicates, and (b) confidence interval around mean CCDF obtained by pooling the three individual replicates (Fig. 8, Ref. 312).

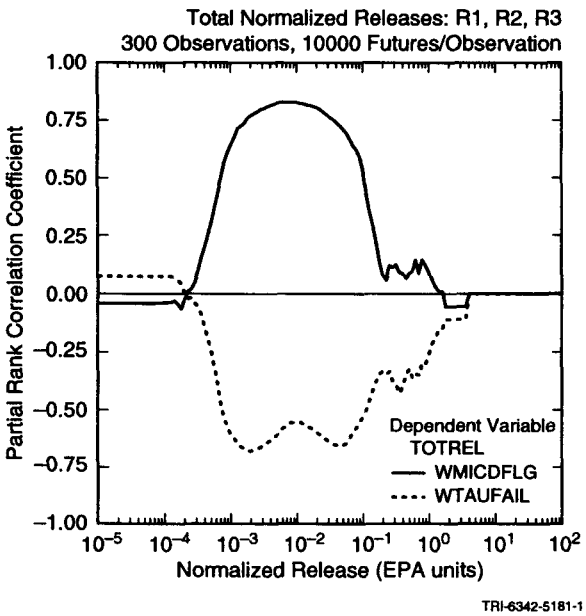

Fig. 7.7. Sensitivity analysis based on PRCCs for CCDFs for normalized release to the accessible environment (Fig. 14, Ref. 324).

The LHS then results in a sequence of values $E(R \mid \mathbf{x}_{su,k})$, $k = 1, 2, \ldots, nLHS = 300$, that can be explored with the previously discussed sensitivity analysis procedures. For example, stepwise regression analysis shows that *WMICDFLG* and *WTAUFAIL* are the dominant variables with respect to the uncertainty in $E(R \mid \mathbf{x}_{su})$, with lesser effects due to a number of additional variables (Table 7.2).

This section briefly describes the 1996 WIPP PA and illustrates uncertainty and sensitivity analysis procedures based on Latin hypercube sampling in the context of this PA. Additional details are available in other presentations.[190, 244, 248, 324]

Table 7.2. Stepwise Regression Analysis with Rank-Transformed Data for Expected Normalized Release Associated with Individual CCDFs for Total Release Due to Cuttings and Cavings, Spallings and Direct Brine Release (Table 5, Ref. 324).

	Expected Normalized Release		
Step[a]	Variable[b]	SRRC[c]	R^{2}[d]
1	*WMICDFLG*	0.60	0.40
2	*WTAUFAIL*	−0.39	0.55
3	*WGRCOR*	0.21	0.59
4	*WPRTDIAM*	−0.19	0.63
5	*HALPOR*	0.17	0.65
6	*BHPRM*	−0.17	0.68
7	*HALPRM*	0.16	0.71
8	*WASTWICK*	0.11	0.72
9	*ANHPRM*	0.09	0.73

[a] Steps in stepwise regression analysis.

[b] Variables listed in order of selection in regression analysis with *ANHCOMP* and *HALCOMP* excluded from entry into regression model because of −0.99 rank correlation within the pairs (*ANHPRM, ANHCOMP*) and (*HALPRM, HALCOMP*).

[c] Standardized rank regression coefficients (SRRCs) in final regression model.

[d] Cumulative R^2 value with entry of each variable into regression model.

8. Discussion

Latin hypercube sampling has become a widely used sampling technique for the propagation of uncertainty in analyses of complex systems. A check of the original article[31] in Science Citation Index or SciSearch can be used to obtain both a list of all citations and also the most recent citations to this technique. This review ends with a discussion of some of the reasons for the popularity of Latin hypercube sampling (Sect. 8.1) and some additional thoughts on the propagation of uncertainty in analyses for complex systems (Sect. 8.2).

8.1 Popularity of Latin Hypercube Sampling

Reasons that have led to the popularity of Monte Carlo techniques in general and Latin hypercube sampling in particular for uncertainty and sensitivity analysis of complex models include (i) conceptual simplicity and ease of implementation, (ii) dense stratification over the range of each sampled variable, (iii) direct provision of uncertainty analysis results without the use of surrogate models as approximations to the original model, (iv) availability of a variety of sensitivity analysis procedures, and (v) effectiveness as a model verification procedure. The preceding reasons are discussed in more detail below.

Conceptual Simplicity and Ease of Implementation. A Monte Carlo approach to the propagation of uncertainty is easy to explain. Further, the definition of Latin hypercube sampling is straightforward, and the reason why its enforced stratification improves the results of an analysis for a given sample size is easy to grasp on an intuitive level. Thus, the presentation of Monte Carlo and Latin hypercube results to individuals of different levels of technical sophistication (e.g., other scientists working in the same or related fields, private or governmental decision makers, the general public) is relatively straightforward. In contrast, some of the other techniques for the propagation and analysis of uncertainty are less transparent (e.g., RSM, FAST, Sobol' variance decomposition, fast probability integration) and thus more difficult to present.

Analyses based on Latin hypercube sampling are typically easy to implement. Software is available to generate LHSs and also to implement the Iman/ Conover restricted pairing technique for the control of correlations within the sample (e.g., Ref. 164). Further, propagation of the sample through the model under consideration is straightforward in most analyses. In practice, this propagation often involves little more than putting a "DO Loop" around the model which (i) reads the individual sample elements, (ii) uses these elements to generate input in the form required by the model, (iii) runs the model, and (iv) saves model results for later analysis.

In contrast, implementation of the other analysis procedures can be considerably more difficult: (i) RSM requires the development of both a suitable experimental design and the construction of a surrogate model, (ii) differential analysis requires the determination of the necessary model derivatives, (iii) FAST and Sobol' variance decomposition require the development and evaluation of suitable integrals involving the model to obtain the associated variance decompositions, and (iv) fast probability integration requires the evaluation and use of model derivatives in the location of the MPP. Not only are the above procedures conceptually and computationally complex but, in many analyses, they can require more computational effort (i.e., model evaluations) than a Monte Carlo analysis with Latin hypercube sampling.

Analyses that involve a single model are relatively easy to implement and explain. Analyses that involve a sequence of linked, and possibly quite complex, models are more difficult to implement and explain. Examples of such analyses are the NRC's reassessment of the risk from commercial nuclear power reactors (i.e., NUREG-1150)[171, 172, 182] and the DOE's PA in support of a CCA for the WIPP.[190, 244, 248, 324] However, in such analyses, a sampling-based approach provides a way to examine results at model interfaces and develop a computational strategy for the overall assembly of the analysis. Analyses using the other techniques described in Sect. 2 seem less useful in the design, integration and ultimate performance of an analysis that involves the propagation of uncertainty through a sequence of linked models.

Dense Stratification over Range of Each Sampled Variable. Latin hypercube sampling results in a denser stratification over the range of each sampled variable than would be obtained with a classical experimental design of the type typically used in conjunction with RSM and a more uniform stratification than would be obtained with random sampling. Further, the random pairing associated with Latin hypercube sampling spreads the sampled points throughout the high-dimensional sample space.

Real analyses typically have a large number of analysis outcomes of interest. Further, these outcomes are often spatially or temporally dependent. The result is that most, if not all, of the sampled variables can be

important to one or more of the analysis outcomes. The dense stratification over the range of each sampled variable with Latin hypercube sampling results in each variable being sampled in a manner that allows its effects to be recognized if such effects exist.

It is a mistake to assume that the important effects associated with a variable only occur at the end points of its range. Instead, it is quite possible that the most important effects associated with a variable could occur in an interior part of its range (e.g., Fig. 6.9a). The dense stratification associated with Latin hypercube sampling allows the identification of such effects when they occur. Further, this stratification also facilitates the identification of interactions involving multiple variables (e.g., Fig. 6.7; also Figs. 8,9, Ref. 170).

Direct Provision of Uncertainty Analysis Results. Because probabilistic weights can be associated with individual sample elements, Latin hypercube sampling, random sampling and stratified sampling can be used to obtain estimates of distribution functions directly from model results. Further, these estimates are unbiased, although some bias may be introduced if the Iman/ Conover restricted pairing technique (Sect. 5.1) is used.

Latin hypercube sampling tends to produce more stable results (i.e., less variation in estimated distribution functions from sample to sample) than random sampling. However, examples can be obtained in which Latin hypercube sampling and random sampling produce results of similar stability by constructing a model in which variations in model behavior take place on a scale that is much smaller than the interval sizes in the LHS that result from the sample size selected for use. Stratified sampling can produce better distribution function estimates than either Latin hypercube or random sampling provided enough information is available to define the strata and calculate the associate strata probabilities. Thus, stratified sampling is typically used only when a substantial knowledge base has already been obtained about the problem under consideration and is usually not appropriate in an initial exploratory analysis. Further, it is difficult to define a meaningful stratified sampling plan when many analysis outcomes are under consideration, as is usually the case in most real analyses.

In contrast to Latin hypercube, random and stratified sampling, fast probability integration is intended primarily for estimating the tails of a distribution rather than the full distribution. Differential analysis in conjunction with the associated Taylor series provides an estimate for model variance rather than the full distribution function; further, the expected values of analysis outcomes are usually taken to be the outcome of the model evaluated at the expected values of the inputs. The FAST approach and Sobol' variance decomposition are also used to estimate expected values and variances rather than full distribution functions, although the calculations used to obtain expected values can also be used to produce estimated distribution functions.

An important characteristic of Latin hypercube and random sampling is that the resultant model evaluations can be used to provide estimated distribution functions for all analysis outcomes. In particular, a different analysis/computational strategy does not have to be developed and implemented for each analysis outcome. As already indicated, real analyses typically have a large number of outcomes of interest, and the necessity to develop a separate investigation for each of them can impose unreasonable demands on both human and computational resources.

Variety of Sensitivity Analysis Procedures. Latin hypercube and random sampling generate a mapping from uncertain analysis inputs to analysis results. Once generated, this mapping can be explored with a variety of techniques, including examination of scatterplots, correlation analysis, regression analysis, rank transformations, tests for nonmonotonic patterns, and tests for random patterns. This variety of techniques allows flexibility in developing a sensitivity analysis that is appropriate for the particular analysis situation under consideration. Again, Latin hypercube sampling is particularly effective in sensitivity analyses with small samples due to its efficient stratification across the range of each uncertain variable.

