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METAMODEL-ASSISTED SENSITIVITY ANALYSIS FOR CONTROLLING THE IMPACT OF INPUT UNCERTAINTY

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ABSTRACT

Given finite real-world data, input models are estimated with error. Thus, the system performance estimation uncertainty includes both input and simulation uncertainties. Built on the global sensitivity analysis proposed by Oakley and O'Hagan, we develop a metamodel-assisted Bayesian framework to quantify the contributions from simulation and input uncertainties. It further estimates the impact from each source of input uncertainty and predicts the value of collecting additional input data, which could guide the data collection to efficiently improve the system response estimation accuracy. The empirical study demonstrates that our approach has promising performance.

1 INTRODUCTION

When stochastic simulation is used to assess the mean response of complex systems, e.g., the expected profit of biopharma supply chains, simulation experiments are often driven by multiple input models. Here, suppose that the parametric families are known and the underlying input parameters are estimated by using the finite real-world data, which introduces the input model estimation error, called input uncertainty. In addition, given limited simulation budget, there exists the simulation estimation error. Thus, it is necessary to quantify the overall estimation uncertainty of system response. Furthermore, it is beneficial to evaluate the relative contribution from simulation uncertainty and each source of input uncertainty. This can be used to guide the additional data collection and efficiently improve the system performance estimation.

This study is built on the metamodel-assisted Bayesian framework introduced in our previous work (Xie et al. 2014). The input uncertainty is quantified by the posterior distribution of input parameters. The uncertainty of system mean response surface is quantified by the posterior distribution characterized by a Gaussian process (GP) metamodel. It is used to efficiently propagate the input uncertainty to system output mean response. Then, given the input and simulation data, the posterior distribution of a compound random variable can quantify the overall estimation uncertainty of system response.

In this paper, we extend the Bayesian framework proposed in Xie et al. (2014) to facilitate the global sensitivity analysis. It can estimate the impact of each input uncertainty and further predict the value of collecting more data from each underlying input model. Here the system response estimation uncertainty is quantified by variance. Built on functional ANOVA introduced in Oakley and O'Hagan (2004), our metamodel-assisted variance decomposition and sensitivity analysis can be used to estimate the contribution from each source of input model estimation uncertainty and simulation uncertainty. We further provide the approach to assess the value of collecting additional data in terms of improving the system performance estimation accuracy. Compared with existing methods, e.g., Ng and Chick (2006), Song and Nelson (2015), our approach demonstrates better performance.

Thus, the contributions of this study can be summarized as follows. First, we propose a fully Bayesian framework to facilitate the global sensitivity analysis. Differing with the sensitivity analysis approach in

Oakley and O'Hagan (2004) proposed for deterministic simulation, we consider stochastic simulation and input uncertainty is quantified by the Bayesian approach. Second, built on the functional ANOVA, we propose an approximation approach to facilitate and simplify the estimation of impact from each input uncertainty and the value of collecting additional data. Third, the empirical study indicates that the proposed framework has the promising performance. It does not rely on the normal assumption on the posterior distributions of input parameters and also the linear form assumption on the system mean response surface. These assumptions typically do not hold in many situations when the amount of real-world data is tight, the input uncertainty is large and the response surface is complex and highly nonlinear.

The paper is organized as follow. Section 2 reviews the related studies in the simulation literature on uncertainty quantification and sensitivity analysis. Section 3 provides the problem description. Built on Xie et al. (2014) and Oakley and O'Hagan (2004), we provide a global metamodel-assisted sensitivity analysis to quantify the the impact of each source of input uncertainty and assess the value of collecting additional data from each input model in Section 5. We perform the empirical study on an $M/M/1/K$ queue example and a bio-pharmaceutical inventory management example in Section 6 and conclude in Section 7.

2 BACKGROUND

Borgonovo and Plischke (2016) provide a detailed review on the recent studies on both local and global sensitivity analysis. In this section, we briefly review related studies, including probabilistic sensitivity analysis for deterministic computer model, stochastic simulation uncertainty quantification, and sensitivity analysis in stochastic simulation studying the contribution from each input model.

We focus on the probabilistic sensitivity analysis, which models input distribution and then analyzes the induced uncertainty in outputs. Among those, variance based methods (Sobol 1993; Wagner 1995) assess the contribution from each input based on expected reduction in output variance when knowing the corresponding input with certainty. Functional ANOVA decomposition (Oakley and O'Hagan 2004) of deterministic input-output mapping can be used to estimate the contribution from each random input. The variance-based sensitivity measures, i.e., first-order effects and total effects, may fail to sum to the total variance and adequately deal with interaction effects of inputs. Owen (2014) suggests a new sensitivity measure, called Shapley value. Song et al. (2016) further analyze this measure and propose a Monte Carlo algorithm to efficiently estimate Shapley effects.

For stochastic simulation, we can use the posterior distributions quantifying the input uncertainty. Various approaches are proposed to propagate the input uncertainty to the output, including the direct simulation approach that runs simulations at posterior samples of input distribution (Chick 2001; Chick and Ng 2002; Zouaoui and Wilson 2004), and metamodel based approaches that model the mean response surface as a function of input parameters (Cheng and Holland 2004; Ng and Chick 2006; Barton et al. 2013).

Furthermore, various approaches were proposed to study the contribution from each input model estimation uncertainty. Freimer and Schruben (2002) propose the analysis of variance (ANOVA) approaches based on fixed effects model and random effects model. They study the effect of input parameter estimation uncertainty on the output response by varying the parameter value over the range of its confidence interval (CI) and suggest where to collect more real-world data. Ng and Chick (2006) approximate input parameter posterior with asymptotic normal distribution and propagate input uncertainty to output by using first-order Taylor expansion of response surface. Given a fixed budget, they proposed an optimization approach to guide the additional data collection so that we can minimize the overall estimation variance. Song and Nelson (2015) employ a linear regression model on the system response and consider the first two moments of the input processes as regressors. The bootstrap is used to estimate each source of input uncertainty. They predict the value of data collection through taking the derivative of system response estimation variance with respect to the sample size of input data.

