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COMPARING ADAPTIVE SAMPLING ALGORITHMS ON PROBABILISTIC EVALUATIONS OF RARE SCENARIOS

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Abstract

The consideration of uncertainties in nuclear safety analyses can be achieved in the framework of best-estimate-plus-uncertainty (BEPU) approaches using Monte Carlo simulations. For each simulation run, a set of input parameter values is sampled according to a multivariate probability distribution and applied to a deterministic simulation code. SUSA is an established software for uncertainty and sensitivity analyses, covering such BEPU analyses from input parameter sampling to simulations and statistical evaluation, for instance, of tolerance intervals for the simulation outcome.
A classical Monte Carlo sampling approach becomes resource intensive for analyses focused on the evaluation of scenarios with rare events in the simulation outcome space (rare scenarios). These events can typically only be reached from small regions of the input parameter space. A large number of simulations would be required to identify the region of interest in the input parameter space and accurately quantify the probability of the rare event.
To perform probabilistic evaluations of rare scenarios with reasonable computational effort, adaptive sampling techniques can be used. Thereby, machine learning algorithms are used to iteratively adapt the sampling range of input parameters to those that most effectively increase the robustness and accuracy of the probabilistic evaluation.
Recently, two adaptive sampling approaches have been implemented in SUSA. One approach uses a support vector regression metamodel in the context of a subset simulation and the other approach uses a combination of a genetic adaptive sampling algorithm with an ensemble of classification algorithms. In this contribution, both algorithms are compared while getting applied to benchmark examples as well as to an accident scenario in a nuclear power plant.

Keywords: Adaptive Sampling, Uncertainty Quantification, Safety Analysis, SUSA.

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1 INTRODUCTION

So-called best-estimate-plus-uncertainty (BEPU) approaches have been developed to account for uncertainties in safety analyses of postulated accidents at a nuclear power plant (NPP). In such BEPU approaches, a deterministic simulation model of the scenario is applied, and the influence of the uncertain parameters supplied as input to the simulation is examined using Monte Carlo (MC) sampling methods. The simulation results of each set of sampled input parameters are then used for statistical evaluations of the resulting uncertainty. The software used in this work, SUSA (Software for Uncertainty and Sensitivity Analyses) [1], provides the tools for such BEPU analyses, from sampling the values of the uncertain parameters based on given univariate distributions and dependencies between the parameters (e. g. correlations, conditional distributions, functional relationships), the application of the sampled parameter sets to a simulation code, and the statistical evaluation of the simulation results.

To evaluate the probability of a rare event in the simulation outcome space which can be derived only from a small range of the input parameter space, a classical MC sampling approach becomes inefficient. A large number of simulation runs would be required to obtain a sufficient number of these unwanted rare events to perform an accurate probabilistic evaluation. For complex models, such as the thermal-hydraulic model of an NPP, even a single simulation run can be time consuming, and computing a large number of simulations would not be feasible. Therefore, adaptive sampling techniques have been developed to reduce the number of simulation runs while obtaining a probability estimate of high precision.

Currently, two adaptive sampling techniques have been implemented in SUSA. In this work, both approaches are briefly presented before being compared using two benchmark applications, a biometric dose model and the Ishigami function. Finally, a loss-of-coolant accident (LOCA) scenario in an NPP is considered, where the rare undesired event is defined as an exceedance of the peak cladding temperature (PCT) of 1200 °C.

2 ADAPTIVE SAMPLING APPROACHES IN SUSA

Adaptive sampling algorithms have been developed to reduce the number of samples required for analyses of rare events by iteratively adapting the sample range to the analysis objectives. Given a dataset of sampled input parameter sets, e.g., from a classical MC sample, with the corresponding results of their simulation runs, the idea of adaptive sampling methods is to iteratively train and refine a metamodel, e.g., a machine learning algorithm, to predict the simulation outcomes of interest until a precise computation of the desired analysis target (e. g. probability of the rare event) is achieved.

At each iteration, the metamodel is refined by identifying regions of the input parameter space that are either most promising to lead to the rare event of interest or that have the greatest predictive uncertainties. Simulation runs are performed using the most promising parameter sets from the identified regions, expanding the training data set for the metamodels. With this approach, the metamodels are trained with a minimal number of simulation runs while providing accurate estimates of the analysis targets.

