Efficient uncertainty quantification using sequential sampling-based neural networks

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Abstract. Uncertainty quantification (UQ) of an engineered system involves the identification of uncertainties, modeling of the uncertainties, and the forward propagation of the uncertainties through a system analysis model. In this work, a novel surrogate-based forward propagation algorithm for UQ is proposed. The proposed algorithm is a new and unique extension of the recent efficient global optimization using neural network (NN)-based prediction and uncertainty (EGONN) algorithm which was created for optimization. The proposed extended algorithm is specifically created for UQ and is called uqEGONN. The uqEGONN algorithm sequentially and simultaneously samples two NNs, one for the prediction of a nonlinear function and the other for the prediction uncertainty. The uqEGONN algorithm terminates based on the absolute relative changes in the summary statistics based on Monte Carlo simulations (MCS), or a given maximum number of sequential samples. The algorithm is demonstrated on the UQ of the Ishigami function. The results show that the proposed algorithm yields comparable results as MCS on the true function and those results are more accurate than the results obtained using space-filling Latin hypercube sampling to train the NNs.

Keywords: Uncertainty quantification · Monte Carlo simulation · efficient global optimization · neural networks · sequential sampling.

1 Introduction

Uncertainty is ubiquitous in engineering design. For example, manufacturing processes create deviations from specifications, the system operating and loading conditions may vary, and some parameters are just inherently variable. Furthermore, the engineering models used in the design can be over simplified which

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introduces uncertainties. All of these can have a direct impact on the engineered system and its performance. Quantifying the impacts of uncertainties on the system is therefore an important part of the engineering design process.

Uncertainty quantification (UQ) of an engineering system can be divided into three major steps [25]. The first step involves identifying the types of uncertainties existing in the problem. For example, are there uncertainties in the system parameters, the design variables, or in the engineering model itself. The second step involves modeling the input parameter uncertainties. In particular, the uncertainties need to be defined in terms of the parameters and variables mathematically, for example using probability theory, and with respect to the quantities of interest (QoI), for example using the mean and standard deviation. The third step involves sampling the input uncertainties and propagating through the system model to yield the output probability distribution of the QoI and computing the associated statistics. This step often involves many evaluations of the QoI to obtain converged values of the statistics.

This work is focused on the third step in the UQ process described above, i.e., the forward propagation of the uncertainty through the system analysis, when dealing with computer simulations of the system. In particular, the goal of this work is to efficiently propagate uncertainties through simulations non-intrusively. In this work, it is assumed the system under consideration has a large number of uncertain parameters and each evaluation of system using the simulation requires the numerical solution of partial differential equations (PDEs). An example of such a system is the aerodynamic analysis of the flow past a civil transport aircraft at transonic speeds requiring a computational fluids dynamics (CFD) simulation which can take on the order of 24 hours on a high-performance computing (HPC) system [17,10]. The key challenges of simulation-based UQ are (1) a large number of uncertain parameters, (2) time-consuming simulations, and (3) many model evaluations.

UQ is a large and active field of research. Methods for forward propagation of uncertainties are many. The four major classes of nonintrusive methods for forward propagation are perturbation methods [24], direct quadrature [18,2], polynomial chaos [12,19], and Monte Carlo simulation (MCS) [7,15]. Perturbation methods use a local Taylor series expansion of the functional output. These methods are limited to local modeling and need at least first-order derivative information. Direct quadrature uses numerical quadrature to evaluate the statistics. This method is limited to low-dimensional problems, although sparse grids enable partially alleviate this issue. Polynomial chaos represent uncertain parameters as a sum of orthogonal basis functions and can yield the statistics and the output distributions. This method is, however, limited to small number of dimensions. Monte Carlo methods approximate the statistics and output distributions using random sampling. These methods are easy to use and are independent of the problem dimension. However, a major weakness is their inefficiency, i.e., many samples are required to obtain converged values of the statistics.

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In surrogate methods, the time-consuming simulations are replaced in the heavy computations of the QoIs with an approximation model, called a surrogate model or simply a surrogate, which is fast to evaluate [20]. This way the computational cost is shifted over to the creation of a surrogate model that can represent the true simulated response as a function of the parameters. In the context of simulation-based UQ, the surrogate needs to represent the uncertain output response of the simulation model in terms of the uncertain input parameter space. If that is possible, then the summary statistics and output distribution can be estimated using the aforementioned forward propagation methods.

