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Use of replicated Latin hypercube sampling to estimate sampling variance in uncertainty and sensitivity analysis results for the geologic disposal of radioactive waste

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ABSTRACT

The 2008 performance assessment (PA) for the proposed repository for high-level radioactive waste at Yucca Mountain (YM), Nevada, used a Latin hypercube sample (LHS) of size 300 in the propagation of the epistemic uncertainty present in 392 analysis input variables. To assess the adequacy of this sample size, the 2008 YM PA was repeated with three independently generated (i.e., replicated) LHSs of size 300 from the indicated 392 input variables and their associated distributions. Comparison of the uncertainty and sensitivity analysis results obtained with the three replicated LHSs showed that the three samples lead to similar results and that the use of any one of three samples would have produced the same assessment of the effects and implications of epistemic uncertainty. Uncertainty and sensitivity analysis results obtained with the three LHSs were compared by (i) simple visual inspection, (ii) use of the *t*-distribution to provide a formal representation of sample-to-sample variability in the determination of expected values over epistemic uncertainty and other distributional quantities, and (iii) use of the top down coefficient of concordance to determine agreement with respect to the importance of individual variables indicated in sensitivity analyses performed with the replicated samples. The presented analyses established that an LHS of size 300 was adequate for the propagation and analysis of the effects and implications of epistemic uncertainty in the 2008 YM PA.

1. Introduction

Latin hypercube sampling is a very effective and popular procedure for the propagation of epistemic uncertainty in analyses of complex systems [1–3]. The effectiveness and resultant popularity of Latin hypercube sampling derives from the fact that a relatively small Latin hypercube sample (LHS) can be used in the generation of a mapping between uncertain analysis inputs and corresponding uncertain analysis results that can then be successfully explored with a variety of uncertainty and sensitivity analysis procedures [4].

Analyses of complex systems typically involve large and computationally demanding models. As a consequence, it is necessary to use an efficient sampling procedure such as Latin hypercube sampling in the propagation of epistemic uncertainty as the number of model evaluations that can be performed is limited by computational cost. For example, the U.S. Nuclear Regulatory Commission's (NRC's) reassessment of risk from commercial nuclear power plants used LHSs of size 200 and 250 from approximately 150 to 200 epistemically uncertain analysis inputs in probabilistic risk assessments (PRAs) for five nuclear power stations [5–11], and the U.S. Department of Energy's (DOE's) performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP) carried out in support of a successful Compliance Certification Application [12,13] to the U.S. Environmental Protection Agency (EPA) used an LHS of size 100 from 57 epistemically uncertain analysis inputs [14]. The indicated reactor PRAs are often referred to as the NUREG-1150 PRAs in consistency with the associated NRC report [11].

The potential effectiveness, and hence appropriateness, of the use of the indicated small sample sizes in complex and important analyses is open to question and needs to be established. In response to this need, a replicated sampling procedure has been proposed to establish the adequacy of the use of small LHSs in the analysis of complex systems [15]. This procedure has been used to establish the adequacy of the LHS sizes in the NUREG-1150 PRAs [16], the WIPP PA [13,17], and an analysis with the MACCS reactor

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accident consequence model [18]. A recently completed large analysis that used replicated Latin hypercube sampling to assess the stability of uncertainty and sensitivity analysis results obtained with a relatively small LHS is the 2008 PA for the proposed Yucca Mountain (YM) repository for high-level radioactive waste [19]. Specifically, this analysis used an LHS of size 300 to propagate 392 epistemically uncertain variables through a complex analysis involving a large number of linked models.

The purpose of this presentation is to describe the use of replicated Latin hypercube sampling in the 2008 YM PA. The following topics are considered: (i) definition and properties of replicated sampling (Section 2), (ii) stability of uncertainty analysis results (Section 3), and (iii) stability of sensitivity analysis results (Sections 4 and 5). The presentation then ends with a summary discussion (Section 6).

This presentation is based on a talk [20] given at the 2010 Sensitivity Analysis of Model Output (SAMO) conference held in Milan, Italy, and is part of a special issue of *Reliability Engineering & System Safety* containing papers presented at this conference. A companion paper in this special issue contains a description of the 2008 YM PA and provides an adequate level of background for this presentation on replicated sampling in the 2008 YM PA [21]. More detailed information on the 2008 YM PA is available in Ref. [19] and in the large number of model-specific reports cited in this reference. A less detailed overview of the 2008 YM PA is available in a sequence of conference papers [22–28]. A special issue of *Reliability Engineering & System Safety* on the 2008 YM PA is also currently in preparation.