3 PROBLEM DESCRIPTION

For complex stochastic systems, the system mean response often depends on multiple input models, denoted by $F \equiv \{F_1, \ldots, F_L\}$, which could include models with component-wise and time-serial dependence. Suppose that the parametric families of input models are known. Thus, F is specified by a finite number of input parameters, denoted by $\boldsymbol{\phi} \equiv (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_L)$, where $\boldsymbol{\phi}_\ell$ is a d_ℓ dimensional vector of parameters for the ℓ-th input distribution F_ℓ and $\boldsymbol{\phi}$ is a $d = \sum_{\ell=1}^{L} d_\ell$ dimensional vector of parameters. Then, the simulation output from the r-th replication can be written as

$$Y_r(\boldsymbol{\phi}) = \mu(\boldsymbol{\phi}) + \varepsilon_r(\boldsymbol{\phi}),$$

where $\mu(\boldsymbol{\phi}) = \mathrm{E}[Y_r(\boldsymbol{\phi})]$ denotes the unknown output mean and $\varepsilon_r(\boldsymbol{\phi})$ represents the simulation error with zero mean. Notice that the simulation output depends on the selection of input parameters.

We are interested in the system mean response at underlying true input models, denoted by $\mu(\boldsymbol{\phi}^c)$. The unknown true input parameters $\boldsymbol{\phi}^c$ are estimated by finite real-world data. Let m_ℓ denote the size of i.i.d. real-world observations from the ℓ-th input model, denoted by $\mathbf{X}_{\ell,m_\ell} \equiv \{X_{\ell,1}, X_{\ell,2}, \ldots, X_{\ell,m_\ell}\}$ with $X_{\ell,p} \overset{i.i.d}{\sim} F_\ell^c$ for $p = 1,2,\ldots,m_\ell$. Let $\mathscr{X}_{\mathbf{m}} = \{\mathbf{X}_{\ell,m_\ell}, \ell = 1,2,\ldots,L\}$ be the collection of samples from all L input models in F^c, where $\mathbf{m} = (m_1, m_2, \ldots, m_L)$. The unknown input distributions are estimated from $\mathscr{X}_{\mathbf{m}}$, and the input uncertainty is quantified by the posterior distribution for the input parameters

$$p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}}) \propto p(\boldsymbol{\phi}) p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}).$$

The underlying mean response surface $\mu(\cdot)$ is unknown. Without strong prior belief on the true response surface, a Gaussian process (GP) metamodel is used to model our belief on mean response surface and the metamodel uncertainty is quantified by the posterior distribution of $\mu(\cdot)$. Let $\widetilde{\cdot}$ denote the posterior sample. Thus, the posterior distribution of the compound random variable $\widetilde{\mu}(\widetilde{\boldsymbol{\phi}})$ characterizes the overall estimation uncertainty of mean response $\mu(\boldsymbol{\phi}^c)$.

In Xie et al. (2014), we introduced a GP metamodel-assisted Bayesian framework to construct a percentile credible interval (CrI) quantifying the overall system mean response estimation uncertainty and further estimate the relative contributions from input and simulation uncertainties. It can be used to guide running more simulations when the overall uncertainty is too large and the simulation uncertainty dominates the input uncertainty. However, in the real applications, we could face the situations where the amount of real-world data is very limited. For example, in the biopharmaceutical manufacturing, we often produce a few batches of drug substance each year and bio-drugs tend to have short life cycle (say 1.5–3 years). Thus, it is critically important to quantify the impact of our limited knowledge on each source of uncertainty impacts on the system performance estimation. Therefore, built on Xie et al. (2014) and Oakley and O'Hagan (2004), in this paper, we develop a global sensitivity analysis to estimate the impact from each source of input uncertainty quantified by the posterior $p(\boldsymbol{\phi}_\ell|\mathbf{X}_{\ell,m_\ell})$ and predict the value of collecting additional data (say Δm_ℓ) from the ℓ-th input model with $\ell = 1,2,\ldots,L$.

4 METAMODEL-ASSISTED BAYESIAN UNCERTAINTY QUANTIFICATION

Here, we briefly review the metamodel-assisted Bayesian uncertainty quantification framework proposed in Xie et al. (2014). Since each simulation run could be computationally expensive, a GP or stochastic kriging (SK) metamodel is employed to efficiently propagate the input uncertainty to the output. Specifically, the simulation output from the r-th replication can be modeled as

$$Y_r(\boldsymbol{\phi}) = \beta_0 + W(\boldsymbol{\phi}) + \varepsilon_r(\boldsymbol{\phi}),$$

where our belief on the unknown mean response $\mu(\cdot)$ is modeled by a GP, $M(\boldsymbol{\phi}) \equiv \beta_0 + W(\boldsymbol{\phi})$ with $W(\boldsymbol{\phi})$ representing a mean-zero GP, and the simulation estimation uncertainty is $\varepsilon(\boldsymbol{\phi}) \sim \mathrm{N}(0, \sigma_\varepsilon^2(\boldsymbol{\phi}))$.

