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ROBUST SIMULATION BASED OPTIMIZATION WITH INPUT UNCERTAINTY

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ABSTRACT

Simulation-based Optimization (SbO) assumes that the simulation model is valid, and that the probability distributions used therein are accurate. However, in practice, the input probability distributions (input models) are estimated by sampling data from the real system. The errors in such estimates can have a profound impact on the optimal solution obtained by SbO. The existing two-stage framework for SbO under computational budget constraint considers only the stochastic uncertainty. In our variant, we consider the input model parameter uncertainty as well. Our algorithmic procedure is based on the stochastic kriging metamodel-assisted bootstrapping with an efficient global optimization technique which sequentially searches the optimum and incorporates Optimal Computational Budget Allocation (OCBA). This framework is also used for determining tighter worst-case bounds of the SbO with input uncertainty. The proposed framework is illustrated with the M/M/1 queuing model.

1 INTRODUCTION

We consider the following stochastic optimization problem:

$$\min_{x \in S, P \in \Theta} y(x), \tag{1}$$

where

- $y(x) := E_P[Y(x,\xi)]$
- $Y(x,\xi)$ is a real-valued function of two variables x and ξ
- x is a decision variable which belongs to a bounded continuous set S
- ξ is a random vector having an input probability distribution P (viz for exponential input probability distribution P).
- Θ is an ambiguity set of input probability distribution P, and is defined as follows:

  $$\Theta = \{P \in \mathbb{D} : D(P||P_0) \leq \eta\},$$

  where $D(\cdot||\cdot)$ is the Kullback-Leibler divergence between two probability distributions, P_0 is a known nominal distribution (fitted from the historical data), η is a measure of input model misspecification due to lack of knowledge or inadequacy in sample data and $\mathbb{D}$ is the set of all possible probability distributions on sample data.

We assume that the expected value function $y(x)$ is well defined for every $x \in S$ and $P \in \Theta$. Let $\{\xi_1, \xi_2, \ldots, \xi_r\}$ be an independent and identically distributed (i.i.d.) sample of size r drawn from P. Then the expected value function can be approximated by the sample average function $\bar{y}(x) := \frac{1}{r}\sum_{j=1}^{r} Y(x,\xi_j)$. Thus, the

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corresponding optimization problem is:

$$\min_{x \in S, P \in \Theta} \bar{y}(x). \tag{2}$$

In many cases, the underlying distribution P on ξ that controls the expectation $E_P[Y(x,\xi)]$ is not known precisely and is estimated based on a sample data from a real system. For example, in a queuing model, the inter-arrival time distribution is often estimated from the historical data of customer arrivals; and in an inventory model, the demand distribution is estimated from the past sales data. This causes uncertainty in the estimation of P. Uncertainty in P causes additional variability in the output response of the simulation experiment. Various methods have been proposed in the literature for quantifying the impact of input model uncertainty on output system performance, such as the delta method given by Cheng and Holland (1997), Cheng and Holland (1998); the bootstrapping method by Cheng (1994), Cheng (1995), Barton and Schruben (2001); the Bayesian model averaging method by Chick (2001), Zouaoui and Wilson (2003); and more recently, the meta-model assisted bootstrapping method by Barton, Nelson, and Xie (2014), Xie and Nelson (2014). The pros and cons of the four methods for quantifying input uncertainty mentioned above have been briefly explained by Barton (2012), Song, Nelson, and Pegden (2014). Input model uncertainty has also been quantified by Song, Nelson, and Hong (2015), Corlu and Biller (2015) in case of finding the best x among a finite set of x.

When the true distribution P^{true} of ξ is known, the optimality gap between formulations (1) and (2), given by $O = \mid y(x^*) - \bar{y}(x^*) \mid$, tends to zero only when $r \to \infty$. This uncertainty is caused due to inherent random number streaming inside the simulation model. To reduce uncertainty, we need to perform a large number of simulation experiments, which can be computationally expensive and time-consuming.