Sensitivity analyses in differential analysis and RSM are typically based on assessing either the effects of perturbations away from base values or fractional contributions to variance. In either case, the resultant sensitivity analyses are no better than the surrogate models (i.e., Taylor series or response surfaces) over the range of uncertainty under consideration. Fast probability integration is primarily an uncertainty analysis procedure and is usually not used in sensitivity analysis.

The FAST approach and Sobol' indices provide very appealing sensitivity analysis results. In particular, they provide a complete decomposition of variance into the components due to individual variables and interactions between variables. Unfortunately, if the model under consideration is expensive to evaluate or a large number of analysis outcomes are being investigated, the computational cost of implementing these procedures may be prohibitive. Although the FAST approach and

the Sobol' variance decomposition are calculated under the assumption that model inputs are independent, variance decomposition procedures exist that can be used with correlated inputs.[135-137]

Model Verification. Sampling-based uncertainty and sensitivity analysis provides a very powerful tool in model verification. Here, model verification is used to mean checking the correctness of the implementation of a model and/or an analysis and thus is distinct from model validation, which involves checking the capability of the model and/or analysis to represent the physical system under study. Propagation of a sample through an analysis provides a very extensive exercising of its many components. Gross errors will often be revealed by the failure of the analysis for some sample elements or possibly by the appearance of clearly erroneous results. Further, subtler errors are often revealed in sensitivity analyses (e.g., a variable having a small negative effect when the underlying physics implies that it should have a small positive effect or when a variable is shown to affect an analysis result on which it should have no effect).

Sensitivity analysis provides a way to examine a large number of analysis outcomes for anomolous behavior in a very rapid manner. Further, relatively small effects can be observed. Sampling-based sensitivity analysis is much more effective in searching for analysis errors than simply running the model for a limited number of cases and then examining the results of these calculations. A sampling-based sensitivity analysis should be included as part of any serious model/analysis verification effort. Latin hypercube is particularly effective in model verification due to the dense stratification across the range of each sampled variable.

8.2 Additional Thoughts

Uncertainty and sensitivity analyses for complex systems are typically iterative. An initial study is often performed to gain perspectives on (i) the behavior of the model(s) involved, (ii) strategies for carrying out a final and defensible analysis, and (iii) the most important variables with respect to the uncertainty in outcomes of interest. In such preliminary analyses, rather crude characterizations of variable uncertainty may be adequate. Once system behavior is better understood and the more important variables with respect to this behavior are identified, resources can be focused on improving the characterization of the uncertainty in these important variables. Further, iterative analyses facilitate quality assurance by providing repeated opportunities to check the correctness of model and analysis implementation. Sampling-based approaches to uncertainty and sensitivity analysis are particularly effective in iterative analyses due to the extensive exercising of the model(s) and associated analysis structure and the availability of a variety of uncertainty and sensitivity analysis results.

Concern is often expressed about the computational cost of carrying out a Monte Carlo analysis. In most analyses, the human cost of developing the model, carrying out the analysis, and documenting and defending the analysis will be far greater than the computational cost (i.e., for CPU time) of performing the necessary calculations. Latin hypercube sampling was developed to improve the quality of uncertainty and sensitivity analysis results relative to those that could be obtained with a random sample of the same size. However, if the model is inexpensive to evaluate, a large sample size can be used, and whether Latin hypercube or random sampling is used will have little effect on either the cost of the analysis or the quality of the results obtained.

Some individuals express a broad, almost philosophical, dislike for Monte Carlo analysis procedures. This makes little sense. Monte Carlo procedures are just a way of carrying out a numerical integration and developing a mapping between model inputs and outputs. There may be reasons to question the model in use or the distributions assigned to uncertain variables, but these are not reasons to question Monte Carlo procedures themselves. Of course, a Monte Carlo analysis has to be carried out with a sufficiently large sample to produce results with a resolution appropriate for the purposes of the analysis. Replicated sampling provides one way to investigate the robustness of analysis outcomes and thus the appropriateness of the sample size selected for use; further, the individual replicates can be pooled to produce the final presentation results of the analysis.

Many large analyses involve a separation of subjective (i.e., epistemic) uncertainty and stochastic (i.e., aleatory) uncertainty (e.g., the NUREG-1150 probabilistic risk assessments (PRAs) and the WIPP PA as previously mentioned). In such analyses, a common strategy is to use Latin hypercube sampling to propagate the effects of subjective uncertainty, and random or stratified sampling to propagate the effects of stochastic uncertainty. With this approach, the effect of stochastic uncertainty is being calculated conditional on individual LHS elements. Typical analysis outcomes are distributions of CCDFs, with the individual CCDFs arising from stochastic uncertainty and the distributions of CCDFs arising from subjective uncertainty. The efficient stratification associated with Latin hypercube

sampling is important in analyses of this type due to the possibly large computational effort required in the determination of the effects of stochastic uncertainty.

Random or stratified sampling is often a better choice than Latin hypercube sampling for the incorporation of stochastic uncertainty into an analysis. With random sampling, it is possible to build up a sample by selecting one sampled value at a time. In contrast, Latin hypercube sampling requires the entire sample to be selected at one time. As a result, random sampling often works better than Latin hypercube sampling when the values to be sampled are closely linked to effects that derive from previously sampled values (e.g., when the stopping point for a sampling process is determined by previously sampled values). The WIPP PA used random sampling to incorporate the effects of stochastic uncertainty due to the need to determine the effects of randomly occurring drilling intrusions over a 10,000 yr period. With stratified sampling, it is possible to force the inclusion of low-probability but high-consequence events into the analysis. The NUREG-1150 PRAs used stratified sampling implemented by event trees to assure the inclusion of, and also to calculate the probability of, low-probability/high-consequence accidents.

No approach to the propagation and analysis of uncertainty can be optimum for all needs. For example and depending on the particular problem, stratified sampling or fast probability integration can be more appropriate than Latin hypercube sampling for the estimation of the extreme quantiles of a distribution. Likewise, differential analysis may be the preferred approach if it is necessary to determine the effects of small perturbations away from base-case values, and the FAST approach or Sobol' variance decomposition may be the preferred approach if it is necessary to determine a complete variance decomposition. However, it is the authors' view that Monte Carlo analysis with Latin hypercube sampling is the most broadly applicable approach to the propagation and analysis of uncertainty and often the only approach that is needed.

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Appendix A

On a Better Method for Selecting Input Variables
W.J. Conover
May, 1975

Comment Supplied by W.J. Conover on Sept. 3, 2001:

This entire manuscript, including remarks, was supported by Los Alamos National Laboratories, and submitted to Ron Lohrding in May, 1975. He was the Group Leader who got me working on this problem. This was not reviewed, and therefore contains a few typos. I worked alone on this research while at Texas Tech, and am the sole author of this report. Parts of it appeared later in the *Technometrics* paper. Otherwise, this was never published.

On a better method for selecting input variables

W.J. Conover

1. Description of the problem: A set of input variables $(X_1,\ldots,X_K) = \underset{\sim}{X}$ enters a system and emerges as an output variable $Y = h(\underset{\sim}{X})$. The distribution function $F(\underset{\sim}{x})$ of $\underset{\sim}{X}$ is known, but the system $h(\cdot)$ is unknown. The problem is to determine information concerning the output Y, such as obtaining estimates of

a) E(Y),

b) Var(Y),

c) the percentiles of Y, and

d) the distribution function of Y.

Obviously information may be obtained about Y only by observing Y for several selected values of $\underset{\sim}{X}$. We are limited to N values of $\underset{\sim}{X}$. How should we select those N values in order to obtain the most information about Y?

The term "most information" is vague. Let's be more specific and say that we are interested in information about E(Y) and wish to choose the input in order to minimize the variance of an unbiased estimator of E(Y). It is reasonable to think that this choice of inputs will also give good estimates for the other quantities we wish to estimate.

2. Random sample: One way of selecting the inputs is to select a random sample of size N. That is, a set of pseudo-random uniform

random numbers is generated on a computer, and a suitable inverse function $F^{-1}(\cdot)$ is used to operate on the uniform variates to obtain a pseudo-random value of $\underset{\sim}{X}$, which is used as an input to obtain a value Y. The process is repeated N times to obtain $\underset{\sim}{X}_1,\ldots,\underset{\sim}{X}_N$, and hence $Y_1,\ldots,Y_N$. The Y_i's constitute a random sample and the entire body of statistical literature may be used to estimate the mean, variance, percentiles, and distribution function of Y.

The only way to obtain an unbiased estimator for the mean E(Y) is by choosing the inputs in such a way that every possible input (and, hence, output also) has some chance, however remote, of occuring. If some region of possible values of $\underset{\sim}{X}$ is excluded from the sampling plan, no probability statements may be made concerning E(Y), Var(Y), or other moments of Y. With the random sample, every possible input has some chance of being selected, and hence every possible output has some chance of being obtained. If we let

$$\bar{Y}_R = \frac{1}{N} \sum_{i=1}^{N} Y_i \tag{2.1}$$

be the estimator, it is well known that the estimator is unbiased,

$$E(\bar{Y}_R) = E(Y) \tag{2.2}$$

and the variance of $\bar{Y}_R$ is given by

$$Var(\bar{Y}_R) = \frac{1}{N} Var(Y). \tag{2.3}$$

We will consider one method of selecting input variables to be better than another if the corresponding variance of the estimator is smaller. This leads us to stratified sampling.