A parametric form of the spatial covariance, denoted by $\Sigma(\boldsymbol{\phi},\boldsymbol{\phi}') = \mathrm{Cov}[W(\boldsymbol{\phi}),W(\boldsymbol{\phi}')] = \tau^2 r(\boldsymbol{\phi}-\boldsymbol{\phi}')$, is typically assumed, where τ^2 denotes the variance and $r(\cdot)$ is a correlation function that depends only on the distance $\boldsymbol{\phi}-\boldsymbol{\phi}'$. Based on Xie et al. (2010), we use the product-form Gaussian correlation function, $r(\boldsymbol{\phi}-\boldsymbol{\phi}') = \exp\left(-\sum_{j=1}^{d}\theta_j(\phi_j-\phi_j')^2\right)$ in the empirical study, where $\boldsymbol{\theta}=(\theta_1,\theta_2,\ldots,\theta_d)$ represents the correlation parameters. Then, the prior of $M(\boldsymbol{\phi})$ can be represented by a Gaussian process $M(\boldsymbol{\phi}) \sim \mathrm{GP}(\beta_0,\tau^2 r(\boldsymbol{\phi}-\boldsymbol{\phi}'))$.

To reduce the uncertainty of our belief on system mean response surface $\mu(\boldsymbol{\phi})$, we choose an experiment design consisting of pairs $\mathscr{D} \equiv \{(\boldsymbol{\phi}^q,n_q), q=1,2,\ldots,k\}$ at which to run simulations and collect observations, where $(\boldsymbol{\phi}^q,n_q)$ denotes the location and the number of replications, respectively, at the q-th design point. The simulation outputs at $\mathscr{D}$ are $\mathbf{Y}_{\mathscr{D}} \equiv \left\{(Y_1(\boldsymbol{\phi}^q),Y_2(\boldsymbol{\phi}^q),\ldots,Y_{n_q}(\boldsymbol{\phi}^q)); q=1,2,\ldots,k\right\}$ and the sample mean at design point $\boldsymbol{\phi}^q$ is $\bar{Y}(\boldsymbol{\phi}^q) = \sum_{j=1}^{n_q} Y_j(\boldsymbol{\phi}^q)/n_q$. Let the sample means at all k design points be $\bar{\mathbf{Y}}_{\mathscr{D}} = (\bar{Y}(\boldsymbol{\phi}^1),\bar{Y}(\boldsymbol{\phi}^2),\ldots,\bar{Y}(\boldsymbol{\phi}^k))^T$. The simulations at different design points are independent and the variance of $\bar{\mathbf{Y}}_{\mathscr{D}}$ is represented by a $k\times k$ diagonal matrix $C = \mathrm{diag}\left\{\sigma_\varepsilon^2(\boldsymbol{\phi}^1)/n_1, \sigma_\varepsilon^2(\boldsymbol{\phi}^2)/n_2,\ldots,\sigma_\varepsilon^2(\boldsymbol{\phi}^k)/n_k\right\}$.

Let Σ be the $k\times k$ spatial covariance matrix of the design points and let $\Sigma(\boldsymbol{\phi},\cdot)$ be the $k\times 1$ spatial covariance vector between each design point and a fixed prediction point $\boldsymbol{\phi}$. If the parameters $(\tau^2,\boldsymbol{\theta},C)$ are known, given all simulation outputs, the metamodel uncertainty can be characterized by a refined GP,

$$M_p(\boldsymbol{\phi}) \sim \mathrm{GP}(u_p(\boldsymbol{\phi}),\sigma_p^2(\boldsymbol{\phi})),$$

where $u_p(\cdot)$ is the minimum mean squared error (MSE) linear unbiased predictor

$$u_p(\boldsymbol{\phi}) = \widehat{\beta}_0 + \Sigma(\boldsymbol{\phi},\cdot)^\top(\Sigma+C)^{-1}(\bar{\mathbf{Y}}_{\mathscr{D}} - \widehat{\beta}_0\cdot\mathbf{1}), \tag{1}$$

and the corresponding variance is

$$\sigma_p^2(\boldsymbol{\phi}) = \tau^2 - \Sigma(\boldsymbol{\phi},\cdot)^\top(\Sigma+C)^{-1}\Sigma(\boldsymbol{\phi},\cdot) + \boldsymbol{\eta}^\top[\mathbf{1}^\top(\Sigma+C)^{-1}\mathbf{1}]^{-1}\boldsymbol{\eta}, \tag{2}$$

where $\widehat{\beta}_0 = [\mathbf{1}^\top(\Sigma+C)^{-1}\mathbf{1}]^{-1}\mathbf{1}^\top(\Sigma+C)^{-1}\bar{\mathbf{Y}}_{\mathscr{D}}$ and $\boldsymbol{\eta} = \mathbf{1}-\mathbf{1}^\top(\Sigma+C)^{-1}\Sigma(\boldsymbol{\phi},\cdot)$ (see Ankenman et al. (2010)). The unknown parameters $(\tau^2,\boldsymbol{\theta})$ are estimated by MLEs, denoted by $(\widehat{\tau}^2,\widehat{\boldsymbol{\theta}})$. The sample variance is used as an estimate for the simulation variance at design points C. By plugging $(\widehat{\tau}^2,\widehat{\boldsymbol{\theta}},\widehat{C})$ into Equations (1) and (2), we can obtain the estimated mean $\widehat{u}_p(\boldsymbol{\phi})$ and variance $\widehat{\sigma}_p^2(\boldsymbol{\phi})$.

The input uncertainty is quantified by the posterior $p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$ and the metamodel uncertainty is quantified by the posterior distribution of $\mu(\cdot)$ specified by the GP, $M_p(\boldsymbol{\phi}) \sim \mathrm{GP}(u_p(\boldsymbol{\phi}),\sigma_p^2(\boldsymbol{\phi}))$. Thus, given the input and simulation data $\mathscr{X}_{\mathbf{m}}$ and $\mathbf{Y}_{\mathscr{D}}$, the posterior distribution of the compound random variable $M_p(\widetilde{\boldsymbol{\phi}})$ characterizes the overall estimation uncertainty of $\mu(\boldsymbol{\phi}^c)$. Xie et al. (2014) proposed a procedure to build a percentile CrI quantifying the system overall estimation uncertainty as follows.