Jone and Welch (1998) have proposed an efficient global optimization algorithm based on kriging metamodel (i.e. regression model fitted to input/output data) for solving deterministic optimization problems. Dellino, Kleijnen, and Meloni (2008) have proposed a robust simulation-based optimization by combining Taguchi's approach and kriging metamodel. Ankenman, Nelson, and Staum (2010) have proposed a Stochastic Kriging (SK) metamodel for stochastic simulation experiment which incorporates the inherent stochastic uncertainty in the metamodel. Quan et al. (2013) have proposed a two-stage framework for performing SbO via kriging metamodel with computational budget constraints which incorporates only stochastic uncertainty. The two-stages are those of allocation and search. Their proposed algorithm gives a split up of the computational budget to each of the stages. Mehdad and Kleijnen (2015) proposed a stochastic intrinsic kriging for simulation optimization but there is no significant improvement in the optimal solution compared to stochastic kriging.

The main motivation of this paper is to provide an efficient algorithm for performing simulation-based optimization with input uncertainty and estimating tighter worst-case bounds of the optimal solution. The worst-case bounds provide an interval for the optimal solution of a simulation based optimization problem with input uncertainty. Our algorithmic procedure for solving the above problem is as follows:

(i) Generate an ambiguity set by bootstrap re-sampling of the sample data from the real system.
(ii) Perform simulation experiments with a few samples $(x,P) \in (S,\Theta)$ and estimate the output responses.
(iii) Fit an SK metamodel with (x,P) and its output response.
(iv) The optimal (x,P) which gives the minimum output response is obtained by sequentially minimizing the SK metamodel over (S,Θ).

The key contribution of this paper is to provide a combination of the stochastic kriging metamodel-assisted bootstrapping with the aforementioned two-stage framework for finding the optimum. This improves the performance of robust simulation optimization with computational budget constraints for providing a tighter worst-case lower bound of the SbO with input uncertainty. We also propose a new algorithmic procedure for sequentially solving a min-max formulation to obtain the worst-case upper bound of SbO with input uncertainty.

The layout of the paper is as follows. Section 2 explains fitting the collected data to the input probability distribution model. Section 3 describes the stochastic kriging metamodel. Section 4 discusses the efficient global optimization algorithm. Section 5 contains the proposed algorithms for performing SbO with input uncertainty. Section 6 explains the M/M/1 queuing simulation model example considered in the paper. Section 7 presents numerical results and the related discussion on the techniques.

2 INPUT MODELING

When the true distribution P^{true} of ξ is not known, it is estimated by fitting the given i.i.d. sample data $\xi = (\xi_1, \xi_2 \ldots, \xi_{n_0})$ to a suitable theoretical probability distribution (Barton and Schruben 2001). In this paper, we assume that the true distribution of a given data $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$ belongs to a known parametric family of theoretical distributions (viz exponential distribution with the parameter, λ). Sufficiently large sample data is required for an accurate estimation of the distribution parameter. But, collecting a large amount of data is costly. In order to improve the accuracy of parameter estimations using limited sample data, bootstrap re-sampling can be employed.

2.1 Bootstrap Re-sampling Approach

In this subsection, we review the bootstrapping approach of simulation input modeling by Cheng (1994), Cheng (1995), Barton and Schruben (2001). Bootstrapping is a technique for reusing data to estimate the statistics of interest by re-sampling sets of data from a given i.i.d. sample data $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$. The re-sampled data are fitted to a distribution P and its parameter (say, $\hat{\lambda}$) is estimated. Let a random sample $\xi_1 = (\xi_{11}, \xi_{12}, \ldots, \xi_{1n_0})$ of size n_0 be drawn with replacement from a given i.i.d. sample data $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$. Using this bootstrap sample ξ_1, the parameter value $\hat{\lambda}_1$ is estimated as the original $\hat{\lambda}$. Repeated sampling and estimation yields independent estimates $\hat{\lambda}_i,\ i = 1, 2, \ldots, B$ where B is the total number of bootstraps.

2.2 Kullback-Leibler Divergence

The Kullback-Leibler (KL) divergence between two distributions P and P_0 is the expectation of logarithmic difference between them. In our case P is the unknown input probability distribution and P_0 is the known nominal probability distribution. If P and P_0 belong to a continuous family of distributions, then the KL divergence between them is given as

$$D(P||P_0) = \int_{-\infty}^{\infty} p(\xi) \log\left(\frac{p(\xi)}{p_0(\xi)}\right) d\xi, \tag{3}$$

where p and p_0 are the densities corresponding to P and P_0. p_0 is obtained by fitting the given data $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$ to a known parametric family of theoretical distributions and p is obtained using the bootstrap re-sampled data described in the previous subsection.