3. A stratified sample: Let the range space $\mathcal{S}$ of $\underset{\sim}{X}$ be partitioned into I subspaces $\mathcal{S}_1,\ldots,\mathcal{S}_I$. Denote the size of $\mathcal{S}_i$ by p_i, where

$$p_i = P(\underset{\sim}{X} \in \mathcal{S}_i) \tag{3.1}$$

A stratified sampling scheme consists of drawing a random sample of size n_i from $\mathcal{S}_i$, for each $i = 1,\ldots,I$. Obviously $N = \sum_{i=1}^{N} n_i$ and $\sum_{i=1}^{N} p_i = 1$. Denote the input variables by $\underset{\sim}{X}_{i,j}$; $i = 1,\ldots,I$; $j = 1,\ldots,n_i$. Let $Y_{ij} = h(\underset{\sim}{X}_{ij})$, and choose as an estimator

$$\bar{Y}_S = \sum_{i=1}^{I} \sum_{j=1}^{n_i} \frac{p_i}{n_i} h(\underset{\sim}{X}_{ij}) = \sum_{i=1}^{I} \frac{p_i}{n_i} \sum_{j=1}^{n_i} Y_{ij}. \tag{3.2}$$

Then $\bar{Y}_S$ is an unbiased estimator of E(Y). This may be seen as follows,

$$E(\bar{Y}_S) = \sum_{i=1}^{I} \sum_{j=1}^{n_i} \frac{p_i}{n_i} E[h(\underset{\sim}{X}_{ij})] = \sum_{i=1}^{I} p_i E[h(\underset{\sim}{X}_i)] \tag{3.3}$$

where $\underset{\sim}{X}_i = \underset{\sim}{X} | \mathcal{S}_i$, because the $\underset{\sim}{X}_{ij}$ are identically distributed for $j = 1,\ldots,n_i$. Note that the distribution function of $\underset{\sim}{X}_{ij}$ is given by $F_{ij}(\underset{\sim}{x})$, which satisfies

$$dF_{ij}(\underset{\sim}{x}) = \frac{1}{p_i} dF(\underset{\sim}{x}) \quad \text{if } \underset{\sim}{x} \in \mathcal{S}_i$$

$$= 0 \qquad \text{if } \underset{\sim}{x} \notin \mathcal{S}_i$$

From (3.3) and the above relationship we obtain

$$E(\bar{Y}_S) = \sum_{i=1}^{I} \int_{\mathcal{S}_i} h(\underset{\sim}{x}) dF(\underset{\sim}{x}) = \int_{\mathcal{S}} h(\underset{\sim}{x}) dF(\underset{\sim}{x}) = E(Y). \qquad (3.4)$$

Furthermore, by independence we have

$$\begin{aligned} Var(\bar{Y}_S) &= \sum_{i=1}^{I} \sum_{j=1}^{n_i} \left(\frac{p_i}{n_i}\right)^2 Var\{h(\underset{\sim}{X}_{ij})\} \\ &= \sum_{i=1}^{I} \frac{p_i^2}{n_i} Var\{h(\underset{\sim}{X}_i)\} \end{aligned} \qquad (3.5)$$

At this point we may examine the portion of (3.5) which arises from the random sample of size n_i from subspace $\mathcal{S}_i$, namely

$$\frac{p_i^2}{n_i} Var\{h(\underset{\sim}{X}_i)\} \qquad (3.6)$$

and compare it with what would happen to that portion if $\mathcal{S}_i$ were further subdivided into subspaces, let's say subspaces $\mathcal{S}_{ij}$ of equal size $p_{ij} = p_i/n_i$, $j = 1,\ldots,n_i$. Then (3.6) would be replaced by

$$\sum_{j=1}^{n_i} p_{ij}^2 Var\{h(\underset{\sim}{X}_{ij})\} = \frac{p_i^2}{n_i^2} \sum_{j=1}^{n_i} Var(h(\underset{\sim}{X}_{ij})) \qquad (3.7)$$

where $\underset{\sim}{X}_{ij}$ now represents $\underset{\sim}{X}|\mathcal{S}_{ij}$. It is easy to see that (3.7) is smaller than (or equal to) (3.6):

$$\frac{p_i^2}{n_i}\mathrm{Var}\{h(\underset{\sim}{X}_i)\} - \frac{p_i^2}{n_i^2}\sum_{j=1}^{n_i}\mathrm{Var}(h(\underset{\sim}{X}_{ij}))$$

$$= \frac{p_i^2}{n_i^2}\{n_i E[h^2(\underset{\sim}{X}_i)] - n_i E^2[h(\underset{\sim}{X}_i)] - \sum_{j=1}^{n_i} E[h^2(\underset{\sim}{X}_{ij})] + \sum_{j=1}^{n_i} E^2[h(\underset{\sim}{X}_{ij})]\}$$

$$= \frac{p_i^2}{n_i^2}\{\sum_{j=1}^{n_i} E^2[h(\underset{\sim}{X}_{ij})] - n_i E^2[h(\underset{\sim}{X}_i)]\}$$

$$= \frac{p_i^2}{n_i^2}\{\sum_{j=1}^{n_i}[E(h(\underset{\sim}{X}_{ij})) - \frac{1}{n_i}\sum_{k=1}^{n_i} E(h(\underset{\sim}{X}_{ik}))]^2\} \geq 0. \qquad (3.8)$$

Therefore any stratified sampling scheme with $n_i > 1$ can be improved, i.e., the term $\mathrm{Var}(\bar{Y}_S)$ can be decreased, by stratifying into finer subdivisions until all n_i equal 1.

Thus we are led to the following improved design. Subdivide the sample space $\mathcal{S}$ of $\underset{\sim}{X}$ into N subspaces $\mathcal{S}_1,\ldots,\mathcal{S}_N$ and randomly sample one value of $\underset{\sim}{X}$ from each $\mathcal{S}_i$. Let the estimator be

$$\bar{Y}_S = \sum_{i=1}^{N} p_i h(\underset{\sim}{X}_i) \qquad (3.9)$$

which is an unbiased estimator of E(Y). The variance of $\bar{Y}_S$ is, from (3.5),

$$\mathrm{Var}(\bar{Y}_S) = \sum_{i=1}^{N} p_i^2\,\mathrm{Var}\{h(\underset{\sim}{X}_i)\}. \qquad (3.10)$$

If the strata $\mathcal{S}_i$ are selected so that all the p_i are equal, then (3.10) represents an improvement over (2.3):

$$\mathrm{Var}(\bar{Y}_R) - \mathrm{Var}(\bar{Y}_S) = \frac{1}{N}\mathrm{Var}(Y) - \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Var}\{h(\underset{\sim}{X}_i)\} \geq 0 \qquad (3.11)$$

as was illustrated in showing (3.8). Therefore stratified sampling results in an estimate $\bar{Y}_S$ that is at least as good as the estimate $\bar{Y}_R$ obtained using a random sample, if the strata have equal size $p_i = 1/N$.

In fact, the best stratified design is obtained by stratifying so that every stratum has the same value for

$$p_i^2\,\mathrm{Var}(h(\underset{\sim}{X}_i)) = [\frac{1}{N}\sum_{i=1}^{N} p_i\{\mathrm{Var}(h(\underset{\sim}{X}_i))\}^{1/2}]^2 . \qquad (3.12)$$

This is seen by noting the identity from (3.10),

$$\mathrm{Var}(\bar{Y}_S) = \sum_{i=1}^{N}[p_i\sqrt{\mathrm{Var}(h,\underset{\sim}{X}_i)} - \frac{1}{N}\sum_{j=1}^{N} p_i\sqrt{\mathrm{Var}(h(\underset{\sim}{X}_i))}]^2 + \frac{1}{N}[\sum_{i=1}^{N} p_i\sqrt{\mathrm{Var}(h(\underset{\sim}{X}_i))} \qquad (3.13)$$

which reveals that $\mathrm{Var}(\bar{Y}_S)$ is minimized when (3.12) holds. Unfortunately the numerical value of (3.12) depends to a great extent on the particular partition $\{\mathcal{S}_i\}$ employed. The best partition of $\mathcal{S}$ is one which also partitions the range of Y into nonoverlapping subsets, but this is very difficult to do when so little is known about the function $h(\underset{\sim}{X})$. This suggests that an optimal design would be one in which each choice for $\underset{\sim}{X}$ as an input depends on the in-

formation obtained from previous inputs and their corresponding outputs. Such a sequential design is not easy to work with from the standpoint of statistical theory, so we will not pursue it further. We will restrict our attention to designs in which the $\mathcal{S}_i$'s have equal probability p_i, because this guarantees us a design no worse than that obtained from random sampling, as we demonstrated in (3.11).

4. A random stratified sample: Attempts to reduce the variance of an unbiased estimator of E(Y) have led us to stratified sampling with equal sized strata. Now two other features of the system should be considered. One is that the output of the system is essentially a monotonic function of its inputs. Without loss of generality we may assume it is monotonicly increasing. The other feature is that although many variables may be used as input variables many times only a few of these (perhaps one or two) input variables will account for most (or nearly all) of the variation of the output variables. Exactly which input variables are most important might not be known, but a proper choice of input variables should reveal their identity.

Suppose one component X_1 of $\underset{\sim}{X}$ dominates the output Y. Then the results of the previous section indicate that the range of X_1 should be partitioned into N intervals I_i of equal probability, i.e., $P(X_1 \in I_i) = \frac{1}{N}$. Because $h(\underset{\sim}{X})$ is increasing, these intervals should be connected. That is, we don't want the points in one interval to straddle points from another interval. One point should

be selected at random from each interval, and these N points should be the components which represent X_1 in the N inputs of $\underset{\sim}{X}$ into the system. In this way we not only get a good estimate of the mean of Y, but we also get a good idea of the behavior of Y over the entire range of X_1, and hence $\underset{\sim}{X}$ which is dominated by X_1.

Suppose we don't know which component of $\underset{\sim}{X}$ is the most important. Then several, or perhaps all, components of $\underset{\sim}{X}$ should receive the above treatment. Partition the range of each X_i into intervals I_{ij} of equal probability, so $P(X_i \in I_{ij}) = 1/N$. Select at random one observation from each interval. Use those observations as the inputs into the system. Denote the value obtained from I_{ij} by X_{ij}. Then the inputs $\underset{\sim}{X}_1,\ldots,\underset{\sim}{X}_n$ consist of $\underset{\sim}{X}_k = (X_{1j_1},X_{2j_2},\ldots,X_{Kj_K})$, where the components of $\underset{\sim}{X}_k$ are obtained by combining the elements of $\{X_{ij}\}$ in some random manner. A suitable random manner will be described in the next section.

Note that each point $(X_{1j_1},\ldots,X_{Kj_K})$ represents one K-dimensional subset $\mathcal{S}_{ij} = I_{1j_1}X\ldots XI_{Kj_K}$ of $\mathcal{S}$, and that there are N^K such subsets, which together constitute a partitioning of $\mathcal{S}$. It is only possible to sample from N of these. This suggests that we form groups $\mathcal{S}_i$ of these subsets, N subsets in each group, so that each element of $\{X_{ij}\}$ is represented exactly once in each group. A method for forming these groups is discussed in the next section. Then one of these groups $\mathcal{S}_i$ is chosen in a random manner, so that each group is equally likely to be selected. In this way each portion of $\mathcal{S}$

has some chance of being selected, and the entire range of each X_i, properly stratified, is guaranteed inclusion in the sample. With this in mind we may be comfortable in knowing that no matter which component or components of $\underset{\sim}{X}$ may be dominating the output, the stratification employed in the above design is likely to result in a substantial improvement in the estimate of E(Y) over that obtained by random sampling.