1. Choose an experiment design $\mathscr{D} = \{(\boldsymbol{\phi}^q,n), q=1,2,\ldots,k\}$ with design points generated by using LHD. They are evenly distributed on the smallest ellipsoid covering the most likely posterior samples from $p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$. The number of replications at all design points is the same.
2. Run simulations at design points to obtain outputs $\mathbf{Y}_{\mathscr{D}}$. Compute the sample average $\bar{Y}(\boldsymbol{\phi}^q)$ and sample variance $S^2(\boldsymbol{\phi}^q)$ of the simulation outputs for $q=1,2,\ldots,k$. Fit the SK metamodel parameters $(\beta_0,\tau^2,\boldsymbol{\theta},C)$ to obtain $\widehat{u}_p(\boldsymbol{\phi})$ and $\widehat{\sigma}_p^2(\boldsymbol{\phi})$.
3. Generate $\widetilde{\boldsymbol{\phi}}^{(b)} \sim p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$ for $b=1,2,\ldots,B$. Let $\widehat{\mu}_b \equiv \widehat{u}_p(\widetilde{\boldsymbol{\phi}}^{(b)})$. Draw $\widehat{M}_b \sim \mathscr{N}\left(\widehat{\mu}_b, \widehat{\sigma}_p^2(\widetilde{\boldsymbol{\phi}}^{(b)})\right)$.

Therefore, the posterior samples $\{\widehat{M}_1,\widehat{M}_2,\ldots,\widehat{M}_B\}$ of the compound variable $M_p(\widetilde{\boldsymbol{\phi}})$ with $\widetilde{\boldsymbol{\phi}} \sim p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$ and $M_p(\boldsymbol{\phi}) \sim \mathrm{GP}(u_p(\boldsymbol{\phi}),\sigma_p^2(\boldsymbol{\phi}))$ quantify the overall system mean response estimation uncertainty.

Conditional on $\mathscr{X}_{\mathbf{m}}$ and $\mathbf{Y}_{\mathscr{D}}$, the total estimation uncertainty of $\mu(\boldsymbol{\phi}^c)$ can be decomposed as

$$\sigma_T^2 \equiv \mathrm{Var}[M_p(\widetilde{\boldsymbol{\phi}})] = \mathrm{E}\{\mathrm{Var}[M_p(\widetilde{\boldsymbol{\phi}})|\widetilde{\boldsymbol{\phi}}]\} + \mathrm{Var}\{\mathrm{E}[M_p(\widetilde{\boldsymbol{\phi}})|\widetilde{\boldsymbol{\phi}}]\} = \mathrm{E}[\sigma_p^2(\widetilde{\boldsymbol{\phi}})] + \mathrm{Var}[u_p(\widetilde{\boldsymbol{\phi}})], \tag{3}$$

where $\sigma_M^2 \equiv \mathrm{E}[\sigma_p^2(\widetilde{\boldsymbol{\phi}})]$ and $\sigma_I^2 \equiv \mathrm{Var}[m_p(\widetilde{\boldsymbol{\phi}})]$ quantify the impact from metamodel and input uncertainties. If σ_M^2 dominates, we can run more simulations at the promising region that could reduce the metamodel uncertainty most. If σ_I^2 dominates, we need to find the key sources of input model estimation uncertainty. We can estimate each variance component as follows:

- Total variance: $\widehat{\sigma}_T^2 = \sum_{b=1}^B (\widehat{M}_b - \bar{M})^2/(B-1)$, where $\bar{M} = \sum_{b=1}^B \widehat{M}_b/B$.
- Input variance: $\widehat{\sigma}_I^2 = \sum_{b=1}^B (\widehat{\mu}_b - \bar{\mu})^2/(B-1)$, where $\bar{\mu} = \sum_{b=1}^B \widehat{\mu}_b/B$.
- Metamodel variance: $\widehat{\sigma}_M^2 = \sum_{b=1}^B \sigma_p^2(\widetilde{\boldsymbol{\phi}}^{(b)})/B$.

5 SENSITIVITY ANALYSIS

Motivated by Oakley and O'Hagan (2004), we extend the Bayesian framework proposed in Xie, Nelson, and Barton (2014) so that it can facilitate the global sensitivity analysis and estimate the value of collecting additional real-world input data. According to Equation (3), the contribution of input uncertainty is quantified by $\sigma_I^2 \equiv \mathrm{Var}[u_p(\boldsymbol{\phi})]$. In Section 5.1, we conduct the sensitivity analysis to estimate the impact from each source of input uncertainty characterized by the posterior $p(\boldsymbol{\phi}_\ell|\mathbf{X}_{\ell,m_\ell})$ with $\ell = 1,2,\ldots,L$. It is based on the functional ANOVA. An approximation approach is proposed to quickly estimate the impact from each input uncertainty. Then, for each dominant source of input uncertainty, in Section 5.2, we predict the value of collecting additional data, say Δm_ℓ, which can guide the data collection to efficiently improve the estimation accuracy of the mean response $\mu(\boldsymbol{\phi}^c)$.