3 STOCHASTIC KRIGING

In this section, we review the stochastic kriging metamodeling technique proposed by Ankenman, Nelson, and Staum (2010). Stochastic kriging is a metamodeling (i.e. regression model fitted for input/output data) methodology developed for stochastic simulation experiment. The stochastic simulation output response $Y_j(x)$ on replication j at a design point x is:

$$Y_j(x) = f(x)^T \beta + M(x) + \varepsilon_j(x), \tag{4}$$

where $f(x)$ is a vector of known functions on x, β is a vector of unknown parameter of compatible dimension, $M(x)$ represents the parameter uncertainty and $\varepsilon_j(x)$ represents sampling variability inherent in a stochastic simulation. To generate a global predictor, consider a set of input points $x_i,\ i=1,\ldots,n$ where r is the number of replications on input design x_i. Let the sample mean be $\bar{Y}(x)=\frac{1}{r}\sum_{j=1}^{r}Y_j(x)$ and let $\bar{Y}=(\bar{Y}(x_1),\bar{Y}(x_2),\ldots,\bar{Y}(x_n))^T$. As in typical spatial correlation models, a linear prediction of the form $w_0(x_0)+w(x_0)^T\bar{Y}$ is considered, where $w_0(x_0)$ and $w(x_0)$ are weights that depend on a design point x_0. The optimal value of these weights is obtained by minimizing the mean squared error of predictor. The linear predictor at x_0 is:

$$\hat{Y}(x_0)=\beta_0+\sum\nolimits_M(x_0,\cdot)^T\left[\sum\nolimits_M+\sum\nolimits_\varepsilon\right]^{-1}(\bar{Y}-\beta_0 1_{n\times 1}), \tag{5}$$

where β_0 is a vector of the unknown parameter of compatible dimension, $\sum_M(x_0,\cdot)$ is an $n\times 1$ covariance vector between prediction point x_0 and all input points, $\sum_M$ represents the $n\times n$ covariance matrix, $Cov(M(x_i),M(x_j))$, across all input points $x_i,\ i=1,\ldots,n$ and $\sum_\varepsilon$ is the diagonal matrix of intrinsic output variance. The covariance between two input points is estimated by, $\sum_M(x_i,x_j)=\tau^2R(\theta,x_i,x_j)$, where τ^2 is the variance of $M(x)$ over all input.

These $\sum_M$ and $\sum_M(x_0,\cdot)$ often uses the Gaussian correlation function $R(\theta,x_i,x_j)=\exp-(\sum_{j=1}^{d}(\theta_l|x_{il}-x_{jl}|^{p_l})$, where θ_l is the parameter which determines the rate of decrease of correlation as we move along the l^{th} coordinate, d is the dimension of the input vector and p_l determines the smoothness of function in the l^{th} coordinate. The parameters of the stochastic kriging model (β_0,τ^2,θ) are estimated using maximum likelihood function derived based on the assumption that $\sum_\varepsilon$ is known. For a fixed input point, the likelihood function of (β_0,τ^2,θ) is obtained by maximum likelihood approximation is:

$$\begin{aligned} l(\beta_0,\tau^2,\theta) &= -\ln\left[(2\pi)^{n/2}\right]-0.5\ln\left[|\tau^2R_M(\theta)+\sum\nolimits_\varepsilon|\right] \\ &\quad -0.5(\bar{Y}-\beta_0 1_{n\times 1})^T\left[\tau^2R_M(\theta)+\sum\nolimits_\varepsilon\right]^{-1}(\bar{Y}-\beta_0 1_{n\times 1}), \end{aligned} \tag{6}$$

where $R_M(\theta)$ is a correlation matrix of M across all input points.

Given the input/output data $Y_j(x_i),\ i=1,\ldots,n;\ j=1,\ldots,r$ the stochastic kriging meta model is fitted as follows:

- Estimate the sample mean and sample variance of the output response $(\bar{Y}(x_i),\sigma^2(x_i)), i=1,\ldots,n$ and let $\sum_\varepsilon=diag[\sigma^2(x_1)/r,\ldots,\sigma^2(x_n)/r]$.
- Maximize the likelihood function $l(\beta_0,\tau^2,\theta)$ to obtain the parameters (β_0,τ^2,θ) of the stochastic kriging metamodel.
- Predict $Y(x_0)$ by the metamodel

$$\hat{Y}(x_0)=\beta_0+\sum\nolimits_M(x_0,\cdot)^T\left[\sum\nolimits_M+\sum\nolimits_\varepsilon\right]^{-1}(\bar{Y}-\beta_0 1_{n\times 1}), \tag{7}$$

with mean square error is

$$\hat{\sigma}^2(x_0)=\tau^2+\sum\nolimits_M(x_0,\cdot)^T\left[\sum\nolimits_M+\sum\nolimits_\varepsilon\right]^{-1}\sum\nolimits_M(x_0,\cdot)+\delta\delta^T(1_{n\times 1}^T\left[\sum\nolimits_M+\sum\nolimits_\varepsilon\right]^{-1}1_{n\times 1})^{-1}, \tag{8}$$

where $\delta=1-(1_{n\times 1}^T[\sum_M+\sum_\varepsilon]^{-1}\sum_M(x_0,\cdot))$.

4 EFFICIENT GLOBAL OPTIMIZATION ALGORITHM

In this section, we summarize the Efficient Global Optimization (EGO) algorithm for both deterministic as well as stochastic simulation optimization problems. In order to improve the accuracy of the optimal solution obtained by SbO with input uncertainty under computational budget constraints, the optimal computational budget allocation technique can be employed.

4.1 EGO for Deterministic Simulation

Here, we summarize EGO for deterministic simulation by Jone and Welch (1998). EGO uses the expected improvement criteria for bringing the balance between local and global search of the optimum solution. The algorithm can be described as follows:

1. Fit a kriging meta-model with the initial set of input design points $Y(x_i),\ i = 1,\ldots,n$.
2. Find x by maximizing Expected Improvement (EI) function. The EI is estimated by assuming that the prediction at any x follows a normal distribution. It is estimated by,

$$EI(x) = (fmin - \hat{Y}(x))\phi\left(\frac{fmin - \hat{Y}(x)}{\hat{\sigma}(x)}\right) + \hat{\sigma}(x)\phi\left(\frac{fmin - \hat{Y}(x)}{\hat{\sigma}(x)}\right), \tag{9}$$

   where $fmin$ is the minimum of all $Y(x_i)$ values, $\phi(\cdot)$ is the standard normal density, $\hat{Y}(x)$ is the predicted optimal objective value and $\hat{\sigma}(x)$ is the predicted standard deviation at x.
3. If the EI is less than 1%, then the minimum is suggested as the best optimum $(x^*, Y(x^*))$. Otherwise, the simulation experiment is performed with x found in step 2. This new point is added to set of initial points, the kriging meta-model is reconstructed again including the new point and the above procedure is repeated.

4.2 EGO for Stochastic Simulation

In this subsection, we summarize the EGO algorithm for stochastic simulation by Quan et al. (2013). The algorithmic procedure is same as in Subsection 4.1 for deterministic simulation. The two major differences in the case of stochastic simulation are that the ordinary kriging metamodel is replaced by stochastic kriging metamodel and EI criteria is replaced by Modified Expected Improvement (MEI). The MEI is estimated by assuming that, the prediction at any x follows normal distribution. It is estimated by,

$$MEI(x) = (fmin - \hat{Y}(x))\phi\left(\frac{fmin - \hat{Y}(x)}{\hat{\sigma}(x)}\right) + \hat{\sigma}(x)\phi\left(\frac{fmin - \hat{Y}(x)}{\hat{\sigma}(x)}\right), \tag{10}$$

where $fmin$ is the minimum of predicted $\hat{Y}(x_i)$ values $i = 1,\ldots,n$, $\phi(\cdot)$ is a standard normal density, $\hat{Y}(x)$ is the predicted optimal objective value and $\hat{\sigma}(x)$ is the predicted standard deviation at x.

4.3 Simulation Budget Allocation

Computational budget allocation technique for simulation-based optimization by Chen et al. (2000) is a highly efficient technique. It provides a more rigorous way of determining the input design point with the best response. Theorem 1 provided by Chen et al. (2000), assumes that we have the sample mean and sample standard deviation at the all input design points $\bar{Y}(x_i), \sigma^2(x_i), i = 1,\ldots,n$. As computational budget goes to infinity, the probability of correct selection can be approximately maximized when,

$$\frac{r_i}{r_j} = \left(\frac{\sigma(x_i)/\Delta_{b,i}}{\sigma(x_j)/\Delta_{b,j}}\right)^2,\ i,j \in 1,\ldots,n;\ i \neq j \neq b, \tag{11}$$

$$r_b = \sigma(x_b)\sqrt{\sum_{i=1,i\neq b}^{n} \frac{r_i^2}{\sigma^2(x_i)}}, \tag{12}$$

where r_i is the number of replication allocated to input design x_i, r_b is the number of replication allocated to input design with lowest sample mean, x_b is the input design with the lowest sample mean and $\Delta_{b,i}$ is the difference between the lowest sample mean and the sample mean at input design x_i.