The estimator $\bar{Y}$ is equally likely to equal any of the $\bar{Y}_i$, where $\bar{Y}_i$ represent the sample mean obtained from $\mathcal{S}_i$, $i = 1,\ldots,N^{K-1}$. That is,

$$\bar{Y}_i = \frac{1}{N} \sum_{j \in \mathcal{S}_i} h(\underset{\sim}{X}_{ij}), \quad i = 1,\ldots,N^{K-1}, \tag{4.1}$$

where the summation over $j \in \mathcal{S}_i$ indicates the summation over the N particular subsets that constitute $\mathcal{S}_i$.

Note that the distribution function of $\bar{Y}$ is given by

$$P(\bar{Y} \leq y) = \sum_{i=1}^{N^{K-1}} P(\bar{Y}_i \leq y) \cdot P(\bar{Y} = \bar{Y}_i)$$

$$= \frac{1}{N^{K-1}} \sum_i P(\bar{Y}_i \leq y) \tag{4.2}$$

Therefore the expected value of $\bar{Y}$ equals

$$E(\bar{Y}) = \int y dF_{\bar{Y}}(y) = \frac{1}{N^{K-1}} \sum_i \int y dF_{\bar{Y}_i}(y) = \frac{1}{N^{K-1}} \sum_i \frac{1}{N} \sum_{j \in \mathcal{S}_i} \int h(\underset{\sim}{x}) dF_{ij}(\underset{\sim}{x}) \tag{4.3}$$

where the distribution function $F_{ij}(\underset{\sim}{x})$ of $\underset{\sim}{X}_{ij}$ satisfies

$$\begin{aligned} dF_{ij}(\underset{\sim}{x}) &= N^K dF(\underset{\sim}{x}) \quad \text{if } \underset{\sim}{x} \in \mathcal{B}_{ij} \\ &= 0 \qquad\quad \text{if } \underset{\sim}{x} \notin \mathcal{B}_{ij}. \end{aligned} \tag{4.4}$$

Therefore

$$E(\bar{Y}) = \frac{1}{N^K} \sum_i \sum_{j \in \mathcal{B}_i} \int_{\mathcal{B}_{ij}} h(\underset{\sim}{x}) N^K dF(\underset{\sim}{x}) = \int_{\mathcal{B}} h(\underset{\sim}{x}) dF(\underset{\sim}{x})$$

$$= E(Y) \tag{4.5}$$

and $\bar{Y}$ is an unbiased estimator of $E(Y)$. In a similar manner we get

$$\begin{aligned} Var(\bar{Y}) &= E(\bar{Y} - E(Y))^2 = \int (y - E(Y))^2 dF_{\bar{Y}}(y) \\ &= \frac{1}{N^{K-1}} \sum_i \int (y - E(Y))^2 dF_{\bar{Y}_i}(y) \\ &= \frac{1}{N^{K-1}} \sum_i [E(\bar{Y}_i^2) - 2E(Y)E(\bar{Y}_i) + E^2(Y)]. \end{aligned} \tag{4.6}$$

By adding and subtracting $E^2(\bar{Y}_i)$ inside the brackets we obtain

$$Var(\bar{Y}) = \frac{1}{N^{K-1}} \sum_i Var(\bar{Y}_i) + \frac{1}{N^{K-1}} \sum_i [E(\bar{Y}_i) - E(Y)]^2 \tag{4.7}$$

as the variance of the estimator.

Direct comparisons of (4.7) and (3.10) are difficult to make except in particular cases. In the particular case for which this sampling scheme was designed, namely where one of the input variables

tends to dominate the output variables, (4.7) tends to equal (3.10).

5. A method of stratifying: If the input values $\{X_{ij}\}$, i = 1,...,k, j = 1,...,N are grouped in a completely random manner into input variables $\underset{\sim}{X}_1,\ldots,\underset{\sim}{X}_N$, it is possible to achieve some undesireable situations. For example, if by chance the smallest values of X_1 and X_2 were put into the process together, and the same with the second smallest values, third smallest, and so on, it would be difficult to distinguish between the effects of X_1 and X_2 on the output because their effects were confounded. If X_1 were the dominant input variable, X_2 would appear to be equally important merely because of the unfortunate choice of design. Because the output is a monotonic function of each input variable, it is prudent to match the input variables in such a way that they appear to be uncorrelated. One such way is the following.

Let the different levels of each input variable be denoted, as before, by X_{ij}, where $X_{i1}<\ldots< X_{iN}$. Let $X_{11},X_{12},\ldots,X_{1N}$ represent the "pattern" for X_1. The pattern for X_2 is formed by placing X_{21} as a "seed", and attaching X_{22},X_{23}, etc. alternately to the right, then the left, of the pattern already formed: X_{21}, then X_{21}, X_{22}, then X_{23}, X_{21}, X_{22}, etc., until the pattern for X_2 is established

$$\ldots,X_{25}, X_{23}, X_{21}, X_{22}, X_{24},\ldots \quad .$$

The pattern for X_3 is established by using two seeds for two clusters,

X_{31} X_{32}

then adding to the left of each cluster, right to left,

X_{34}, X_{31} X_{33}, X_{32}

then adding to the right of each cluster, left to right,

$\ldots, X_{34}, X_{31}, X_{35}, \ldots$ $X_{33}, X_{32}, X_{36}, \ldots$

and so on. The pattern for X_4 is established with three seeds, forming three clusters as described above, and so on. This may be extended easily for up to (N/2) + 1 random variables. Since we anticipate that N will exceed twice the number of input variables no difficulty is expected, but another scheme could be used with more input variables.

Once the patterns are established, the matching, i.e., the subspace $\mathcal{S}_i$, is determined as follows. One of the digits from 1 to N is selected at random, say R_2. Then the first R_2 elements in the pattern for X_2 are removed from the front of the pattern (left side), and added to the back of the pattern (right side) without disturbing the relative order of the R_2 elements. This new order determines the order in which the various values of X_2 are placed into the system. The same procedure is repeated by selecting an integer R_3 for X_3, R_4 for X_4. etc. The natural ordering for X_1 may be used without loss of generality. Thus one of the N^{K-1} subspaces $\mathcal{S}_i$ is selected in a random manner. The subspaces $\mathcal{S}_i$ themselves are formed so that a simple graph of Y vs. X_i should reveal the extent of the influence of each input variable on the output.

As an example consider K = 4 and N = 8. The pattern for X_1 is

$$X_{11}, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{18}.$$

The pattern for X_2 is

$$X_{27}, X_{25}, X_{23}, X_{21}, X_{22}, X_{24}, X_{26}, X_{28};$$

for X_3 it is

$$X_{38}, X_{34}, X_{31}, X_{35}, X_{37}, X_{33}, X_{32}, X_{36};$$

and for X_4 it is

$$X_{46}, X_{41}, X_{47}, X_{45}, X_{42}, X_{48}, X_{44}, X_{43}.$$

The first pattern remains intact. By selecting random numbers between 1 and 8, the final order for the other patterns is determined. Suppose the random numbers selected were 2, 2, and 8 (or 0). The new orders are as follows:

X_1: $X_{11}, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{18}$

X_2: $X_{23}, X_{21}, X_{22}, X_{24}, X_{26}, X_{28}, X_{27}, X_{25}$

X_3: $X_{31}, X_{35}, X_{37}, X_{33}, X_{32}, X_{36}, X_{38}, X_{34}$

X_4: $X_{46}, X_{41}, X_{47}, X_{45}, X_{42}, X_{48}, X_{44}, X_{43}.$

The first input is $(X_{11}, X_{23}, X_{31}, X_{46})$, the second is $(X_{12}, X_{21}, X_{35}, X_{41})$ and so on.

This procedure has no claim to optimality. Any procedure for pairing the input variables may be used, as long as the procedure avoids embarassing patterns, and as long as the probability of $X_{i_1 j_1}$ being paired with $X_{i_2 j_2}$, $i_1 \neq i_2$, remains 1/N for all com-

binations of subscripts.

6. An estimate of the variance of Y: In the case of random sampling the usual estimator of the variance is $S_R^2\, N/(N-1)$ where

$$S_R^2 = \frac{1}{N} \sum_{i=1}^{N} (Y_i - \bar{Y}_R)^2 \quad . \tag{6.1}$$

It is well known that

$$E(S_R^2) = Var(Y) - Var(\bar{Y}) \tag{6.2}$$

which, from (2.3), becomes

$$E(S_R^2) = (1 - \tfrac{1}{N}) Var(Y) \tag{6.3}$$

which has a small known bias. Therefore $S_R^2\, N/(N-1)$ is an unbiased estimator of the variance of Y.

With stratified sampling the bias is smaller than in (6.3), but is unknown and therefore not able to be removed. Let the estimator of the variance be

$$S_S^2 = \frac{1}{N} \sum_{i=1}^{N} (h(\underset{\sim}{X}_i) - \bar{Y}_S)^2 = \frac{1}{N} \sum_{i=1}^{N} h^2(\underset{\sim}{X}_i) - (\bar{Y}_S)^2 \tag{6.4}$$

where $\bar{Y}_S$ is given by (3.9) with $p_i = 1/N$. Then

$$E(S_S^2) = \frac{1}{N} \sum_{i=1}^{N} E[h^2(\underset{\sim}{X}_i)] - E(\bar{Y}_S^2) = E(Y) - E(\bar{Y}_S^2). \tag{6.5}$$

Because of (3.4) this becomes

$$E(S_S^2) = Var(Y) - Var(\bar{Y}_S) \tag{6.6}$$

which, because of (3.11), shows that

$$(1 - \frac{1}{N})Var(Y) \leq E(S_S^2) \leq Var(Y). \tag{6.7}$$

Thus S_S^2 has a slight but unknown bias as an estimator for Var(Y).