5.1 Variance Decomposition

Based on the function ANVOA (Oakley and O'Hagan 2004), we first decompose the function $u_p(\cdot)$ into main effects and interactions of the input components. Let $\mu^b = u_p(\widetilde{\boldsymbol{\phi}}^{(b)})$ with $\widetilde{\boldsymbol{\phi}}^{(b)} \sim p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$. Let $\mathscr{U} = u_p(\widetilde{\boldsymbol{\phi}})$ with $\widetilde{\boldsymbol{\phi}} \sim p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$. Then,

$$\mu^b = \mathrm{E}(\mathscr{U}) + \sum_{\ell=1}^L z_\ell(\widetilde{\boldsymbol{\phi}}_\ell^{(b)}) + \sum_{\ell<p} z_{\ell,p}(\widetilde{\boldsymbol{\phi}}_\ell^{(b)},\widetilde{\boldsymbol{\phi}}_p^{(b)}) + \sum_{\ell<p<q} z_{\ell,p,q}(\widetilde{\boldsymbol{\phi}}_\ell^{(b)},\widetilde{\boldsymbol{\phi}}_p^{(b)},\widetilde{\boldsymbol{\phi}}_q^{(b)}) + \ldots + z_{1,\ldots,d}(\widetilde{\boldsymbol{\phi}}^{(b)}), \tag{4}$$

with $z_\ell(\widetilde{\boldsymbol{\phi}}_\ell^{(b)}) = \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)}) - \mathrm{E}(\mathscr{U})$, $z_{\ell,p}(\widetilde{\boldsymbol{\phi}}_\ell^{(b)},\widetilde{\boldsymbol{\phi}}_p^{(b)}) = \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)},\boldsymbol{\phi}_p = \widetilde{\boldsymbol{\phi}}_p^{(b)}) - \mathrm{E}(\mathscr{U}) - z_\ell(\widetilde{\boldsymbol{\phi}}_\ell^{(b)}) - z_p(\widetilde{\boldsymbol{\phi}}_p^{(b)})$, $\mathrm{E}(\mathscr{U}) = \int_{\boldsymbol{\phi}} u_p(\boldsymbol{\phi}) dG_{\boldsymbol{\phi}}$, $\mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)}) = \int_{\boldsymbol{\phi}_{-\ell}} u_p(\boldsymbol{\phi}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)}) dG_{\boldsymbol{\phi}_{-\ell}}$, $\mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)},\boldsymbol{\phi}_p = \widetilde{\boldsymbol{\phi}}_p^{(b)}) = \int_{\boldsymbol{\phi}_{-\ell,-p}} u_p(\boldsymbol{\phi}|\boldsymbol{\phi}_\ell = \widetilde{\boldsymbol{\phi}}_\ell^{(b)},\boldsymbol{\phi}_p = \widetilde{\boldsymbol{\phi}}_p^{(b)}) dG_{\boldsymbol{\phi}_{-\ell,-p}}$ where $G_{\boldsymbol{\phi}}$ is the cumulative distribution function (c.d.f) of the posterior distribution $p(\boldsymbol{\phi}|\mathscr{X}_{\mathbf{m}})$; $\boldsymbol{\phi}_{-\ell}$ denotes the parameters in $\boldsymbol{\phi}$ except those for the ℓ-th input model, $G_{\boldsymbol{\phi}_{-\ell}}$ is the c.d.f of the posterior distribution for $\boldsymbol{\phi}_{-\ell}$, $\boldsymbol{\phi}_{-\ell,-p}$ denotes the parameters in $\boldsymbol{\phi}$ except those of the ℓ-th and p-th input models, $G_{\boldsymbol{\phi}_{-\ell,-p}}$ is the c.d.f of the posterior distribution for $\boldsymbol{\phi}_{-\ell,-p}$.

Since the main effect usually accounts for almost all the estimation variance of system response in many real-world systems (Oakley and O'Hagan 2004), we approximate Equation (4) as

$$\mu^b \approx \mathrm{E}(\mathscr{U}) + \sum_{\ell=1}^L z_\ell(\widetilde{\boldsymbol{\phi}}_\ell^{(b)}). \tag{5}$$

Let $W_\ell(m_\ell) = \mathrm{Var}(z_\ell(\boldsymbol{\phi}_\ell)|\mathscr{X}_{\mathbf{m}})$ be the variance contributed by the input uncertainty of parameter $\boldsymbol{\phi}_\ell$. Let G_ℓ to be the c.d.f of the posterior distribution $p(\boldsymbol{\phi}_\ell|\mathscr{X}_{\mathbf{m}})$. Then,

$$W_\ell(m_\ell) = \mathrm{Var}(z_\ell(\boldsymbol{\phi}_\ell)|\mathscr{X}_{\mathbf{m}}) = \int_{\boldsymbol{\phi}_\ell} z_\ell^2(\boldsymbol{\phi}_\ell) dG_\ell - \left[\int_{\boldsymbol{\phi}_\ell} z_\ell(\boldsymbol{\phi}_\ell) dG_\ell\right]^2 = \int_{\boldsymbol{\phi}_\ell} \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell)^2 dG_\ell - \mathrm{E}^2(\mathscr{U}). \tag{6}$$

To facilitate the sensitivity analysis and avoid the complexity required to calculate the integral term $\int_{\boldsymbol{\phi}_\ell} \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell)^2 dG_\ell$, we first approximate $\mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell)$ in Equation (6) by the first order Taylor's expansion at the maximum a posterior (MAP) estimate of $p(\boldsymbol{\phi}_\ell|\mathscr{X}_{\mathbf{m}})$, denoted by $\widehat{\boldsymbol{\phi}}_\ell$

$$\mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell) \approx \alpha_\ell + \boldsymbol{\gamma}_\ell^\top \boldsymbol{\phi}_\ell, \tag{7}$$

where

$$\boldsymbol{\gamma}_\ell = \left.\frac{\partial \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \boldsymbol{\phi}_\ell)}{\partial \boldsymbol{\phi}_\ell}\right|_{\boldsymbol{\phi}_\ell = \widehat{\boldsymbol{\phi}}_l} = \int_{\boldsymbol{\phi}_{-\ell}} \left.\frac{\partial u_p(\boldsymbol{\phi}|\boldsymbol{\phi}_\ell = \boldsymbol{\phi}_\ell)}{\partial \boldsymbol{\phi}_\ell}\right|_{\boldsymbol{\phi}_\ell = \widehat{\boldsymbol{\phi}}_\ell} dG_{\boldsymbol{\phi}_{-\ell}}, \tag{8}$$