5 SbO WITH INPUT UNCERTAINTY

We discuss the robust simulation optimization with input uncertainty and the proposed algorithm for solving the simulation-based optimization described in (1). We have considered the following formulation for determining the robust simulation optimization bounds:

$$\min_{x \in S} VaR_{\alpha}(E_P[Y(x,\xi)]), \tag{13}$$

where $VaR_{\alpha}(E_P[Y(x,\xi)])$ is the value of risk at α quantile of the mean output response, defined as

$$VaR_{\alpha}(E_P[Y(x,\xi)]) = \inf\{t : F(t) \geq \alpha\},$$

where F is the cumulative distribution function of $E_P[Y(x,\xi)]$. If $E_P[Y(x,\xi)]$ is a continuous random variable, then the α-level VaR is evaluated as $VaR_{\alpha}(E_P[Y(x,\xi)]) = F^{-1}(\alpha)$. The objective function of (13) is determined by fitting an empirical cumulative distribution function of $E_P[Y(x,\xi)]$ over ambiguity set Θ at a particular x and estimate its value $F^{-1}(\alpha)$. The formulation in (13) at $\alpha = \frac{1}{N}$ is equal to the formulation given below:

$$\min_{x \in S} \min_{P \in \Theta} E_P[Y(x,\xi)], \tag{14}$$

where N is the number of elements in the ambiguity set Θ. The following equality will always hold,

$$\min_{x \in S, P \in \Theta} E_P[Y(x,\xi)] = \min_{x \in S} \min_{P \in \Theta} E_P[Y(x,\xi)]. \tag{15}$$

Hence, we have proposed Algorithm 1 for solving the optimization problem on the left hand side of equation (15).

In our algorithm we have used bootstrap resampling on the given sample data to find the accurate estimate of the ambiguity set Θ. The SbO experiment is performed over the ambiguity set and bound constraints on the decision variable x. In order to determine the global optimum, we have used stochastic kriging metamodel for fitting the output response of the simulation experiments with few input design points. We have implemented an efficient global optimization algorithm for sequentially searching the optimal solution. Finally, we have applied an optimal allocation computational budget technique for efficiently allocating the available computational budget during the search stage. The following terminology is used in the algorithm below:

- T is the total computational budget
- r is the number of replications available at each iteration
- r_{min} is the minimum number of replications
- j is the current iteration $j = 1,\ldots,I,\ I = \lceil (T - nr)/r \rceil$
- $r_S(j)$ is the number of replications available for search stage at iteration j
- $r_A(j)$ is the number of replications available for allocation stage at iteration j.

Algorithm 1 Algorithm for SbO with input uncertainty

1: **Determining the valid range of uncertain parameter:** Given an i.i.d. sample $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$ of size n_0, perform bootstrap resampling on the given sample (as mentioned in the Subsection 2.1).
2: Estimate the ambiguity set $\Theta = \{P \in \mathbb{D} : D(P||P_0) \leq \eta\}$ (as described in the Subsection 2.2). Compute the minimum and maximum value of the estimated parameter in Θ. Use these values as a bound for estimated parameter $\hat{\lambda}$.
3: **Initialization:** Generate an initial input design $(x, \hat{\lambda})$ of size n using Latin Hypercube sampling.