To identify promising candidate parameter samples, there is a tradeoff between exploring the unknown parameter space and tending to predict results near the desired region of interest (rare event). In both cases, a metric or distance measure must be defined in the multidimensional parameter space or metamodel related predictions to sort the candidates and evaluate how promising they are. Since the desired region of interest may also depend on multiple simulation outcome variables, this approach is also applicable to identify possible input parameter sets that lead to a combined rare event.

For simplicity, the desired region of interest in the example applications of this paper depends on only a single simulation outcome variable. This also simplifies the metamodels, which only need to predict the final state of a single simulation variable. However, in general, metamodels can also be trained to predict multiple parameters of the simulation outcome for more complex applications.

Choosing how to build the metamodel and identifying the most promising parameter samples are the key challenges of adaptive sampling approaches and the main differences. The following subsections describe the different approaches implemented in SUSA that solve these challenges, including the adjustable termination criteria of the algorithms.

2.1 Subset Simulation with Support Vector Regression (SuSSVR)

Subset Simulation (SuS) is a combined sampling and simulation approach for small failure probabilities described as the product of much larger conditional probabilities of intervening events approaching the actual failure event, while the conditional samples for each intervening event are sampled using Marcov Chain Monte Carlo simulation [2,3]. In the adaptive sampling algorithm implemented in SUSA, Support Vector Regression (SVR) is used as a metamodel within the Subset Simulation to predict the simulation outcome, as described in [4].

This SuSSVR algorithm consists of three iteration cycles. In a first cycle, the algorithm is repeated until at least a certain percentage of the training dataset, e.g., 10%, is in the desired region of interest. In a second cycle, the goal of the algorithm is to converge to a robust metamodel, i.e., a robust prediction of the SVR. Adjustable threshold parameters are given for the so-called switching rate, i.e., the mean fraction of parameter sets in the last subset sample that were classified differently in the last – say 5 - iterations and the mean rate of change of the rare event probabilities calculated in the last iterations. In both cycles, the new parameter candidates for runs with the actual simulation code and, thus, for the training dataset, are selected from the last subset sample obtained in an iteration step (random or cluster-based selection). The last cycle is iterated using a larger subset sample size to obtain a robust rare event probability estimate. The number of iterations in the last cycle is 10 or more to get information on the variation of the probability estimate due to the random sampling. Since no refinement of the metamodel is performed and thus no further simulation run with the actual simulation code is required, this cycle is comparatively fast.

2.2 GASA-PRECLAS Algorithm

The Genetic Adaptive Sampling Algorithm combined with the Probability Estimation using an Ensemble of Classification Algorithms (GASA-PRECLAS) presented in [5] consists of two iteration cycles and divides the sampling problem into two parts, each of which is solved using an optimized algorithm. First, the GASA algorithm is used to effectively explore the parameter space to obtain a training dataset with a certain number of samples in the region of interest, e.g., n=5 samples. The GASA algorithm provides the training data so that the classifiers in the second cycle can distinguish between interesting and uninteresting events. Its aim is comparable to the first cycle of the SuSSVR algorithm. If there are multiple regions of interest that are separated from each other, this should also be taken into account when choosing the termination criterion of the GASA algorithm, i.e., the number of samples in the desired region of interest should be increased.

The second cycle uses a combination of classification algorithms as a metamodel to predict whether a parameter sample leads to a rare event. A Bayesian approach is used to calculate the probability distribution for the likelihood of the rare event based on a large parameter sample generated at each iteration and the corresponding predictions of the fitted classification

metamodels. The adjustable termination criteria refer to the variation of the calculated probability distribution of the rare event over the last – say 5 - iterations. The use of an ensemble of classification algorithms reduces the impact of the uncertainties of a single classification algorithm and the impact of an incorrect prediction. Combined with the Bayesian calculation of the probability distribution, an additional refinement loop for the probability estimate and its uncertainty - as in the SuSSVR algorithm - is not necessary. At each iteration step, the new parameter candidates for the actual simulation runs are selected from the large parameter sample which is also the basis for the estimation of the rare event probability. The selection of the candidates is based on criteria associated with the fitted metamodels and calculated for each element of the parameter sample.

3 COMPARISON ON APPLICATION EXAMPLES

Two benchmark functions are used to analyze the implemented adaptive sampling methods. Both consist of a simple function that can be quickly evaluated. The first example with a biological dose model tests how a very small probability (~1E-06) can be estimated in a 6-dimensional parameter space. The second example with the Ishigami function tests how to identify four separate regions in a strongly non-linear function. Although this is only a three-dimensional problem with a probability of about 1E-03, finding all four maxima of this function is a difficult task that requires advanced sampling algorithms for proper likelihood estimation.