2. Definition and properties of replicated sampling

Analyses of complex systems typically maintain a separation of aleatory uncertainty and epistemic uncertainty, where aleatory uncertainty arises from an inherent variability in the behavior of the system under study and epistemic uncertainty arises from a lack of knowledge about the appropriate values to use for analysis inputs that have fixed but poorly known values [29–39]. Thus, aleatory uncertainty is a property of the system under analysis while epistemic uncertainty is a property of the knowledge base of the individuals performing the analysis. Typically, probability is the mathematical structure used to characterize both aleatory uncertainty and epistemic uncertainty. Alternatives to probability for the representation of epistemic uncertainty such as interval analysis, possibility theory and evidence theory also exist [40–42]; however, these alternatives to probability for the representation of epistemic uncertainty are not, at present, widely used in analyses for complex systems that maintain a distinction between aleatory uncertainty and epistemic uncertainty. Consistent with general practice, the 2008 YM PA uses probability in the characterization of both aleatory uncertainty and epistemic uncertainty.

As indicated in the Introduction, the 2008 YM PA considers 392 epistemically uncertain analysis inputs (see [19], Tables K3-1, K3-2, K3-3, for a complete listing of these variables and their assigned distributions characterizing epistemic uncertainty). As a fundamental part of the 2008 YM PA, it is necessary to propagate the uncertainty in these variables through the analysis in a manner that (i) maintains a separation of the effects of aleatory uncertainty and epistemic uncertainty, (ii) provides an informative display of the epistemic uncertainty in analysis results that derives from epistemic uncertainty in analysis inputs, and (iii) provides a basis for the application of a variety of sensitivity analysis procedures to determine the effects of epistemic uncertainty in individual analysis inputs on analysis results. Further, due to the size and computational cost of the analysis, the propagation procedure had to provide information on a large number of analysis results (see [19], Table K4.1-1) with a relatively small sample size.

Because of its successful application in prior analyses of complex systems (e.g., the previously indicated NUREG-1150 PRAs, the WIPP PA, and the MACCS analysis), Latin hypercube sampling was chosen as the sampling procedure for the propagation of epistemic uncertainty in the 2008 YM PA. As a reminder, Latin hypercube sampling operates in the following manner to generate a sample of size $nLHS$ from the distributions D_1, D_2, …, D_{nE} associated with the elements of the vector $\mathbf{e}=[e_1, e_2, \ldots, e_{nE}]$ of epistemically uncertain analysis inputs. The range of each e_j is exhaustively divided into $nLHS$ disjoint intervals of equal probability and one value e_{ij} is randomly selected from each interval. The $nLHS$ values for e_1 are randomly paired without replacement with the $nLHS$ values for e_2 to produce $nLHS$ pairs. These pairs are then randomly combined without replacement with the $nLHS$ values for e_3 to produce $nLHS$ triples. This process is continued until a set of $nLHS$ nE-tuples

$$\mathbf{e}_i=[e_{i1},e_{i2},\ldots,e_{i,nE}],\quad i=1,2,\ldots,nLHS, \tag{1}$$

is obtained, with this set constituting the LHS. If needed, a restricted pairing technique exists that can be used to induce a specified rank correlation structure in an LHS [43,44].

As previously indicated, the 2008 YM PA used an LHS of size $nLHS=300$ in the propagation of the epistemic uncertainty associated with $nE=392$ analysis inputs. Although this sample was computationally practicable, its small size relative to the number of variables being sampled and propagated was an issue that had to be addressed. Specifically, most analyses with Latin hypercube sampling use a sample size (i.e., $nLHS$) that is larger than the number of epistemically uncertain variables being sampled (i.e., nE). Thus, it is natural to question if an LHS of size $nLHS=300$ from $nE=392$ analysis inputs is sufficiently large to produce meaningful results. As a reminder, the 2008 YM PA was performed as a primary support for what was anticipated would be a very contentious license application to the NRC for the construction of the YM repository. Issues such as adequacy of sample size could not be left unaddressed. In response to this important need, a replicated sampling sample procedure was chosen to address the issue of sample size adequacy [15].

At a conceptual level, the replicated sampling procedure is very simple as it is based on generating nR LHSs with different non-overlapping sequences of random numbers. This results in a random sample of size nR from the universe of all possible LHSs of a given size (i.e., $nLHS$) that could be generated from the epistemically uncertain variables under consideration. The outcomes associated with these nR randomly generated LHSs can then be analyzed to determine if consistent results are being obtained across the nR LHSs. The 2008 YM PA used $nR=3$ replicated LHSs of size $nLHS=300$ from $nE=392$ epistemically uncertain analysis inputs. These replicated samples were then used to assess the stability of sampling-based results obtained in the 2008 YM PA. For notational convenience, these three samples will be represented by

$$R_r:\mathbf{e}_{ri},\quad i=1,2,\ldots,nLHS=300, \tag{2}$$

for $r=1, 2, 3$.

The uncertainty and sensitivity analysis results obtained in the 2008 YM PA are based on the presentation and exploration of results obtained with LHSs of the form indicated in Eqs. (1) and (2). A related approach to uncertainty and sensitivity analysis is known as Bayesian Analysis of Computer Code Outputs (BACCO) [45–47]. The BACCO approach involves two steps: (i) a sample of the uncertain analysis inputs and the associated model evaluations are used to construct an emulator that provides a statistical