Kriging is a widely used surrogate modeling method capable of approximating nonlinear responses [3]. An advantage of using kriging prediction is that it comes with its own prediction uncertainty. This enables the sequential (adaptive) sampling of the parameters space to enhance the kriging prediction surrogate. A widely used approach for sequential sampling is the efficient global optimization (EGO) algorithm [9]. A weakness of kriging is that it is limited to small data sets. Deep neural networks (DNNs) [6], on the other hand, scale more efficiently for large data sets [16,21] and while still being handle nonlinear responses. A major limitation, however, is that uncertainty estimates are not readily available for a single prediction [16], and it is necessary to make use of an ensemble of NNs with a range of predictions [14,23,5] or use dropout to represent model uncertainty [4] and these algorithms are computationally very intensive.

A recently created EGO algorithm with neural network (NN)-based prediction and uncertainty (called EGONN) partially alleviates some of these challenges [13]. The EGONN algorithm was created for unconstrained global optimization problems. In the algorithm, a NN model approximates a nonlinear high-dimensional objective function with initial samples and then proceeds to sequentially sample the design space and continuously update the NN-based prediction based on a predetermined computational budget or a termination condition is fulfilled. The update is based on an infill sample point determined by the prediction uncertainty of the NN model. In EGONN, a prediction uncertainty model is constructed using another NN that is trained on separate data set based on the current prediction NN model and sample from the true function. The prediction NN and the prediction uncertainty NN are used to maximize the expected improvement infill criterion to determine the next sample point.

In this paper, an extension to the EGONN algorithm to handle UQ problems is proposed. The goal is create an accurate global surrogate model of the true function that can be sampled quickly using MCS to compute the desired statistical information for the purpose of UQ. The proposed extension to EGONN is to model the spatial error of the prediction NN in order to construct the prediction uncertainty model. By maximizing the prediction error NN model, a new sample point is determined and appended to the current data set for training the prediction NN model. Since the prediction is being updated in each sequential sampling cycle it allows for termination of the UQ process based on convergence of the summary statistics. This is another new and unique feature of the proposed algorithm. This is achieved in the following way. In each itera-

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tion of the sequential sampling the current prediction NN is used to perform a MCS to yield the summary statistics and the change in the predicted mean and standard deviation with respect to the previous iteration is calculated. The algorithm terminates if the change in the statistics is below a pre-specified tolerance or a pre-specified maximum number of function evaluations has been reached. The proposed EGONN for UQ (uqEGONN) algorithm is demonstrated on two analytical test functions and compared against MCS of the true function.

The next section describes the proposed uqEGONN algorithm. The following section presents the numerical results of applying the proposed algorithm to an analytical test functions. Concluding remarks and possible next steps in this work are presented in the last section.

2 Methods

A surrogate-based forward propagation approach for simulation-based UQ is proposed. The proposed uqEGONN algorithm is given in Algorithm 1. Initially, two separate data sets, $(\mathbf{X}, \mathbf{Y})$ and $(\mathbf{X}, \mathbf{Y})_u$, are generated using design of experiments, such as space-filling Latin hypercube sampling (LHS). $(\mathbf{X}, \mathbf{Y})$ is for training a prediction model NN_y and $(\mathbf{X}, \mathbf{Y})_u$ is for training a prediction uncertainty model NN_u. The next steps in the algorithm comprise the sequential sampling. In the first step, the NN_y is fit to the current training data set $(\mathbf{X}, \mathbf{Y})$. In the second step, NN_y is evaluated at $\mathbf{X}$ and $\mathbf{X}_u$ to yield $\widehat{\mathbf{Y}}$ and $\widehat{\mathbf{Y}}_u$, respectively. This data is used to compute the spatial prediction errors $\mathbf{S} = \sqrt{(\mathbf{Y} - \widehat{\mathbf{Y}})^2}$ and $\mathbf{S}_u = \sqrt{(\mathbf{Y}_u - \widehat{\mathbf{Y}}_u)^2}$. The data is then appended as $\widetilde{\mathbf{X}} = \mathbf{X} \cup \mathbf{X}_u$, and $\widetilde{\mathbf{S}} = \mathbf{S} \cup \mathbf{S}_u$. The prediction uncertainty model NN_u is fit to the data set $(\widetilde{\mathbf{X}}, \widetilde{\mathbf{S}})$. A new sampling point $\mathbf{P}$ is now found by maximizing the prediction uncertainty model $\widehat{\mathbf{S}}(\mathbf{x}) = NN_u(\mathbf{x})$. The new sample point $\mathbf{P}$ is appended to $\mathbf{X}$ and the corresponding function value $y(\mathbf{P})$ is appended to $\mathbf{Y}$. The prediction model NN_y is used in a MCS to yield the summary statistics, the mean μ and standard deviation σ.