and $\alpha_\ell = \mathrm{E}(\mathscr{U}|\boldsymbol{\phi}_\ell = \widehat{\boldsymbol{\phi}}_\ell) - \boldsymbol{\gamma}_\ell^\top \widehat{\boldsymbol{\phi}}_\ell$. Then, by plugging (7) into Equation (6), the impact from the ℓ-th input uncertainty can be estimated by

$$W_\ell(m_\ell) \approx (\alpha_\ell^2 - \mathrm{E}^2(\mathscr{U})) + 2\alpha_\ell \sum_{i=1}^{d_\ell} \gamma_{\ell,i} \mathrm{E}(\phi_{\ell,i}|\mathscr{X}_{\mathbf{m}}) + \sum_{i=1}^{d_\ell}\sum_{j=1}^{d_\ell} \gamma_{\ell,i}\gamma_{\ell,j} \mathrm{E}(\phi_{\ell,i}\phi_{\ell,j}|\mathscr{X}_{\mathbf{m}}), \tag{9}$$

where $\gamma_{\ell,i}$ is the i-th element in $\boldsymbol{\gamma}_\ell$ and $\phi_{\ell,i}$ is the i-th parameter in $\boldsymbol{\phi}_\ell$ for $i = 1,\ldots,d_\ell$, $\mathrm{E}(\phi_{\ell,i}|\mathscr{X}_{\mathbf{m}})$ and $\mathrm{E}(\phi_{\ell,i}\phi_{\ell,j}|\mathscr{X}_{\mathbf{m}})$ are the posterior mean and cross-moment of the parameters $\boldsymbol{\phi}_\ell$.

Then, we present a quick way to approximate the posterior moments in Equation (9). Let $g(\cdot)$ be a smooth, positive function. Set $L(\boldsymbol{\phi}_\ell) = [\log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]/m_\ell$ and $L^\star(\boldsymbol{\phi}_\ell) = [\log(g(\boldsymbol{\phi}_\ell)) + \log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]\ /m_\ell$. The studies in Tierney and Kadane (1986), Tierney et al. (1989) proposed accurate approximations of the posterior mean of any function $g(\boldsymbol{\phi}_\ell)$,

$$\widehat{\mathrm{E}}(g(\boldsymbol{\phi}_\ell)|\mathscr{X}_{\mathbf{m}}) = \left(\frac{|\Omega^\star|}{|\Omega|}\right)^{1/2} \exp\left(m_\ell(L^\star(\widehat{\boldsymbol{\phi}}_\ell^\star) - L(\widehat{\boldsymbol{\phi}}_\ell))\right),$$

where the posterior modes $\widehat{\boldsymbol{\phi}}_\ell$ and $\widehat{\boldsymbol{\phi}}_\ell^\star$ maximize $L(\boldsymbol{\phi}_\ell)$ and $L^\star(\boldsymbol{\phi}_\ell)$ correspondingly, Ω and $\Omega^\star$ are the negative of inverse Hessian matrices of $L(\boldsymbol{\phi}_\ell)$ and $L^\star(\boldsymbol{\phi}_\ell)$ at $\widehat{\boldsymbol{\phi}}_\ell$ and $\widehat{\boldsymbol{\phi}}_\ell^\star$. For Equation (9), the function $g(\cdot)$ is $\phi_{\ell,i}$ or $\phi_{\ell,i}\phi_{\ell,j}$.

Then, we calculate $\boldsymbol{\gamma}_\ell$ by applying (8). Since $u_p(\boldsymbol{\phi}) = \widehat{\beta}_0 + \Sigma(\boldsymbol{\phi},\cdot)^\top(\Sigma + C)^{-1}(\bar{\mathbf{Y}}_{\mathscr{D}} - \widehat{\beta}_0 \cdot \mathbf{1})$, we can calculate the derivative,

$$\frac{\partial u_p(\boldsymbol{\phi}|\boldsymbol{\phi}_\ell = \boldsymbol{\phi}_\ell)}{\partial \boldsymbol{\phi}_\ell} = \frac{\partial \Sigma(\boldsymbol{\phi},\cdot)^\top}{\partial \boldsymbol{\phi}_\ell}(\Sigma + C)^{-1}(\bar{\mathbf{Y}}_{\mathscr{D}} - \widehat{\beta}_0 \cdot \mathbf{1}).$$

For the Gaussian correlation function $r(\boldsymbol{\phi} - \boldsymbol{\phi}') = \exp\left(-\sum_{j=1}^d \theta_j(\phi_j - \phi_j')^2\right)$ used in the empirical study, we have $\frac{\partial \Sigma(\boldsymbol{\phi},\cdot)^\top}{\partial \boldsymbol{\phi}_\ell}$ is a $d_\ell \times k$ matrix with the $(i,q)-$th element, $\tau^2 \exp\left(-\sum_{j=1}^d \theta_j(\phi_j - \phi_j^q)^2\right)\left(-2\theta_{\ell,i}(\phi_{\ell,i} - \phi_{\ell,i}^q)\right)$.