Finally, a thermal-hydraulic code simulating a LOCA scenario in an NPP is used as a more realistic and complex application example where a single simulation run requires several hours. This example considers a high-dimensional parameter space (35 uncertain parameters) and demonstrates the need for an adaptive sampling algorithm, as a classic MC sampling would require at least 1E04 or more simulation runs, which is not feasible.

3.1 Benchmark Example: Biologic Dose Model

In this example, it is assumed that during the normal operation of an NPP small concentrations of radionuclides are released and enter the food chain of a population group. To calculate the maximum annual dose-equivalent of an individual of the population group, the following simple deterministic model is applied:

$$y = c \cdot (x_{rate1} \cdot x_{conc1} + x_{rate2} \cdot x_{conc2}) \cdot exp(-0.2 \cdot dt), \quad (1)$$

The description of the parameters and their distributions is listed in Table 1.

Name	Symbol	Distribution	Distribution parameter
Dose conversion factor	c	Normal	Mean=3.29E-08, std=1.11E-08, Min=1.E-08, Max=5.E-08
Consumption rate of meal 1	x_{rate1}	Log-Uniform	Min=10, Max=100
Radio-Concentration in meal 1	x_{conc1}	Uniform	Min=10, Max=35
Consumption rate of meal 2	x_{rate1}	Log-Normal	Mean=4.7552, std=0.1993, Min=0.5, Max=400
Radio-Concentration in meal 2	x_{conc2}	Uniform	Min=10, Max=30
Delay time	dt	Triangular	Mode=8, Min=0.5, Max=20

Table 1: Uncertain parameters and their distributions for the Biologic Dose Model.

The region of interest is defined by the maximum annual dose equivalent exceeding 0.25 mSv, which means that in Eq. (1) the result y exceeds 2.5E-04. A simple MC sample of the

formula with 1E08 samples identified 386 samples above the threshold. The resulting 95% confidence interval using Pearson and Clopper is [3.48E-06, 4.26E-06].

Both algorithms start with an initial training pool of 50 samples using simple MC sampling. In addition, both algorithms use a maximum variation of probability calculation over the last four iterations of 0.1 for the second learning cycle, defining the robustness of the metamodel. The additional threshold for the switching rate of the SuSSVR algorithm was set to 2.5%. In order to accumulate enough rare events of interest in the training sample in the first learning cycle, a termination criterion of at least 10% was used for the SuSSVR approach, while an absolute value of at least 5 rare events was set for the GASA-PRECLAS algorithm.

The SuSSVR algorithm terminated after 165 additional calculations of the simulation function and estimated a probability for the region of interest within the interval [3.16E-06, 4.19E-06]. The GASA-PRECLAS algorithm terminated after 180 additional simulation runs, estimating a probability inside the interval [3.52E-06, 7.05E-06].

Both algorithms require almost the same number of additional calculations and estimate compatible intervals for the probability, which could mean that both algorithms pass this benchmark test without problems or further adjustments. However, the low probability of about 1E-06 reveals limitations of the PRECLAS algorithm . Since this algorithm actually estimates the probability based on a simple random sample of parameter values and corresponding predictions of the metamodels, 1E08 sample elements are required for a robust probability estimate. Furthermore, to select new parameter candidates, all 1E08 parameter sample elements must be graded according to specific selection criteria. While this amount of data can still be processed with high computing power, applications with even smaller probabilities thus producing larger amount of data introduces runtime and memory problems. In future developments, am advanced sampling method, such as importance sampling, should be introduced to solve this problem. However, this procedure is based on expert judgement derived from the available training dataset and needs to be improved. These problems do not arise with the SuSSVR approach, because the Subset Simulation does not need a large sample to predict a low probability.

3.2 Benchmark Example: Ishigami Function

The Ishigami function is often used for benchmarking advanced sampling methods and sensitivity indices. It is defined by the following formula

$$y = sin(x_1) + c_1 \cdot sin^2(x_2) + c_2 \cdot x_3^4 \cdot sin(x_1). \quad (2)$$

The distribution of each of the three parameters x_1, x_2, x_3 is a uniform distribution between the limits $[-\pi, \pi]$ and the constants are $c_1 = 7$ and $c_2 = 0.1$. The region of interest in this case is defined by the function result y exceeding the threshold of 15. A simple MC sampling of the function using 1E06 samples identified 3071 samples above the chosen threshold, resulting in a 95% confidence interval of [2.96E-03, 3.18E-03] using Pearson and Clopper.