The algorithm terminates if the absolute relative change in the mean, calculated as $|\mu^{(i)} - \mu^{(i-1)}|/|\mu^{(0)}|$, is less than a predefined tolerance τ_μ, and the absolute relative change in the standard deviation, calculated as $|\sigma^{(i)} - \sigma^{(i-1)}|/|\sigma^{(0)}|$, is less than a predefined tolerance τ_σ, or if the number of sequential sample cycles exceeds N_{max}. In this work, the values of tolerance are set to $\tau_\mu = 0.005$ and $\tau_\sigma = 0.005$, and the maximum number of sequential samples is $N_{max} = 100$.

In this work, LHS is used to generate the initial sampling data set. The neural networks in uqEGONN are implemented within Tensorflow [1]. In this work, both NN_y and NN_u have two hidden layers and each with 8 neurons. The number of epochs is set to 10,000 and hyperbolic tan is used as activation function. All the NNs are trained using the Adam optimizer [11] with a learning rate of 0.001. For maximizing the infill criterion, differential evolution [22] is used with a population size of 210. The mutation and recombination is set to

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0.8 and 0.9, respectively, with a maximum of 200 generations. MCS is performed using random sampling.

Algorithm 1 Uncertainty quantification with EGONN (uqEGONN)

Require: initial data sets $(\mathbf{X}, \mathbf{Y})$ and $(\mathbf{X}, \mathbf{Y})_u$
  repeat
    fit NN_y to data $(\mathbf{X}, \mathbf{Y})$
    use NN_y to get $\widehat{\mathbf{Y}}$ at $\mathbf{X}$ and $\widehat{\mathbf{Y}}_u$ at $\mathbf{X}_u$
    compute prediction errors: $\mathbf{S} \leftarrow \sqrt{(\mathbf{Y} - \widehat{\mathbf{Y}})^2}$ and $\mathbf{S}_u \leftarrow \sqrt{(\mathbf{Y}_u - \widehat{\mathbf{Y}}_u)^2}$
    combine data: $\widetilde{\mathbf{X}} \leftarrow \mathbf{X} \cup \mathbf{X}_u$, $\widetilde{\mathbf{S}} \leftarrow \mathbf{S} \cup \mathbf{S}_u$
    fit NN_u to data $(\widetilde{\mathbf{X}}, \widetilde{\mathbf{S}})$
    $\mathbf{P} \leftarrow \arg\max \widehat{\mathbf{S}}(\mathbf{x})$
    $\mathbf{X} \leftarrow \mathbf{X} \cup \mathbf{P}$
    $\mathbf{Y} \leftarrow \mathbf{Y} \cup y(\mathbf{P})$
    $\mu, \sigma \leftarrow$ Monte Carlo simulation using NN_y
  until convergence

3 Numerical experiments

This section presents the numerical results of applying the proposed uqEGONN algorithm for the UQ of the Ishigami function [8], which is written as

$$Y = f(x_1, x_2, x_3) = \sin(x_1) + a \sin^2(x_2) + b x_3^4 \sin(x_1), \tag{1}$$

where $a = 7$, $b = 0.1$, and $x_i \sim \mathcal{U}[-\pi, \pi]$ $\forall$ $i = 1, 2, 3$. The convergence of MCS on the true analytical function (1) is shown in Figs. 1(a) and (b). It can be seen that MCS needs around one million samples to reach a converged mean $\mu = 3.50$ and standard deviation $\sigma = 3.72$. Figure 1(b) shows the true output distribution.

Figure 2 shows the convergence of the uqEGONN algorithm as a function of the sequential infill samples for the mean (Fig. 2(a)) and the standard deviation (Fig. 2(b)), as well as using NN modeling with LHS of the total number of samples, i.e., $n_s = n + n_i$, where n is the number of initial samples and n_i is the number of infill samples. It can be seen that the convergence history for both approaches exhibit oscillations which is due to the NN random fit. Also, the figures show that the sequential algorithm achieves more reduction in the both the mean and the standard deviation than the pure LHS approach.