In the random stratified plan described in section 4 we can let the estimator be

$$S^2 = \frac{1}{N} \sum_{j \epsilon \mathcal{S}_i} (h(\underset{\sim}{X}_{ij}) - \bar{Y}_i)^2 = \frac{1}{N} \sum_{j \epsilon \mathcal{S}_i} h^2(\underset{\sim}{X}_{ij}) - (\bar{Y}_i)^2 \tag{6.8}$$

which is simply the sample variance computed from the observations actually obtained. We can show

$$E(S^2) = Var(Y) - Var(\bar{Y}) \tag{6.9}$$

as follows. Because S^2 is equally likely to be any one of the S_i^2, where S_i^2 is the sample variance when the stratum $\mathcal{S}_i$ is known, we have, as in (4.2),

$$P(S^2 \leq y) = \frac{1}{N^{K-1}} \sum_i P(S_i^2 \leq y) \tag{6.10}$$

so that, as in (4.3),

$$E(S^2) = \frac{1}{N^{K-1}} \sum_i E(S_i^2). \tag{6.11}$$

This in turn becomes

$$E(S^2) = \frac{1}{N^{K-1}} \sum_i E\{\frac{1}{N_i} \sum_{j \in \mathcal{S}_i} h^2(\underset{\sim}{X}_{ij}) - (\bar{Y}_i)^2\}$$

$$= \frac{1}{N^K} \sum_i \sum_{j \in \mathcal{S}_i} \int h^2(\underset{\sim}{x}) dF_{ij}(\underset{\sim}{x}) - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_i^2) \tag{6.12}$$

where, as in (4.3), $F_{ij}(\underset{\sim}{x})$ is the distribution function of $\underset{\sim}{X}_{ij}$. Because of (4.4) we have

$$E(S^2) = E(Y^2) - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_i^2). \tag{6.13}$$

We can add and subtract $E^2(Y)$ and use the identity, from (4.5),

$$\frac{1}{N^{K-1}} \sum_i E(\bar{Y}_i) = E(Y) \tag{6.14}$$

to get

$$E(S^2) = E(Y^2) - E^2(Y) - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_i - E(Y))^2. \tag{6.15}$$

However this becomes, using the middle line of (4.6), (6.9) and we have a form for $E(S^2)$ analogous to the cases in random sampling (6.2) and stratified sampling (6.6). Because the purpose of using the random stratified sample is to obtain a small $\mathrm{Var}(\bar{Y})$ without

knowing which input variables are the most important, we can have some assurance that the bias of S^2 is about as small as the bias of S_S^2 in the case of stratified sampling.

7. Changing the input distribution function: It may happen that the entire simulation of the system is conducted under the assumption that the inputs are governed by the distribution function $F(\underset{\sim}{x})$, and then we want to see how the system behaves when the distribution function is $G(\underset{\sim}{x})$ rather than $F(\underset{\sim}{x})$. If $G(\underset{\sim}{x})$ is not drastically different than $F(\underset{\sim}{x})$ it may not be necessary to repeat the simulation.

As before, the sample space $\mathcal{S}$ of the input variable $\underset{\sim}{X}$ is stratified into subspaces $\mathcal{S}_1,\ldots,\mathcal{S}_N$ of size $p_i = P(\underset{\sim}{X} \in \mathcal{S}_i)$. The distribution function of $\underset{\sim}{X}$ is $F(\underset{\sim}{x})$, and of $\underset{\sim}{X}_i = \underset{\sim}{X} | \underset{\sim}{X} \in \mathcal{S}_i$ is $F_i(\underset{\sim}{x})$ where $dF_i(\underset{\sim}{x}) = dF(\underset{\sim}{x})/p_i$ (see section 3). One value is obtained from each $\mathcal{S}_i$ using random sampling methods. These values $\underset{\sim}{X}_i$, $i = 1,\ldots,N$ are fed into the system to obtain $h(\underset{\sim}{X}_i)$, $i = 1,\ldots,N$, which may be used to estimate $E(h(\underset{\sim}{X}))$.

However now we wish to estimate $E(h(\underset{\sim}{Z}))$, where the distribution function of $\underset{\sim}{Z}$ is $G(\underset{\sim}{x})$ different from $F(\underset{\sim}{x})$. Assume that the range space for $\underset{\sim}{Z}$ is the same as for $\underset{\sim}{X}$. Using the same partition of $\mathcal{S}$ as before, let $q_i = P(\underset{\sim}{Z} \in \mathcal{S}_i)$. And consider the estimator

$$\bar{Y}_{S,G} = \sum_{i=1}^{N} q_i h(\underset{\sim}{X}_i) \tag{7.1}$$

where the values for $h(\underset{\sim}{X}_i)$ are the same ones obtained from the original study of the system. Therefore, as in section 3,

$$E(\bar{Y}_{S,G}) = \sum_{i=1}^{N} q_i E\{h(\underset{\sim}{X}_i)\} = \sum_{i=1}^{N} q_i \int_{\mathcal{B}_i} h(\underset{\sim}{x}) \frac{1}{p_i} dF(\underset{\sim}{x}). \quad (7.2)$$

At this point we need to assume something about the relative behavior of $\underset{\sim}{Z}$ and $\underset{\sim}{X}$ within $\mathcal{B}_i$. We assume that the conditional distribution of $\underset{\sim}{Z}$ given $\underset{\sim}{Z} \in \mathcal{B}_i$ is the same as the conditional distribution of $\underset{\sim}{X}$ given $\underset{\sim}{X} \in \mathcal{B}_i$. Under most circumstances, if $G(\underset{\sim}{x})$ is not drastically different than $F(\underset{\sim}{x})$, if both are reasonably smooth functions, and if $\mathcal{B}_i$ is sufficiently small, then the assumption will be very good. In fact, under the conditions stated both $G(\underset{\sim}{x})$ and $F(\underset{\sim}{x})$ may be approximated reasonably well by a uniform distribution within $\mathcal{B}_i$ for each i.

The above assumption implies

$$\frac{dF(\underset{\sim}{x})}{p_i} = \frac{dG(\underset{\sim}{x})}{q_i} \quad , \qquad \underset{\sim}{x} \in \mathcal{B}_i, \; i = 1,\ldots,N \qquad (7.3)$$

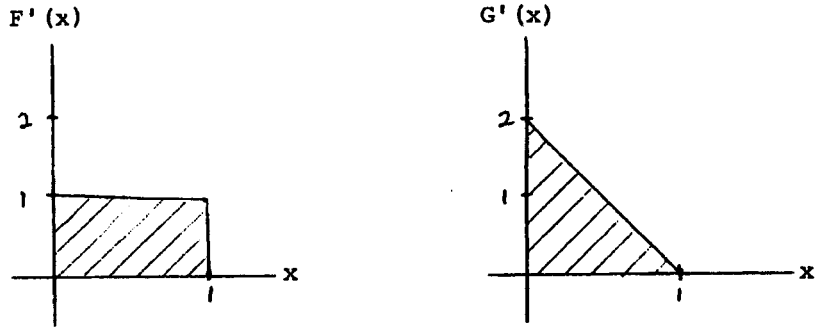
so (7.2) becomes

$$E(\bar{Y}_{SG}) = \sum_{i=1}^{N} q_i \int_{\mathcal{B}_i} h(\underset{\sim}{x}) \frac{1}{q_i} dG(\underset{\sim}{x}) = \sum_{i=1}^{N} \int_{\mathcal{B}_i} h(\underset{\sim}{x}) dG(\underset{\sim}{x})$$

$$= \int h(\underset{\sim}{x}) dG(\underset{\sim}{x}) = E(h(\underset{\sim}{Z})) \qquad (7.4)$$

as desired for an unbiased estimator.

To see how realistic the above assumption might be in a real situation, consider a simple model with $h(x) = x$, $F'(x) = 1$ for $0 < x < 1$, and $G'(x) = 2 - 2x$ in the same region.



Let the N subspaces be given by $\mathcal{S}_i = (\frac{i-1}{N}, \frac{i}{N})$ so that

$$E(X_i) = \int_{\mathcal{S}_i} x dF_i(x) = \int_{\frac{i-1}{N}}^{\frac{i}{N}} x \cdot (N) dx = \frac{i-\frac{1}{2}}{N} \quad . \tag{7.5}$$

Then an unbiased estimate of E(X) is $\bar{X}$,

$$E(\bar{X}) = \frac{1}{N} \sum_{i=1}^{N} E(X_i) = \frac{1}{N} \sum_{i=1}^{N} \frac{i-\frac{1}{2}}{N} = \frac{1}{2}. \tag{7.6}$$

Now suppose Z has the distribution G(x) and we wish to estimate $E(h(Z)) = E(Z)$ using

$$\bar{Y}_{S,G} = \sum_{i=1}^{N} q_i h(X_i) \tag{7.7}$$

where

$$q_i = P(Z \in \mathcal{S}_i) = \int_{\frac{i-1}{N}}^{\frac{i}{N}} (2 - 2x) dx = \frac{2N+1-2i}{N^2} \quad . \tag{7.8}$$

To see if this estimate is unbiased consider

$$E(\bar{Y}_{S,G}) = \sum_{i=1}^{N} q_i E(X_i) = \sum_{i=1}^{N} \left(\frac{2N+1-2i}{N^2}\right)\left(\frac{i-\frac{1}{2}}{N}\right) = \frac{1}{3} + \frac{1}{6N^2} \tag{7.9}$$

Is this right?

which is almost equal to the exact $E(Z) = \frac{1}{3}$. Even though $G(x)$ is considerably different than $F(x)$, the bias of $\bar{Y}_{S,G}$ is quite small for any reasonable sample size N.

If we let $\underset{\sim}{Z}_i$ be $\underset{\sim}{Z}$, given $\underset{\sim}{Z} \in \mathcal{S}_i$, then the above assumption is merely that $\underset{\sim}{Z}_i$ has the same distribution as $\underset{\sim}{X}_i$. Then the derivation of (7.4) is greatly simplified:

$$E(\bar{Y}_{S,G}) = \sum_{i=1}^{N} q_i E\{h(\underset{\sim}{X}_i)\} = \sum_{i=1}^{N} q_i E\{h(\underset{\sim}{Z}_i)\} = E\{h(\underset{\sim}{Z})\} \qquad (7.10)$$

with a little help from (7.4). Furthermore

$$\mathrm{Var}(\bar{Y}_{S,G}) = \sum_{i=1}^{N} q_i^2 \mathrm{Var}\{h(\underset{\sim}{X}_i)\} = \sum_{i=1}^{N} q_i^2 \mathrm{Var}\{h(\underset{\sim}{Z}_i)\}. \qquad (7.11)$$

It is not possible at this point to compare (7.11) with the variance that would arise by random sampling, because we have not discussed how to adjust a random sample of $h(\underset{\sim}{X})$'s to estimate $E\{h(\underset{\sim}{Z})\}$. Intuitively one might use the estimator (compare with (2.1))

$$\bar{Y}_{R,G} = \sum_{i=1}^{N} p_i^* Y_i \qquad (7.12)$$

where

$$p_i^* = GF^{-1}\left(\frac{i}{N}\right) - GF^{-1}\left(\frac{i-1}{N}\right) \qquad (7.13)$$

in the univariate case (K = 1), but justification of (7.13), or an extension of (7.13) to the multivariate case, is not easy to do and won't be discussed further.