4: Run a simulation experiment at all the initial input design $(x_i, \hat{\lambda}_i),\ i = 1, \ldots, n$ for r replications and estimate the corresponding sample mean $\bar{Y}(x_i, \hat{\lambda}_i)$ and sample variance $\sigma^2(x_i, \hat{\lambda}_i)$ of the output response for each $i = 1, \ldots, n$.
5: **Validation:** Fit a stochastic kriging metamodel to the set $\{\bar{Y}(x_i, \hat{\lambda}_i),\ \sigma^2(x_i, \hat{\lambda}_i)\}$, $i = 1, \ldots, n$ (as described in the Section 3). Use leave-one-out cross validation method to check the quality of initial fitting. For searching and allocation stage, use the sequential search algorithm proposed by Quan (2013).
6: Set $j = 1, r_A(0) = 0$
7: **while** $j \leq I$ **do** $r_A(j) = r_A(j-1) + \min(\frac{r - r_{min}}{I}, T - nr - (j-1)r)$
8: **if** $(T - nr - (j-1)r - r_A(j)) > 0$ **then** $r_S(j) = r - r_A(j)$
9: **Search stage:** Find a new point which maximize the MEI function in equation (10). Run a simulation experiment at new point for $r_S(j)$ replication.
10: **Allocation stage:** Allocate $r_A(j)$ replications among all the sampled points using equation (11) and (12).
11: Fit a stochastic kriging metamodel to the set $\{\bar{Y}(x_i, \hat{\lambda}_i), \sigma^2(x_i, \hat{\lambda}_i)\},\ i = 1, \ldots, n + j$.
12: **end if**
13: **end while**
14: The input design point with the lowest sample mean at the end of the iteration is taken as a global optimum.

In order to obtain the accurate worst-case upper bound of SbO with input uncertainty, the formulation in (13) at $\alpha = 1$ is as given below,

$$\min_{x \in S} \max_{P \in \Theta} E_P[Y(x, \xi)]. \tag{16}$$

We have proposed Algorithm 2 for solving the formulation in (16). The algorithmic procedure is same as Algorithm 1 till the initialization stage. After initialization, we fit a separate stochastic kriging metamodel for each $x_i,\ i = 1, \ldots, n$ using the set of $\{\bar{Y}(x_i, \hat{\lambda}_w), \sigma^2(x_i, \hat{\lambda}_w)\},\ w = 1, \ldots, m$. First, we want to find the maximum value of output response for given x over Θ. The maximum output response $\hat{Y}_{max}(x_i)$ and corresponding variance at each x_i is obtained by maximizing the stochastic kriging metamodel $\hat{Y}(x_i, \hat{\lambda})$ over Θ. Next, we want to find a point x which gives the minimum value of $\hat{Y}_{max}(x)$. For that, we fit an another stochastic kriging metamodel using the maximum output response and its variance. We have used efficient global optimization algorithm for sequentially searching the optimal solution. The following terminology is used in algorithm below:

- $\hat{Y}(x_i, \hat{\lambda})$ is the prediction of stochastic kriging metamodel at input parameter $\hat{\lambda}$ when the design point is x_i
- m is the number of input parameters $\hat{\lambda}$.

Algorithm 2 Algorithm for determining the worst-case upper bound of SbO with input uncertainty

1: **Determining valid range of uncertain parameter:** Given an i.i.d. sample $\xi = (\xi_1, \xi_2, \ldots, \xi_{n_0})$ of size n_0. Perform bootstrap resampling on the given sample (as mentioned in the Subsection 2.1).
2: Estimate the ambiguity set $\Theta = \{P \in \mathbb{D} : D(P||P_0) \leq \eta\}$ (as described in the Subsection 2.2). Compute the minimum and maximum values of the estimated parameter in Θ. Use these values as bounds for estimated parameter $\hat{\lambda}$.
3: **Initialization:** Generate an initial input design point x of size n and $\hat{\lambda}$ of size m using Latin Hypercube sampling technique.

4: Run a simulation experiment at all the possible combination of $x_i,\ i=1,\dots,n$ and $\hat{\lambda}_w,\ w=1,\dots,m$ for r replications and estimate the corresponding mean and variance of the output performance $\{\bar{Y}(x_i,\hat{\lambda}_w),\sigma^2(x_i,\hat{\lambda}_w)\},\ i=1,\dots,n;\ w=1,\dots,m$.

5: **Validation:** Fit a stochastic kriging metamodel to x_i using the set of $\{\bar{Y}(x_i,\hat{\lambda}_w),\sigma^2(x_i,\hat{\lambda}_w)\}$, $w=1,\dots,m$. Use leave-one-out cross validation method to check the quality of initial fitting.

6: Perform the above step for each $x_i,\ i=1,\dots,n$.

7: **Optimize:** Obtain the maximum output response $\hat{Y}_{max}(x_i)$ and the corresponding variance $\hat{\sigma}^2(x_i)$ over ambiguity set for each $x_i,\ i=1,\dots,n$ by solving optimization formulation given below:

$$\max_{\hat{\lambda}\in\Theta}\hat{Y}(x_i,\hat{\lambda}).$$

8: Fit the stochastic kriging metamodel to the set of $\{\hat{Y}_{max}(x_i),\hat{\sigma}^2(x_i)\},\ i=1,\dots,n$.