Figures 3 to 5 show the progression in the convergence of the mean and the standard deviation as the number of samples increases. It can seen that the sequential algorithm reaches close to the true mean and true standard deviation values using 50 initial samples and 70 infills. The LHS approach does not give get

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as close to the true values using 120 samples. It can also be seen that the output distribution of the sequential approach is closer to the true output distribution than the pure LHS approach.

4 Conclusion

A novel surrogate-based forward propagation algorithm for simulation-based uncertainty quantification (UQ) is proposed. The unique features of the algorithm are (1) the sequential updating of the neural network (NN) predictions of the nonlinear function responses and the associated prediction uncertainty, (2) automated termination criteria based on the absolute relative change in the summary statistics, and (3) the elimination of testing data sets and the arbitrary choice of convergence metric values such as those based on the root mean squared error.

The demonstration example shows that comparable summary statistics and probability density function are obtained as those of the true function at a low computational cost. Furthermore, it was shown that the proposed algorithm yields more accurate results than those of using design of experiments methods without the sequential sampling to construct the NNs.

Future steps in this work include testing the proposed algorithm on higher dimensional analytical functions, and on simulation-based problems with the goal of characterizing its properties with respect to the dimensionality. The effects of the ratio of the number of samples of the initial sampling plan to the number of sequential infill points needs to be investigated. Another important future direction is the automation of the hyperparameter tuning of the NN architecture and training algorithm. This is important because the optimal architecture may change as the number of training data points increase in the sequential sampling.

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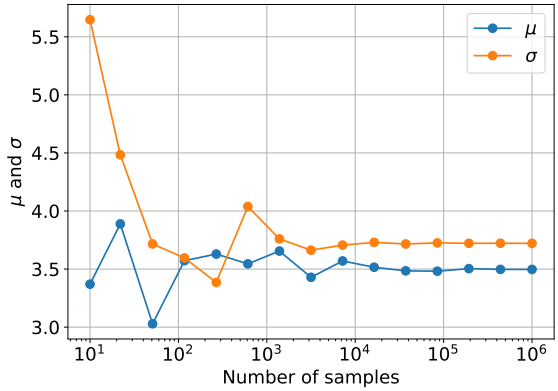

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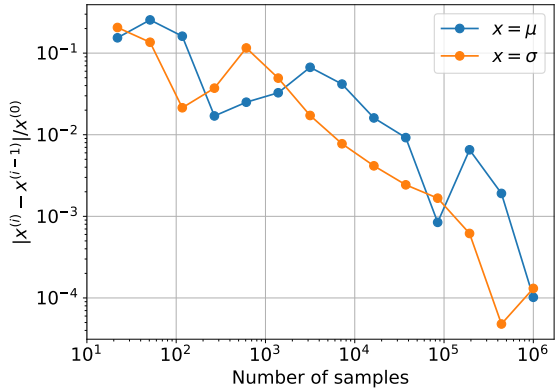

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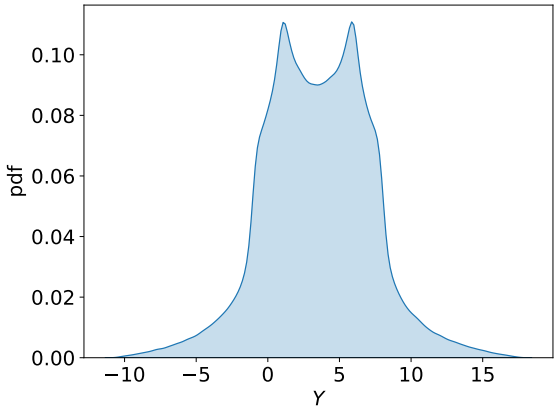

(c)

Fig. 1: Monte Carlo simulation convergence history of the true Ishigami function.