If we use

$$S^2_{S,G} = \sum_{i=1}^{N} q_i (h(\underset{\sim}{X}_i) - \bar{Y}_G)^2 \qquad (7.14)$$

as an estimator of $\mathrm{Var}(h(\underset{\sim}{Z}))$, it is easy to show that $S^2_{S,G}$ is biased:

$$\begin{aligned} E(S^2_{S,G}) &= E\{ \sum_{i=1}^{N} q_i h^2(\underset{\sim}{X}_i) - (\bar{Y}_G)^2 \} \\ &= \sum_{i=1}^{N} q_i \int_{\mathcal{S}_i} h^2(\underset{\sim}{x}) dF_i(\underset{\sim}{x}) - E\{(\bar{Y}_G)^2\} \\ &= \sum_{i=1}^{N} \int_{\mathcal{S}_i} h^2(\underset{\sim}{x}) dG(\underset{\sim}{x}) - E^2(h(\underset{\sim}{Z})) - E(\bar{Y}_G)^2 + E^2(h(\underset{\sim}{Z})) \\ &= \mathrm{Var}(h(\underset{\sim}{Z})) - \mathrm{Var}(\bar{Y}_G). \end{aligned} \qquad (7.15)$$

However, efforts at determining the approximate extent of the bias have not been very informative.

Now let us turn our attention to the random stratified sample described in section 4. Consider the same partions $\mathcal{S}_{ij}$ described in section 4, selected in the same manner described in sections 4 and 5. Let q_{ij} be the probability of $\underset{\sim}{Z}$ being in $\mathcal{S}_{ij}$. Again we use the assumption of this section, that the conditional distribution of $\underset{\sim}{Z}$, given $\underset{\sim}{Z} \in \mathcal{S}_{ij}$, is the same as $\underset{\sim}{X}_{ij} = \underset{\sim}{X} | \underset{\sim}{X} \in \mathcal{S}_{ij}$. Because $\mathcal{S}_{ij}$ is a relatively small portion of $\mathcal{S}$, the range space of $\underset{\sim}{X}$, for even moderately large N, this assumption should be reasonable for fairly

smooth distribution functions that do not differ radically from each other.

Let the estimator of $E(h(\underset{\sim}{Z}))$ be

$$\bar{Y}_G = \sum N^{K-1} q_{ij} h(\underset{\sim}{X}_{ij}), \tag{7.16}$$

the weighted average of the same observations recorded in the original simulation study. Then $\bar{Y}_G$ is equally likely to come from each of the $\mathcal{S}_i$, $i = 1,\ldots,N^{K-1}$. As in section 4 we have

$$P(\bar{Y}_G \leq y) = \frac{1}{N^{K-1}} \sum_i P(\bar{Y}_{G,i} \leq y) \tag{7.17}$$

where

$$\bar{Y}_{G,i} = \sum_{j \in \mathcal{S}_i} N^{K-1} q_{ij} h(\underset{\sim}{X}_{ij}) = \bar{Y}_G | \mathcal{S}_i. \tag{7.18}$$

The unbiasedness of $\bar{Y}_G$ is shown as follows.

$$\begin{aligned} E(\bar{Y}_G) &= \int y dF_{\bar{Y}_G}(y) = \frac{1}{N^{K-1}} \sum_i \int y dF_{\bar{Y}_{G,i}}(y) \\ &= \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_{G,i}) = \frac{1}{N^{K-1}} \sum_i \sum_{j \in \mathcal{S}_i} N^{K-1} q_{ij} E\{h(\underset{\sim}{X}_{ij})\} \\ &= \sum_i \sum_j q_{ij} \int h(\underset{\sim}{x}) dF_{ij}(\underset{\sim}{x}) \\ &= \sum_i \sum_j q_{ij} \int_{\mathcal{S}_{ij}} h(\underset{\sim}{x}) \frac{1}{q_{ij}} dG(\underset{\sim}{x}) \\ &= \int_{\mathcal{S}} h(\underset{\sim}{x}) dG(\underset{\sim}{x}) = E\{h(\underset{\sim}{Z})\}. \end{aligned} \tag{7.19}$$

The variance of $\bar{Y}_G$ is found as in (4.6) and (4.7);

$$\mathrm{Var}(\bar{Y}_G) = \frac{1}{N^{K-1}} \sum_i E\{\bar{Y}_{G,i} - E(\bar{Y}_G)\}^2$$

$$= \frac{1}{N^{K-1}} \sum_i \mathrm{Var}(\bar{Y}_{G,i}) + \frac{1}{N^{K-1}} \sum_i [E(\bar{Y}_{G,i}) - E(\bar{Y}_G)]^2. \tag{7.20}$$

The details are given in (4.6) and (4.7).

To estimate the variance of $h(\underset{\sim}{Z})$, consider

$$S_G^2 = \sum_j N^{K-1} q_{ij} (h(\underset{\sim}{X}_{ij}) - \bar{Y}_G)^2 \tag{7.21}$$

where the summation extends over the points actually observed. Note that S_G^2 is equally likely to be computed from any of the strata $\mathcal{S}_i$. So

$$E(S_G^2) = \frac{1}{N^{K-1}} \sum_i E(S_{G,i}^2) \tag{7.22}$$

where

$$S_{G,i}^2 = \sum_{j \in \mathcal{S}_i} N^{K-1} q_{ij} (h(\underset{\sim}{X}_{ij}) - \bar{Y}_{G,i})^2$$

$$= \sum_{j \in \mathcal{S}_i} N^{K-1} q_{ij} h^2(\underset{\sim}{X}_{ij}) - (\bar{Y}_{G,i})^2 \tag{7.23}$$

is S_G^2 given $\mathcal{S}_i$. The expected value of S_G^2 becomes

$$E(S_G^2) = \sum_i \sum_{j \in \mathcal{S}_i} q_{ij} \int h^2(\underset{\sim}{x}) dF_{ij}(\underset{\sim}{x}) - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_{G,i}^2)$$

$$= \sum_i \sum_j \int_{S_{ij}} h^2(\underset{\sim}{x})\, dG(\underset{\sim}{x}) - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}^2_{G,i})$$

$$= E[h^2(\underset{\sim}{Z})] - E^2[h(\underset{\sim}{Z})] + E^2[h(\underset{\sim}{Z})] - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}^2_{G,i})$$

$$= \mathrm{Var}\{h(Z)\} - \frac{1}{N^{K-1}} \sum_i E(\bar{Y}_{G,i} - E[h(\underset{\sim}{Z})])^2 \qquad (7.24)$$

because of the second line in (7.19). The above equation combines with the first line of (7.20) to give

$$E(S^2_G) = \mathrm{Var}\{h(\underset{\sim}{Z})\} - \mathrm{Var}(\bar{Y}_G) \qquad (7.25)$$

to show that S^2_G is a biased estimator of the variance of $h(\underset{\sim}{Z})$, tending to underestimate the true variance.

8. Estimating quantiles: Up to this point we have not used the fact that Y is a monotonic function of each of the components of $\underset{\sim}{X} = (X_1,\ldots,X_K)$, except in section 4 where we discussed the reason for using a random stratified sample rather than an ordinary stratified sample. However, the fact that Y is monotonically increasing in each X_i, $i = 1,\ldots,K$, is of considerable help in estimating the distribution function of Y, and hence in estimating the quantiles of Y.

Let $\underset{\sim}{x} = (\underset{\sim}{x}_1,\ldots,\underset{\sim}{x}_K)$ be an observed value of $\underset{\sim}{X}$ used as an input to obtain $y = h(\underset{\sim}{x})$ as an output. Because of the monotonicity property of Y we have

$$F_Y(y) = P(Y \leq y) \geq P(X_1 \leq x_1, \ldots, X_K \leq x_k) = F(\underset{\sim}{x}) \qquad (8.1)$$

and

$$P(Y > y) \leq P(X_1 > x_1, \ldots, X_K > x_K) \ . \qquad (8.2)$$

These combine to give

$$F(\underset{\sim}{x}) \leq P(Y \leq y) \leq 1 - P(X_1 > x_1, \ldots, X_K > x_K). \qquad (8.3)$$

Note that (8.3) gives absolute bounds on the distribution function of Y for any known input $\underset{\sim}{x}$ and output y, without regard to what sampling scheme if any is used to obtain $\underset{\sim}{x}$.

As a numerical example consider the eight points obtained in section 5. The actual values obtained would be random values within the octants designated for each variable. For the sake of illustration let us assume that the observed value of each X_{ij} falls right at its median, and that the X_{ij} are mutually independent. Therefore we are choosing

$$P(X_{ij} \leq x_{ij}) = \frac{j-1/2}{8} \ , \quad j = 1, \ldots, 8. \qquad (8.4)$$

This leads to the following upper and lower bounds.

Table 1. An example of upper and lower bounds for $P(Y \leq y)$.

$\underset{\sim}{X}_j$	L(y)=lower bound	U(y)=upper bound
$(X_{11},X_{23},X_{31},X_{46})$	.0008	.8112
$(X_{12},X_{21},X_{35},X_{41})$	.0004	.6876
$(X_{13},X_{22},X_{37},X_{47})$	.0387	.9804
$(X_{14},X_{24},X_{33},X_{45})$	.0336	.9048
$(X_{15},X_{26},X_{32},X_{42})$	.0136	.9097
$(X_{16},X_{28},X_{36},X_{48})$	.4154	.9996
$(X_{17},X_{27},X_{38},X_{44})$	.2708	.9988
$(X_{18},X_{25},X_{34},X_{43})$	.0721	.9894

The bounds in Table 1 may be sharpened somewhat after observing the values of Y, because the distribution function of Y, and hence the upper and lower bounds, are increasing functions of y. That is, the actual lower and upper bounds $L^*(y)$ and $U^*(y)$ satisfy

$$L^*(y) = \max_{y_i \leq y} L(y_i)$$
$$U^*(y) = \min_{y_i \geq y} U(y_i) \qquad (8.5)$$

where $y_1,\ldots,y_N$ denote the observed points. If the observed y_i are in the same order as in Table 1, indicating perfect agreement in order with X_1, then the lower and upper bounds would be the following.

