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Computation of Sensitivity Indices with different routines for Latin Hypercube Designs

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Abstract

Complex mathematical simulations are performed to understand the various phenomena in physics, chemistry, etc. Usually these models consist of several input variables and sensitivity analysis explains the variation of computer code output due to the changes in the input values. We have used the software package, Gaussian Emulation Machine for sensitivity analysis (GEM-SA), (Kennedy and O'Hagan, 2006) for performing sensitivity analysis and chosen Rosenbrock function as a test problem. In this paper we have studied the effect of different available software routines for Latin hypercube designs (LHD) on values of the variance-based sensitive indices, total sensitive indices and roughness parameters for the test problem. We have used MATLAB, R software and GEM-SA modules for LHD.

Keywords: Bayesian analysis; Computer model; Sensitivity analysis; Latin hyperspace design;

1. Main text

Large computer simulations are performed in many areas of science and engineering for the study of physical systems, optimization of the designs, etc. The output of these simulations usually depends in a complex way on several input variables. Sensitivity and uncertain analysis are important techniques for understanding the variation of the output on the changes in the input variables. An introduction of global sensitivity analysis was given by Saltellia et al. (2004). Two important measures of sensitivity analysis are variance-based sensitivity indices and total sensitivity indices. A Bayesian approach to probabilistic sensitivity analysis was developed by Oakley and O'Hagan (2004). In this method, the sensitivity of model output variation is decomposed into components representing main effects and interactions of the input variables. One of the advantages of these methods is that it requires far fewer runs than that are needed for Monte-Carlo based methods. Based on this approach, a software package Gaussian Emulation Machine for Sensitivity Analysis (GEM-SA) was developed by Marc Kennedy for the Center for Terrestrial Carbon dynamics (CTCD) (Kennedy and O'Hagan, 2006).

One of the requirements of Gaussian emulations is that the design for the input point should have good space filling property. Designs based on maximin LHD fulfill this requirement. Some of the commonly available routines for LHD are available in these software products: 1) GEM-SA 2) MATLAB and 3) R software. To study the effect of these software routines on values of the sensitivity indices, we have chosen Rosenbrock function as a test problem. The multi-dimensional Rosenbrock function is given by.

$$f(x) = \sum_{i=1}^{N-1} [(1 - x_i)^2 + 100(x_{i+1} - x_i^2)^2] \quad \forall x \in R^N \quad (1)$$

LHD design points are generated between range (-2, 2) for following test cases:

- a) 2 input variables with 100, 200 and 400 training points.
- b) 4 input variables with 100, 200 and 400 training points.

It is found that for the case a) with the 2 inputs, all the routines for LHD give almost nearly equal values for the variance-based sensitive indices and total sensitive indices. For the case b) with 4 inputs, there is a large difference in the values generated with all the routines with 100 and 200 training points. The roughness parameters and the sensitivity indices are nearly equal for MATLAB and R routines for LHD with 400 training points. The difference between the values for sensitivity indices generated by GEM-SA is around 10 % with the other routines in this case (see, Table 1).

Table1: Sensitivity indices for third input variable x_3 from test case b) with 400 training points.

	MATLAB	GEM-SA	R Software
Variance (%)	28.57	29.85	28.89
Total Effect	42.65	43.28	41.77
Roughness Parameter	6.64	12.63	6.92

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