Both algorithms again start with an initial training data set of 50 parameter samples and corresponding results. The termination criteria are the same as for the biological dose example. However, the termination criteria for the first cycle had to be adjusted because both algorithms had difficulty finding all four maxima. Therefore, a larger number of samples in the region of interest was required for this exploration cycle (120 events for the GASA algorithm and 20% for the SuSSVR approach).

The SuSSVR algorithm terminated after 170 additional function evaluations, resulting in an estimated probability within the interval [2.5E-03, 3.2E-03]. The GASA-PRECLAS algorithm terminated after 312 additional evaluations, resulting in an estimated probability within the interval [1.75E-03, 3.61E-03].

In this benchmark example, the GASA algorithm performs slightly better in exploring the uncertain parameter space than the first cycle of the SuSSVR algorithm. How the GASA algorithm targets the region of interest while exploring the rest of the parameter space is shown in Figure 1, which illustrates the evolution of the training data set for the GASA-PRECLAS algorithm.

However, the necessary adjustments in the SuSSVR and in the GASA algorithm show the limitations of both exploration algorithms. Without the increased number of training data in the desired region of interest, the GASA algorithm or the first cycle of the SuSSVR algorithm would not have found all four separated regions and would have underestimated the rare event probability. This can be explained by the fact that neither approach is designed to find multiple separated regions of interest. Only the higher statistics and thus higher probability of finding all maxima prevented an underestimation of the probability. This can be improved, e.g., by introducing prior knowledge about four separate maxima or by adding an optional parameter that controls whether the new samples should be more biased towards one (already found) region of interest or towards the exploration of the unknown parameter space.

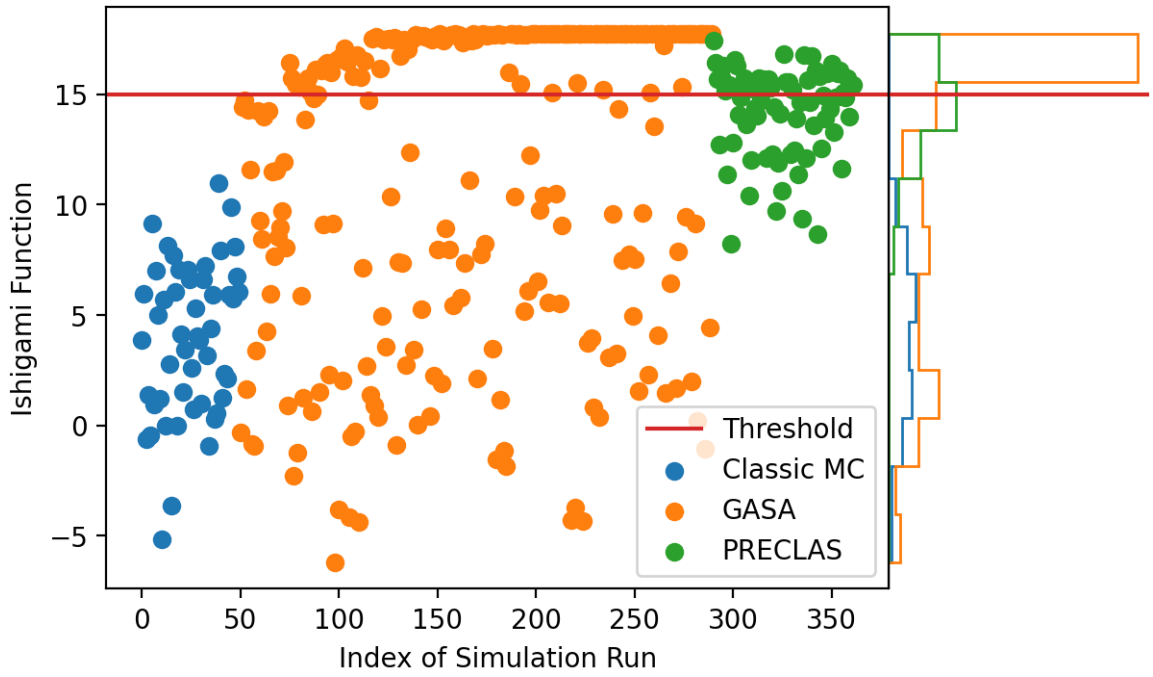

Figure 1: Development of the Ishigami function evaluations during the adaptive sampling of the GASA-PRECLAS algorithm. After the initial 50 samples using classic MC sampling (blue), the GASA algorithm (orange) required 240 additional function evaluations and the PRECLAS algorithm (green) required 72.