Table 2. Illustration when Y agrees in order with X_1.

y_j=point	L*(y)	U*(y)	$P(X_1 \leq x_{1_j})$
y_1	.0008	.6876	.0625
y_2	.0008	.6876	.1875
y_3	.0387	.9048	.3125
y_4	.0387	.9048	.4375
y_5	.0387	.9097	.5625
y_6	.4154	.9894	.6875
y_7	.4154	.9894	.8125
y_8	.4154	.9894	.9375

Because Y agrees with the order of X_1, and therefore with no other X_i's, it is reasonable to assume that the input X_1 has a dominating effect on Y. This leads to using $P(X_1 \leq x_{1j})$ as an estimate of $P(Y \leq y_j)$. A similar table could be devised for the case where the order of $\{y_j\}$ was in perfect agreement with the order of any-one of the X_i's.

1. Remark following section 3, p. 7.

An inequality concerning $\mathrm{Var}(\bar{Y}_S)$ may be obtained as follows. For convenience we will now let $Y_i = h(\underset{\sim}{X}_i)$. As before $p_i = P(\underset{\sim}{X} \in S_i)$. From (3.9) and (3.10) we have

$$\begin{aligned}
\mathrm{Var}\{\bar{Y}_S\} &= \sum_{i=1}^{N} p_i^2 \mathrm{Var}\{Y_i\} = \sum_{i=1}^{N} p_i^2 E(Y_i^2) - \sum_{i=1}^{N} p_i^2 [E(Y_i)]^2 \\
&\leq \max_i p_i \sum_{i=1}^{N} p_i E(Y_i^2) - \frac{1}{N}[E(Y)]^2 - \sum_{i=1}^{N} [p_i E(Y_i)]^2 + \frac{1}{N}[\sum_{j=1}^{N} p_j E(Y_j)]^2 \\
&= \max_i p_i E(Y^2) - \frac{1}{N}[E(Y)]^2 - \sum_{i=1}^{N} \{p_i E(Y_i) - \frac{1}{N}\sum_{j=1}^{N} p_j E(Y_j)\}^2 \\
&= \max_i p_i \mathrm{Var}(Y) + (\max_i p_i - \frac{1}{N}) E^2(Y) - \sum_{i=1}^{N} \{p_i E(Y_i) - \frac{E(Y)}{N}\}^2 .
\end{aligned} \tag{3.14}$$

Note that if $p_i = 1/N$ for all i, we have

$$\mathrm{Var}\{\bar{Y}_S\} = \frac{1}{N} \mathrm{Var}(Y) - \sum_{i=1}^{N} \{E(Y_i) - E(Y)\}^2/N^2. \tag{3.15}$$

2. Remark following section 4, p. 11.

The expression for $\mathrm{Var}(\bar{Y})$ may be written in various forms. Let Y_i represent $h(\underset{\sim}{X}_i) = h(\underset{\sim}{X}) \,|\, \underset{\sim}{X} \in S_i$, and let $Y_{ij} = h(\underset{\sim}{X}_{ij})$. Then (4.1) may be substituted into (4.7) to obtain one of the more useful forms:

$$\mathrm{Var}(\bar{Y}) = \frac{1}{N^{K+1}} \sum_i \sum_j \mathrm{Var}(Y_{ij}) + \frac{1}{N^{K-1}} \sum_i [E(Y_i) - E(Y)]^2 \tag{4.8}$$

which follows easily because of $E(Y_i) = E(\bar{Y}_i)$. For each S_{ij} the term $Var(Y_{ij})$ may be expected to be much smaller than the term $Var(Y)$, because the monotonicity property greatly restricts the range of Y_{ij} relative to Y. Therefore under most circumstances the first $\sum\sum$ above should be quite small compared with $Var(\bar{Y}_R)$. That is,

$$\frac{1}{N}\{\underset{i,j}{\text{ave}}\ Var(Y_{ij})\} << \frac{1}{N}\{Var(Y)\} \tag{4.9}$$

under usual conditions. If the strata S_i are selected so $E(Y_i) = E(Y)$ for all i the remaining terms disappear and $\bar{Y}$ becomes much more accurate than $\bar{Y}_R$ as an estimator of E(Y). This result, combined with (6.9), shows that the bias of S^2 should be quite small under reasonable circumstances.

Also, if all of the variation in Y is due to one component X_j of $\underset{\sim}{X}$, then $E(Y_i) = E(Y)$ and (4.8) reduces to (3.10) with $p_i = 1/N$.

3. Remark following section 6, p. 17.

The following example illustrates some of the ideas thus far presented. Consider $\underset{\sim}{X} = (X_1,\ldots,X_K)$ where the X_i are i.i.d. standard uniform random variables and let $Y = \sum_{i=1}^{K} a_i X_i$ represent the linear response surface. Then

$$E(Y) = \frac{1}{2}\sum_{i=1}^{N} a_i \tag{6.16}$$

and

$$Var(Y) = \frac{1}{12}\sum_{i=1}^{N} a_i^2 \tag{6.17}$$

are the parameters we wish to estimate.

The sample mean $\bar{Y}_R$ from random sampling has a variance, from (2.3)

$$\mathrm{Var}(\bar{Y}_R) = \frac{1}{12N} \sum_{i=1}^{N} a_i^2. \tag{6.18}$$

If we use the random strata sampling plan with cells of equal size $1/N^K$, the variance of Y_{ij} is given by

$$\mathrm{Var}(Y_{ij}) = \mathrm{Var}\{\sum_{\ell=1}^{K} a_\ell X_{\ell,(i,j)}\} = \sum_{\ell=1}^{K} a_\ell^2 \mathrm{Var}\{X_{\ell(i,j)}\}. \tag{6.19}$$

Because the X_i's are i.i.d., each component $X_{\ell,(i,j)}$ has a uniform marginal distribution with variance

$$\mathrm{Var}\{X_{\ell,(i,j)}\} = \int_{\frac{j-1}{N}}^{\frac{j}{N}} [x-\frac{j-1/2}{N}]^2 N \cdot dx = \frac{1}{N^2} \int_0^1 [y-\frac{1}{2}]^2 dx = \frac{1}{12N^2}, \tag{6.20}$$

and (6.19) becomes

$$\mathrm{Var}(Y_{ij}) = \frac{1}{12N^2} \sum_{i=1}^{K} a_i^2. \tag{6.21}$$

Also, for any additive model $Y' = \sum_{i=1}^{K} f_i(X_i)$ we have $E(Y_i) = E(Y)$. In our case this becomes

$$E(Y_i) = E(\bar{Y}_i) = \frac{1}{N} \sum_{\ell=1}^{K} \sum_{j=1}^{N} E(a_\ell X_{\ell,(i,j)}) = \frac{1}{N} \sum_{\ell=1}^{K} a_\ell \sum_{j=1}^{N} E(X_{\ell,(i,j)})$$

$$= \frac{1}{N} \sum_{\ell=1}^{K} a_\ell \sum_{j=1}^{N} \frac{j-1/2}{N} = \frac{1}{2} \sum_{i=1}^{K} a_i. \tag{6.22}$$

Thus (4.8) becomes, from (6.21), (6.22), and (6.16),

$$\mathrm{Var}(\bar{Y}) = \frac{1}{12N^3} \sum_{i=1}^{K} a_i^2. \tag{6.23}$$

The random strata sampling plan reduces the variance of the estimator of the mean by a factor of $1/N^2$ compared with random sampling in this example. For any reasonable sample size this represents a considerable improvement.

The maximum and minimum values for $X_{\ell,(i,j)}$ are $\frac{j}{N}$ and $\frac{j-1}{N}$ respectively. Therefore the maximum and minimum values of $\bar{Y}$ become

$$\max \bar{Y} = \frac{1}{N} \sum_{\ell=1}^{K} a_\ell \sum_{j=1}^{N} \max X_{\ell,(i,j)} = \frac{N+1}{2N} \sum_{i=1}^{K} a_\ell = \frac{N+1}{N} E(Y)$$

and

$$\min \bar{Y} = \frac{N-1}{N} E(Y) \tag{6.24}$$

which leads to 100% confidence bounds on $E(Y)$,

$$\frac{N}{N+1} \bar{Y} \leq E(Y) \leq \frac{N}{N-1} \bar{Y}, \tag{6.25}$$

independent of the coefficients $\{a_i\}$.

The estimator S^2 of the variance $\mathrm{Var}(Y)$ has a very small bias, because of the small size of $\mathrm{Var}(\bar{Y})$ compared with $\mathrm{Var}(Y)$. From (6.9) we have

$$E(S^2) = (1 - \frac{1}{N^3})\mathrm{Var}(Y). \tag{6.26}$$

4. Remark following section 7, p. 24.

We can write $\mathrm{Var}(\bar{Y}_G)$, given by (7.20), in several useful forms. First we will develop one analogous to (4.8).

It is easy to show that

$$E(\bar{Y}_{G,i}) = N^{K-1} \sum_{j \in S_i} q_{ij} E\{h(\underset{\sim}{Z}_{ij})\} = N^{K-1} q_i E(Y_{G,i}) \quad (7.26)$$

where $q_i = P(\underset{\sim}{Z} \in S_i)$ and $E(Y_{G,i})$ is the mean of $h(\underset{\sim}{Z})$, given $\underset{\sim}{Z} \in S_i$. We also have from (7.18),

$$\mathrm{Var}(\bar{Y}_{G,i}) = \sum_{j \in S_i} (N^{K-1} q_{ij})^2 \mathrm{Var}\, h(\underset{\sim}{Z}_{ij}). \quad (7.27)$$

These and (7.19) combine in (7.20) to give

$$\mathrm{Var}(\bar{Y}_G) = \frac{1}{N^{K-1}} \sum_i \sum_j (N^{K-1} q_{ij})^2 \mathrm{Var}\, h(\underset{\sim}{Z}_{ij}) + \frac{1}{N^{K-1}} \sum_i [N^{K-1} q_i E(Y_{G,i}) - E(Y)]^2 \quad (7.28)$$

which reduces to (4.8) when all q_{ij} are equal.