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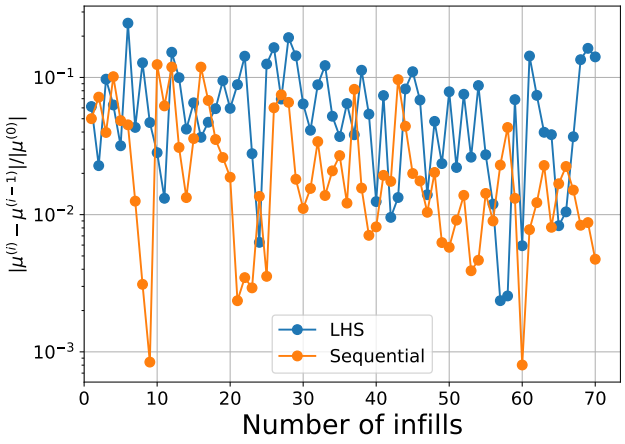
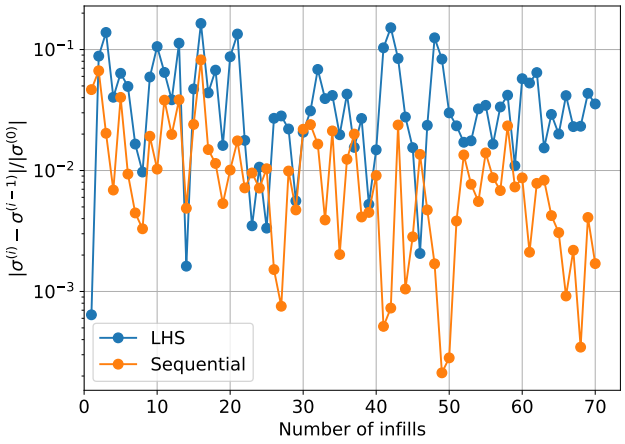


(a)



(b)

Fig. 2: Convergence history of the uqEGONN algorithm (Sequential) and using neural network modeling with Latin hypercube sampling without infills (LHS).

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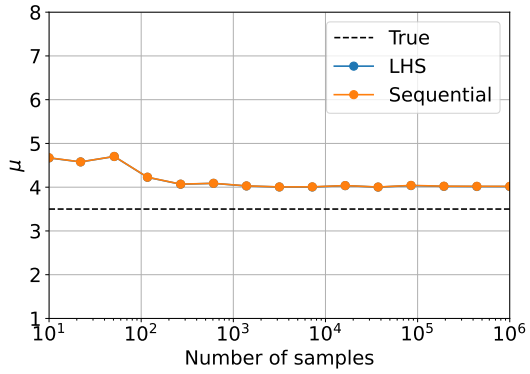

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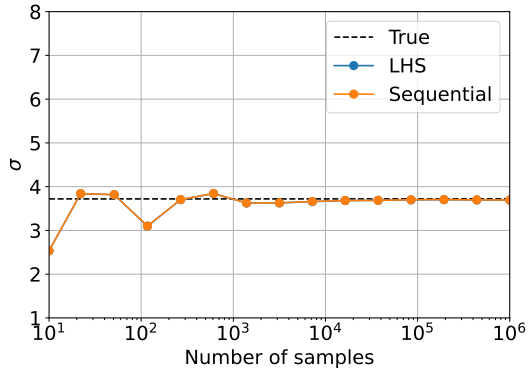

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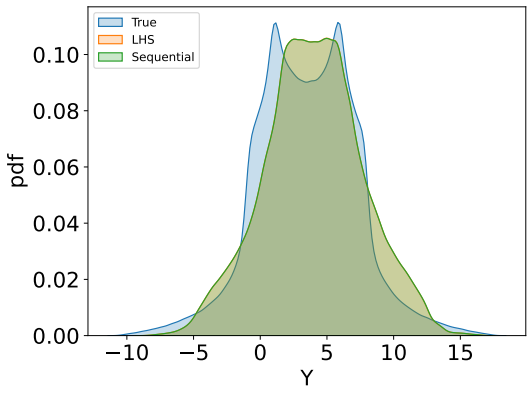

(c)

Fig. 3: Monte Carlo simulations on neural network models trained with the initial data sets ($n_s = 50$) using Latin hypercube sampling (LHS) and the sequential algorithm: (a) mean, (b) standard deviation, and (c) probability density functions of the output.