Let $\boldsymbol{g}_\ell(\boldsymbol{\phi}_{-\ell}) = \left.\frac{\partial u_p(\boldsymbol{\phi}|\boldsymbol{\phi}_\ell = \boldsymbol{\phi}_\ell)}{\partial \boldsymbol{\phi}_\ell}\right|_{\boldsymbol{\phi}_\ell = \widehat{\boldsymbol{\phi}}_\ell}$ to be a d_ℓ dimensional vector. Then, $\boldsymbol{\gamma}_\ell$, $\mathrm{E}(\mathscr{U})$ and α_ℓ in Equation (9) can be estimated by

$$\widehat{\boldsymbol{\gamma}}_\ell \;=\; \frac{1}{B}\sum_{b=1}^B \boldsymbol{g}_\ell(\widetilde{\boldsymbol{\phi}}_{-\ell}^{(b)}),\ \widehat{\mathrm{E}}(\mathscr{U}) = \frac{1}{B}\sum_{b=1}^B u_p(\widetilde{\boldsymbol{\phi}}^{(b)}),\ \widehat{\alpha}_\ell = \frac{1}{B}\sum_{b=1}^B u_p(\boldsymbol{\phi}_\ell = \widehat{\boldsymbol{\phi}}_\ell, \boldsymbol{\phi}_{-\ell} = \widetilde{\boldsymbol{\phi}}_{-\ell}^{(b)}) - \widehat{\boldsymbol{\gamma}}_\ell^\top \widehat{\boldsymbol{\phi}}_\ell.$$

By plugging these estimates $\widehat{\boldsymbol{\gamma}}_\ell$, $\widehat{\alpha}_\ell$, and $\widehat{\mathrm{E}}(\mathscr{U})$ into Equation (9), we can estimate the contribution of the ℓ-th input model estimation uncertainty,

$$\widehat{W}_\ell(m_\ell) = (\widehat{\alpha}_\ell^2 - \widehat{\mathrm{E}}^2(\mathscr{U})) + 2\widehat{\alpha}_\ell \sum_{i=1}^{d_\ell} \widehat{\gamma}_{\ell,i} \widehat{\mathrm{E}}(\phi_{\ell,i}|\mathscr{X}_{\mathbf{m}}) + \sum_{i=1}^{d_\ell}\sum_{j=1}^{d_\ell} \widehat{\gamma}_{\ell,i}\widehat{\gamma}_{\ell,j}(\widehat{\mathrm{E}}(\phi_{\ell,i}\phi_{\ell,j}|\mathscr{X}_{\mathbf{m}})), \tag{10}$$

where $\widehat{\mathrm{E}}(\phi_{\ell,i}|\mathscr{X}_{\mathbf{m}}) = \left(\frac{|\Omega^\star|}{|\Omega|}\right)^{1/2} \exp\left(m_\ell(L^\star(\widehat{\boldsymbol{\phi}}^\star_\ell) - L(\widehat{\boldsymbol{\phi}}_\ell))\right)$ with $L(\boldsymbol{\phi}_\ell) = [\log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]/m_\ell$ and $L^\star(\boldsymbol{\phi}_\ell) = [\log(\phi_{\ell,i}) + \log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]/m_\ell$, $\widehat{\boldsymbol{\phi}}_\ell$ and $\widehat{\boldsymbol{\phi}}^\star_\ell$ maximize $L(\boldsymbol{\phi}_\ell)$ and $L^\star(\boldsymbol{\phi}_\ell)$ respectively, Ω and $\Omega^\star$ are the negative of the inverse Hessian matrices correspondingly.

For most commonly used input distributions with conjugate prior (e.g., exponential family), there are analytical solutions to $\widehat{\boldsymbol{\phi}}_\ell$, $\widehat{\boldsymbol{\phi}}^\star_\ell$, Ω and $\Omega^\star$. Similarly, $\widehat{\mathrm{E}}(\phi_{\ell,i}\phi_{\ell,j}|\mathscr{X}_{\mathbf{m}}) = \left(\frac{|\Omega^\star|}{|\Omega|}\right)^{1/2} \exp\left(m_\ell(L^\star(\widehat{\boldsymbol{\phi}}^\star_\ell) - L(\widehat{\boldsymbol{\phi}}_\ell))\right)$ with $L(\boldsymbol{\phi}_\ell) = [\log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]/m_\ell$ and $L^\star(\boldsymbol{\phi}_\ell) = [\log(\phi_{\ell,i}\phi_{\ell,j}) + \log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell)) + \log(p(\boldsymbol{\phi}_\ell))]/m_\ell$.

5.2 Value of Additional Data

We estimate the relative contribution from each input uncertainty by $\widehat{W}_\ell(m_\ell)$ for $\ell = 1,2,\ldots,L$. It is beneficial to quantify the system response estimation variance reduced by collecting additional data from each input model, say F^c_ℓ, which we refer to the value of more data. Suppose Δm_ℓ additional data are collected from F^c_ℓ. Then, the new input uncertainty $\widehat{W}_\ell(m_\ell + \Delta m_\ell)$ can be estimated according to Equation (10), by replacing the corresponding posterior means with

$$\widehat{\mathrm{E}}(g(\boldsymbol{\phi}_\ell)|\mathscr{X}_{\mathbf{m}}) = \left(\frac{|\Omega^\star|}{|\Omega|}\right)^{1/2} \exp\left((m_\ell + \Delta m_\ell)(L^\star(\widehat{\boldsymbol{\phi}}^\star_\ell) - L(\widehat{\boldsymbol{\phi}}_\ell))\right),$$

where $L(\boldsymbol{\phi}_\ell) = \frac{\log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell))}{m_\ell} + \frac{\log(p(\boldsymbol{\phi}_\ell))}{m_\ell + \Delta m_\ell}$, $L^\star(\boldsymbol{\phi}_\ell) = \frac{\log(p(\mathscr{X}_{\mathbf{m}}|\boldsymbol{\phi}_\ell))}{m_\ell} + \frac{\log(p(\boldsymbol{\phi}_\ell)) + \log(g(\boldsymbol{\phi}_\ell))}{m_\ell + \Delta m_\ell}$, and all other terms are unchanged. Thus, we can estimate the value of collecting Δm_ℓ additional data from F_ℓ with $\ell = 1,2,\ldots,L$,

$$\Delta\widehat{W}_\ell(\Delta m_\ell) = \widehat{W}_\ell(m_\ell) - \widehat{W}_\ell(m_\ell + \Delta m_\ell). \tag{11}$$

The value $\Delta\widehat{W}_\ell(\Delta m_\ell)$ for $\ell = 1,\ldots,L$ can guide the decision making to efficiently reduce the impact of input uncertainty, while accounting for the cost of additional data collection.