Instead of expressing $\mathrm{Var}(\bar{Y}_G)$ as a sum of the variances within the sub-strata S_{ij}, we may wish to write $\mathrm{Var}(\bar{Y}_G)$ in terms of the overall variance of $h(\underset{\sim}{Z})$. First, from (7.18), (we have

$$\mathrm{Var}(\bar{Y}_{G,i}) = \sum_{j \in S_i} (N^{K-1} q_{ij})^2 \int_{S_{ij}} h^2(\underset{\sim}{x}) \frac{1}{q_{ij}} dG(\underset{\sim}{x}) - \sum_{j \in S_i} (N^{K-1} q_{ij})^2 \cdot E^2(h(\underset{\sim}{Z}_{ij})) \quad (7.29)$$

which is substituted into (7.20) to get

$$\begin{aligned}
\mathrm{Var}(\bar{Y}_G) &= \sum_i \sum_j N^{K-1} q_{ij} \int_{S_{ij}} h^2(\underset{\sim}{x})\, dG(\underset{\sim}{x}) - \sum_i \sum_j N^{K-1} E^2\{q_{ij} h(\underset{\sim}{Z}_{ij})\} \\
&\quad + N^{K-1} \sum_i E^2\{q_i Y_{G,i}\} - E^2(h(\underset{\sim}{Z})) \\
&\leq N^{K-1} \max_{i,j} q_{ij} \cdot \mathrm{Var}(h(\underset{\sim}{Z})) + (N^{K-1} \max q_{ij} - \tfrac{1}{N}) E^2 h(\underset{\sim}{Z}) \\
&\quad - \sum_i \sum_j N^{K-1} E^2\{q_{ij} h(\underset{\sim}{Z}_{ij})\} + N^{K-1} \sum_i E^2\{q_i Y_{G,i}\} \\
&\quad + (\tfrac{1}{N} - 1) E^2(h(\underset{\sim}{Z})). \qquad (7.30)
\end{aligned}$$

This may be written either as

$$\begin{aligned}
\mathrm{Var}(\bar{Y}_G) &\leq N^{K-1} (\max_{i,j} q_{ij}) \mathrm{Var}(h(\underset{\sim}{Z})) + (N^{K-1} \max q_{ij} - \tfrac{1}{N}) E^2 h(\underset{\sim}{Z}) \\
&\quad - N^{K-1} \sum_i \sum_j [E\{q_{ij} h(\underset{\sim}{Z}_{ij})\} - \tfrac{1}{N} E\{q_i Y_{G,i}\}]^2 \\
&\quad + (N-1) N^{K-2} \sum_i [E\{q_i Y_{G,i}\} - \frac{1}{N^{K-1}} E\{h(\underset{\sim}{Z})\}]^2 \qquad (7.31)
\end{aligned}$$

or

$$\begin{aligned}
\mathrm{Var}(\bar{Y}_G) &\leq N^{K-1} (\max_{i,j} q_{ij}) \mathrm{Var}(h(\underset{\sim}{Z})) + (N^{K-1} \max q_{ij} - \tfrac{1}{N}) E^2 h(\underset{\sim}{Z}) \\
&\quad - N^{K-1} \sum_i \sum_j [E\{q_{ij} h(\underset{\sim}{Z}_{ij})\} - \frac{1}{N^K} E\{h(\underset{\sim}{Z})\}]^2 \\
&\quad + N^{K-1} \sum_i [E(q_i Y_{G,i}) - \frac{1}{N^{K-1}} E\{h(\underset{\sim}{Z})\}]^2. \qquad (7.32)
\end{aligned}$$

If all q_{ij} are equal, the inequalities in (7.30), (7.31), and (7.32) become equalities, and the expressions simplify to give alternative forms for $\mathrm{Var}(\bar{Y})$, instead of (4.7).

5. Remark following section 8, p. 27.

A further sharpening of the upper and lower bounds is possible by noting that if $h(\underset{\sim}{x}) \leq h(\underset{\sim}{x}_1)$, and $h(\underset{\sim}{x}_1) \leq h(\underset{\sim}{x}_2)$, then $h(\underset{\sim}{x}) \leq h(\underset{\sim}{x}_2)$. That is, order the observed values of $Y = h(\underset{\sim}{X})$,

$$h(\underset{\sim}{x}_1) \leq h(\underset{\sim}{x}_2) \leq \ldots \leq h(\underset{\sim}{x}_N),$$

and let $A_i = \{\underset{\sim}{x} \text{ such that } h(\underset{\sim}{x}) \leq h(\underset{\sim}{x}_i)\}$. Then

$$P(Y \leq y_j) \geq P(\bigcup_{i=1}^{j} A_i). \tag{8.6}$$

Similarly, let $B_i = \{\underset{\sim}{x} | h(\underset{\sim}{x}) > h(\underset{\sim}{x}_i)\}$, so

$$P(Y \leq y_j) \leq 1 - P(\bigcup_{i=j}^{N} B_i). \tag{8.7}$$

In the above example the bounds (the best possible) are given in Table 3, for the same order of y's as before.

Table 3. Optimal bounds for $P(Y \leq y_j)$

y_j = point	L**(y)	U**(y)
y_1	.0008392	.5436249
y_2	.0012359	.6260224
y_3	.0390167	.8460846
y_4	.062088	.854599
y_5	.0689544	.9067231
y_6	.4213714	.9883271
y_7	.5209197	.9886017
y_8	.5305328	.9894257

These bounds are called the best possible, because it is possible for a function $h_1(\underset{\sim}{X})$ to touch each value in L**(y), and for another function $h_2(\underset{\sim}{X})$ to attain each given value of U**(y). It is not possible to make probability statements within those bounds unless some further assumptions are made concerning the form of $h(\underset{\sim}{X})$. Note that the bounds given in Table 3 form a 100% confidence band on the distribution function of Y.

Perhaps it is adviseable to select the values of $\underset{\sim}{X}$ in order to form better (in some sense) bounds on $P(Y \leq y)$. For example, the upper bound U**(y) in the above example never goes lower than .544. If we chose one value of $\underset{\sim}{X} = \underset{\sim}{x}_0$ which represents the "minimum likely value", say the one that gives $P(\underset{\sim}{X} \leq x_0) = .001$, then for reasonable K, say $K \leq 10$, we have $U^{**}(h(\underset{\sim}{x}_0)) \leq .01$, which "closes off" the left side of the band for $P(Y \leq y)$. A similar "maximum likely value" would close off the right side of the band. Perhaps a judicious choice of interior points would provide a narrower band than would be obtained by random stratified sampling. This is an open question.

It should be noted that a change of distribution function from $F(\underset{\sim}{x})$ to $G(\underset{\sim}{x})$ does not cause any difficulties, other than recomputing the bounds L**(y) and U**(y).

Appendix B

The Evolution of Latin Hypercube Sampling

R.L. Iman

February 1980

The Evolution of Latin Hypercube Sampling

compiled by

R. L. Iman

February 1980

Latin hypercube sampling was first suggested by W. J. Conover in the early fall of 1975 when Mike McKay told Conover that LASL had a problem with selecting input values for a computer code which had 200 input variables and took 8 1/2 hours to do a single run (this was a LOCA type computer code).

At the First ERDA Statistical Symposium held at LASL from November 3-5, 1975, McKay gave a presentation which included comments about stratified sampling and referenced some work done by Conover in this area (W. J. Conover, Private Communication, 1975). At this same symposium, Conover, in discussing George Steck's presentation of the work done by Steck and Easterling on the LOCA problem, clearly outlined the scheme now called Latin hypercube sampling although the name was not used.

In the fall of 1975 I started working on the LOCA problem after coming to Sandia in August. In my communications with Conover, I was informed of the efforts at LASL and Conover sent me a copy of his unpublished manuscript entitled "On a Better

Method of Selecting Input Variables" which described in detail how to do LHS and the benefits of LHS although not using the name LHS. I used LHS and repeated the examples given by Steck, Dahlgren, and Easterling (1975). The results were much better fits (i.e., smaller residuals) with fewer (at least 1/3) runs. Thus encouraged I continued using LHS (in a sequential manner) on the LOCA problem as reported in Steck, Iman, and Dahlgren (1976).

In September 1976, McKay, Conover, and Whiteman issued an informal LASL report which compared LHS with random sampling and fractional factorial sampling using a model called SOLA-PLOOP. This was the first written report to use the name Latin hypercube sampling.

In January 1977 a manuscript by McKay, Conover, and Beckman detailing how to do LHS and comparing it with random and stratified sampling was submitted to Technometrics. This article appeared in May 1979.

During 1977 I started work on the waste isolation project and in the fall of that year I started using sequential LHS on the Pathways model with good results. These results along with sensitivity analysis techniques appear in Iman, Helton, and Campbell (1978).

Since that time LHS has been used on the SWIFT transport model, on the NWFT transport model, on a salt dissolution model developed by Herb Shaw at USGS, in a repeated extensive sensitivity analysis on the Pathways model, in a study of the asymptotic

properties of the Pathways model, and on a flow model for the geologically complex (64 input variables) Nevada Test Site. In each case the results were carefully studied by both the modeler and myself with the modeler satisfied with the results each time.

In addition, in a unique application LHS was used to study the numerical dispersion of the NWFT model. This represented the first time that sensitivity analysis techniques had been used in this manner and led to significant changes in the way the model did the calculations with the immediate results that the greatly simplified NWFT model was able to quickly and accurately reproduce the time consuming and costly SWIFT calculations.

At the annual ASA meeting in San Diego in August 1978, a session chaired by Easterling entitled "Statistical Problems in Nuclear Regulation" was held. During this meeting response surface fitting was discussed and during this meeting Dick Beckman from LASL said he had set up every difficult situation he could think of to test LHS and in every case the people at LASL had been able to determine the important variables.

In the summer of 1978 Conover and I started work on a report entitled "Small Sample Sensitivity Analysis Techniques with an Application to Risk Assessment" which generalized LHS w.r.t. to changing input distribution assumptions. This work was presented at the annual ASA meeting in Washington, D.C. in

August 1979. This work was recently expanded to make direct comparisons with random sampling and replicated (sequential) Latin hypercube sampling and has just been completed.

In November 1978, McKay, Ford, Moore, and Witte issued an informal LASL report which used a 72 input variable model called COAL2 as a basis for comparing the ability of LHS and a 3 point sampling scheme to determine important variables with samples of size 10, 15, 20, and 25. "Truth" was determined by comparing the variable selection with a sample of size 100.

In the fall of 1979 a distribution free procedure was developed (Iman and Conover (1980)) that allows dependence among input variables (i.e., correlations) to be included with LHS or random sampling. This is something that cannot be done with fractional factorial sampling. This document is currently undergoing review.

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