3.3 Application to a LOCA Scenario

In this example, the objective is to estimate the probability that the PCT exceeds 1200 °C in a LOCA scenario inside an NPP. A conservative reference model of a pressurized water reactor with four cooling circuits and an electrical power of 1425 MW is used, in which a double-ended guillotine rupture is initiated in the cold section of the main coolant line. The simulation model using ATHLET [6] was developed based on previous analyses [7,8]. 35 uncertain input parameters are considered in this work.

Both algorithms start with an initial training data set of 50 samples and with the same termination criteria as the Biologic Dose Model. The SuSSVR approach terminated after 364

additional simulation runs and estimated a probability between [8.16E-03, 9.36E-03]. The GASA-PRECLAS approach terminated after 103 additional simulation runs with an estimated probability between [1.06E.02, 2.07E-02].

The GASA-PRECLAS algorithm converges earlier. Although the estimated probability intervals of the SuSSVR and GASA-PRECLAS algorithms do not overlap, the intervals are close and their results are consistent. This shows that both algorithms work well also for high-dimensional parameter spaces with 35 dimensions. However, such high-dimensional parameter spaces make the sampling algorithms less and less efficient. Analogous to the Biologic Dose Model results, where an iterative refinement of the parameter space was suggested, an intermediate algorithm during the iteration of the adaptive sampling could reduce the dimensionality by analyzing the influence of the uncertain parameters on the simulation results of interest and remove those that have low influece.

4 CONCLUSION AND OUTLOOK

In this work, two adaptive sampling algorithms implemented in SUSA, the SuSSVR and GASA-PRECLAS algorithms, were compared to two benchmark applications and a LOCA scenario. In general, both approaches require the same order of magnitude of simulation runs to train a robust metamodel and compute a robust prediction for the rare scenario of interest. However, for runtime intensive calculations, already 100 additional simulation runs are expensive. But even when using the same algorithm but with a different seed, larger differences, e.g., of 100 additional simulation runs, can occur.

The probability intervals provided by the two approaches slightly differ. This can be explained by the fact that the parameters defining the termination criteria are not completely identical for the two algorithms. While the threshold for the variation of the probability is set to the same value, the switching rate is defined only in the SuSSVR algorithm. There is no such equivalent termination criterion in the PRECLAS algorithm, since this algorithm includes several classification algorithms that compensate for the uncertainty or switching points of the predictions of a single metamodel. However, it has been shown that the switching point is the most important parameter that determines the number of learning cycles required in the SuSSVR algorithm. For testing purposes, a switch point parameter was also implemented in the PRECLAS algorithm, but this did not lead to a subsequent termination of the iteration cycle.

As for the first cycle in exploring the parameter space, both algorithms performed well when there is only a single contiguous target region. In such applications, an advanced parameter space exploration method is not required. However, if there are multiple target regions that are not connected to each other, the GASA algorithm performs slightly better and can play its advantage of effectively exploiting the parameter space over the first iteration cycle of the SuSSVR algorithm.

As for the second cycle in building a robust metamodel for prediction, both algorithms perform well when the probability is not too small. However, for probabilities below 1e-06, the simple MC sampling in the PRECLAS algorithm requires too many parameter samples and leads to runtime and memory problems. The Subset Simulation, which is used in the SuSSVR algorithm, already prevents such behavior.

In summary, both implemented adaptive sampling algorithms are promising approaches for estimating the probability of a rare scenario. However, there is also room for improvements regarding the modularity of the algorithm. For some applications it might be useful combine the GASA algorithm with the second cycle of the SuSSVR algorithm. Furthermore, the sampling for the pool of parameter samples can be decoupled from the metamodel and decision process. In addition, an analysis of the relevant parameter space in terms of truncating an

uncertain parameter distribution (importance sampling) or identifying irrelevant parameters would be beneficial to simplify the problem iteratively.

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