9: **Search stage:** Find a new point x which maximize the Modified Expected Improvement function in equation (10).

10: If the MEI is less than 1%, then the minimum of $\hat{Y}_{max}(x_i),\ i=1,\dots,n$ is suggested as the best optimum. Otherwise, the simulation experiment is performed with all combination of x (found in step 9) and $\hat{\lambda}_w,\ w=1,\dots,m$ for r replications. Perform steps 5 and 7 at the new point x. This new point x is added to set of initial points. Then steps 8, 9 and 10 are repeated.

6 NUMERICAL EXAMPLE

We will illustrate the above described framework of SbO with input uncertainty on a simple M/M/1 queuing model example. The arrival of customers in the system follows Poisson distribution with rate λ and the service time of the customers follows an exponential distribution with mean time x. The objective is to find a mean service time x that minimizes the cost:

$$\min_{x>0} C(x) = \begin{cases} \min\{E_\lambda[Y(x,\xi)]+\frac{c}{x}, M\}, & \text{if } \lambda x < 1,\\ M, & \text{otherwise,}\end{cases}$$

where c is the cost per unit increase in the service rate, M is the practical limitation on the total cost, ξ represents the inter-arrival time that is exponentially distributed with parameter λ and $Y(x,\xi)$ is the amount of time spend in the system. The theoretical expression for expected amount of time spend in the system $E_\lambda[Y(x,\xi)]$ of M/M/1 queuing model is $\frac{x}{1-\lambda x}$. The unique optimal solution for the above optimization is $x^*=\frac{\sqrt{c}}{\sqrt{c}\lambda+1}$.

In the numerical experiments, it is assumed that the true value of λ is unknown. For the purpose of experimentation, n_0 i.i.d. sample of inter arrival times $\xi_1,\dots,\xi_{n_0}$ are generated from the exponential distribution with parameter λ^{true}. The sample data is fitted to exponential distribution and its corresponding parameter $\hat{\lambda}$ is estimated using maximum likelihood estimate. The above optimization problem is solved under the estimated input probability distribution.

The convergence of Algorithm 1 is evaluated using mean absolute deviation and mean square deviation of the response. We run K independent macro replications, and in each replication k, we generate an i.i.d. sample $\xi_1,\dots,\xi_{n_0}$ of inter arrival times of size n_0 from the exponential distribution with parameter λ^{true}. The above optimization problem solved using Algorithm 1 to obtain optimal solution $\hat{x}_k^*$ for k^{th} macro replication. The Mean Absolute Deviation (MAD) is estimated as follows:

$$MAD=\frac{1}{K}\sum_{k=1}^{K}|\hat{x}_k^*-x^*|, \tag{17}$$

where x^* is the true optimal solution. The Mean Square Deviation (MSD) of the response is estimated as follows:

$$MSD = \frac{1}{K}\sum_{k=1}^{K}\Big(\frac{Y(\hat{x}_k^*) - Y(x^*)}{Y(x^*)}\Big)^2, \tag{18}$$

where $Y(x^*)$ is the true optimal output response and $Y(\hat{x}_k^*)$ is the optimal output response obtained at k^{th} replication.

7 RESULT AND DISCUSSION

This section briefly explains the experimental results that were obtained by performing SbO with input uncertainty of M/M/1 queuing model using Algorithm 1 and Algorithm 2. The M/M/1 queuing simulation model is implemented in MATLAB. The stochastic kriging metamodel is also implemented in MATLAB and its parameter values are estimated by maximizing the likelihood function using `fmincon` solver. For Latin Hypercube Sampling, `lhsdesign` function in the statistical toolbox of MATLAB is used.