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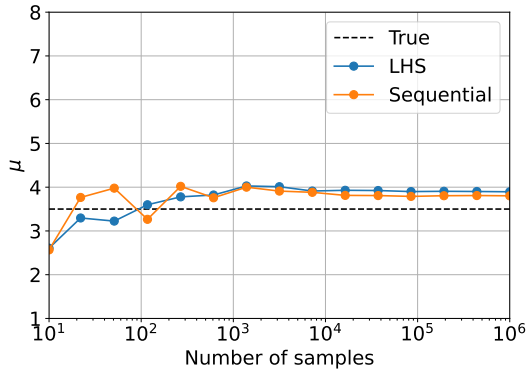

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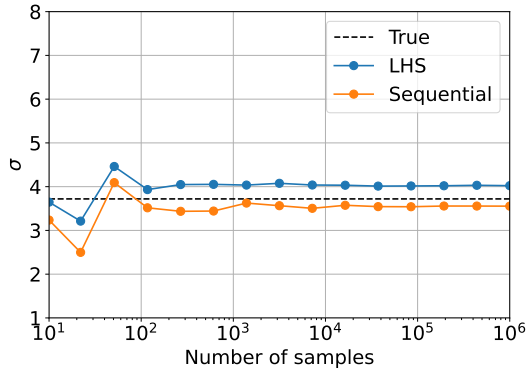

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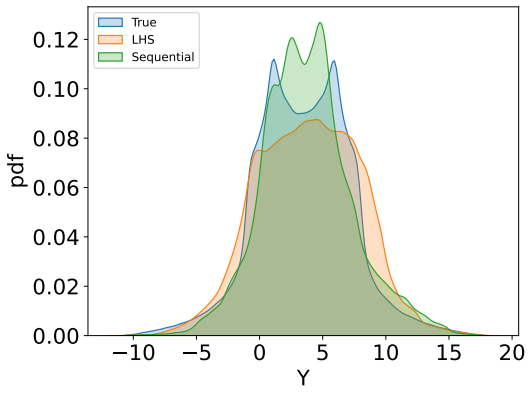

(c)

Fig. 4: Monte Carlo simulations on neural network models trained with the using Latin hypercube sampling (LHS) ($n_s = 85$) and the sequential algorithm ($n = 50$, $n_i = 35$): (a) mean, (b) standard deviation, and (c) probability density functions of the output.

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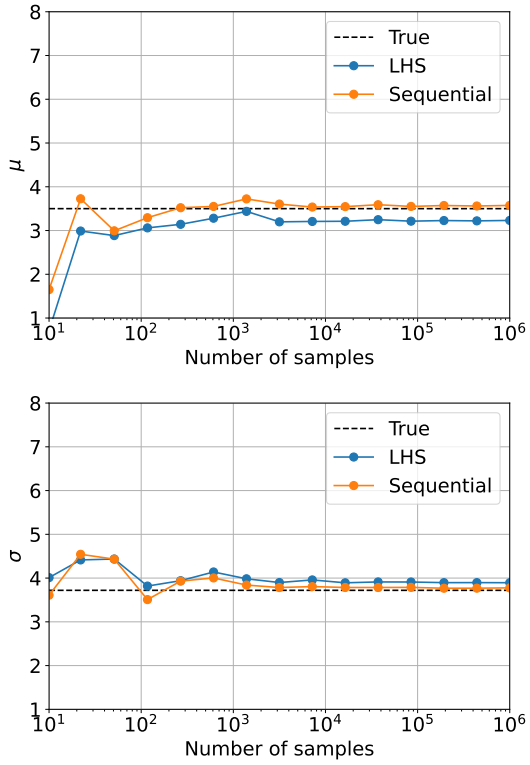
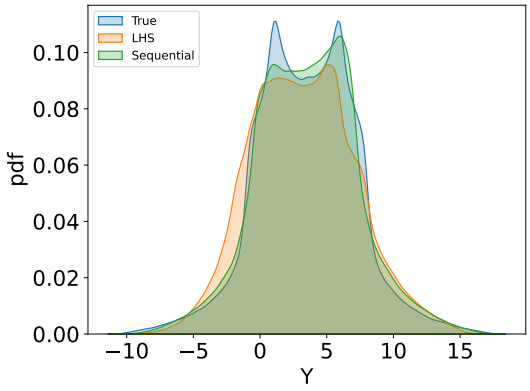


(a)



(b)

Fig. 5: Monte Carlo simulations on neural network models trained with the using Latin hypercube sampling (LHS) ($n_s = 120$) and the sequential algorithm ($n = 50$, $n_i = 70$): (a) mean, (b) standard deviation, and (c) probability density functions of the output.

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