The parameter settings used in the Algorithm 1 for testing the convergence of the optimal solution of formulation (1) are as follows: The interarrival time is exponentially distributed with parameter $(\lambda = 1)$. The cost per unit increase in the service rate c is 1. The practical limitation on the total cost M is 500. The number of i.i.d. sample n_0 drawn from the exponential $(\lambda = 1)$ varies from 10 to 1000. The simulation experiment run length L is 1000. The number of bootstrap B is 1000. The measure η of input model misspecification due to lack of knowledge or inadequacy in sample data is 0.5. The initial number of input design points is $n = 10d$, where, d is the dimension of the design point. In this case, the dimension is $d = 2$ so the number of initial input design points $n = 20$. The total computational budget T is 1200. The number of replications r available at each iteration is 40. The minimum number of replications r_{min} is 10. The number of macro replications K is 100. The true optimal solution of the optimization problem defined in Section 6 for a given interarrival rate $(\lambda = 1)$ is $(x^*, Y(x^*)) = (0.5, 3)$. Table 1 shows the MAD and MSD of the optimum solution obtained by solving the optimization problem illustrated in the Section 6 using Algorithm 1. The numerical result in the Table 1 clearly shows that the MAD and MSD of the optimal solution decreases as the size of the input sample increases. This guarantees that the optimal solution of the above optimization problem converges to the true optimum solution as the size of the input sample increases.

Table 1: MAD and MSD of optimal solutions of M/M/1 Queuing model.

n_0	10	20	50	100	1000
MAD	0.16516	0.10419	0.07097	0.04806	0.0218
MSD	0.02271	0.01582	0.00969	0.00663	0.00104

The worst-case lower bound of the M/M/1 queuing model simulation optimization is obtained by solving the formulation in (1) using Algorithm 1 with the same experimental settings. Except that the number of macro replication K is 1. The worst-case upper bound of the M/M/1 queuing model is obtained by solving the formulation in (16) using Algorithm 2 with the following experimental settings: $\lambda = 1, L = 1000, \eta = 0.5, B = 1000, n = 10, m = 10$ and $r = 40$. Table 2 shows the bounds of the estimated uncertain parameter $\hat{\lambda}$ and the true theoretical worst-case bounds of the optimal solution.

Table 2: Theoretical worst-case bounds.

n_0	10		20		50		100		1000	
	lb	ub	lb	ub	lb	ub	lb	ub	lb	ub
$\hat{\lambda}$	0.5901	3.4075	0.5242	3.0647	0.6282	1.4693	0.7613	1.4423	0.8499	1.0303
x^*	0.6289	0.2269	0.6561	0.2460	0.6142	0.405	0.5678	0.4095	0.5406	0.4925
$Y(x^*)$	2.5901	5.4075	2.5242	5.0647	2.6282	3.4693	2.7613	3.4423	2.8499	3.0303

Table 3 shows the worst-case bounds of the optimal solution of M/M/1 queuing model. The numerical results in the Table 3 clearly shows that the true optimal solution of the underlying M/M/1 queuing model lies within the bounds. The distance between the lower and upper bound of the optimal solution reduces as the sample size n_0 increases.

Table 3: Worst-case bounds obtained by the proposed algorithm.

n_0	10		20		50		100		1000	
	lb	ub	lb	ub	lb	ub	lb	ub	lb	ub
$\hat{x}^*$	0.6176	0.2296	0.5948	0.2312	0.5719	0.3957	0.5415	0.4062	0.5092	0.4959
$Y(\hat{x}^*)$	2.5781	5.3583	2.7162	5.0939	2.6369	3.4579	2.7371	3.4183	2.9692	2.9993

The optimality gap in the Table 4, shows that the proposed algorithm for performing SbO with input uncertainty gives promising worst-case bounds.

Table 4: Optimality gap.

n_0	10		20		50		100		1000	
	lb	ub	lb	ub	lb	ub	lb	ub	lb	ub
$\lvert\hat{x}^* - x^*\rvert$	0.0113	0.0028	0.0612	0.0148	0.0423	0.009	0.026	0.003	0.031	0.003
$\lvert Y(\hat{x}^*) - Y(x^*)\rvert$	0.0119	0.0491	0.1921	0.0293	0.0087	0.011	0.024	0.024	0.119	0.031

8 CONCLUSION AND FUTURE WORK

The algorithmic procedure of performing robust simulation-based optimization with input uncertainty for determining the worst-case bounds is discussed in the paper. The stochastic kriging metamodel assisted bootstrapping is combined with an efficient global optimization with OCBA for determining the worst-case bounds of the optimal solution. The proposed approach is illustrated with an M/M/1 queuing model. The numerical results shows that the proposed algorithm gives tighter worst-case bounds for simulation-based optimization with input uncertainty. The applicability of proposed algorithm for SbO with non-parametric family of input probability distribution and for the case of more than one input probability distributions are to be investigated.

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