6 EMPIRICAL STUDY

In this section, we study an $M/M/1/K$ example and compare the proposed approach with those introduced in Ng and Chick (2006) and Song and Nelson (2015). Then, we use a bio-pharmaceutical inventory problem with five products including multivariate input models to study the performance of our approach.

6.1 An $M/M/1/K$ Queueing Example

We consider an $M/M/1/K$ queueing example with capacity $K = 20$. To evaluate the performance of our approach, suppose that the true arrival and service rates $\lambda^c = 4$ and $\nu^c = 5$ are unknown, and they are estimated from the real-world data $\mathscr{X}_m$. We use the conjugate priors $p(\lambda) = \mathrm{Gamma}(1,1)$ and $p(\nu) = \mathrm{Gamma}(1,1)$. We are interested in the expected waiting time, which has the closed form solution when the arrival and service rates are known (Sztrik, János 2012). For an $M/M/1/K$ queue with utilization rate $\rho = \lambda/\nu$, the expected waiting time is $\mu = \frac{N}{\lambda(1-P_K)} - \frac{1}{\nu}$, where $P_K = \frac{\rho^K}{\sum_{i=0}^K \rho^i}$ is the probability of K customer in queue.

Suppose the amount of real-world data for inter-arrival and service times is the same. There are three factors impacting on the system response estimation variance: (1) the size of input data m; (2) the number of design points used to construct the GP metamodel; and (3) the number of replications at each design point. We set the size of real-world data $m = 50, 100, 500$, the number of design points $k = 20, 80$, and the number of replications $n = 10, 100$. We set the same replications at all design points. At each replication, the run length is 100 with the warm up as 100 in term of number of customers.

We first consider the ratio of $\widehat{\sigma}^2_I/\widehat{\sigma}^2_M$ which measures the relative contribution from input uncertainty compared with the metamodel uncertainty. We report the average of ratios obtained from 100 macro-replications in Table 1. The input uncertainty has dominant impact on the total variance.

Table 1: Ratio between input and metamodel variance.

$\widehat{\sigma}_I^2/\widehat{\sigma}_M^2$		$m=50$	$m=100$	$m=500$
$n=10$	$k=20$	19.764	8.285	3.017
	$k=80$	42.150	17.603	8.536
$n=100$	$k=20$	33.427	12.969	5.382
	$k=80$	76.590	25.587	9.305

Since the input uncertainty has the dominant impact, we study the contribution from each input model and evaluate the robustness of approximations introduced in Equations (5) and (9). The first metric is the relative absolute difference between the input variance $\widehat{\sigma}_I^2$ with $\sum_{\ell=1}^L \widehat{W}_\ell(m_\ell)$, defined by $\mathrm{Err} = \frac{|\widehat{\sigma}_I^2 - \sum_{\ell=1}^L \widehat{W}_\ell(m_\ell)|}{\widehat{\sigma}_I^2}$. We compare the proposed input variance decomposition with that in Ng and Chick (2006) and Song and Nelson (2015). Ng and Chick (2006) considered the local linear metamodel of system mean response. The metamodel uncertainty is quantified by the posterior distribution. Song and Nelson (2015) proposed a linear metamodel for first two moments of each input model. To compare these approaches, we use the same design points and run the same number of replications. Table 2 records the average Err obtained from 100 macro-replications. Our method provides the better estimation accuracy on σ_I^2.

Table 2: Approximation error of input uncertainty for the $M/M/1/K$ example.

Err	Our Method	Ng (2006)	Song (2015)
$m=50$	0.287	0.360	0.443
$m=100$	0.206	0.248	0.291
$m=500$	0.094	0.109	0.122

We then estimate the contribution from each input model. Since there is the closed form of the system mean response (Sztrik, János 2012), we estimate the true component-wise input variance $W_\ell^c(m_\ell)$ for $\ell = 1,2$ according to Equation (6), where the integrations are estimated by using $B=1000$ posterior samples of input parameters. We use the sample variance of B responses to estimate $W_\ell^c(m_\ell)$. The average of the absolute relative error $\mathrm{RelativeError} = \frac{|\widehat{W}_\ell(m_\ell) - W_\ell^c(m_\ell)|}{W_\ell^c(m_\ell)}$ estimated by using 100 macro-replications is reported in Table 3. Our method provides more accurate estimation for the relative contribution from each source of input uncertainty.

Table 3: Relative error of each input model uncertainty.

W_1 (Arrival)	Our Method	Ng (2006)	Song (2015)
$m=50$	0.195	0.288	0.304
$m=100$	0.147	0.190	0.203
$m=500$	0.127	0.141	0.158
W_2 (Service)	Our Method	Ng (2006)	Song (2015)
$m=50$	0.221	0.318	0.373
$m=100$	0.160	0.192	0.209
$m=500$	0.142	0.155	0.170

Finally, we study the value of additional data on reducing the input uncertainty. The value of collecting Δm additional data from F_ℓ^c can be estimated from Equation (11) as $\Delta\widehat{W}_\ell(\Delta m)$ for $\ell = 1,2$. To evaluate the performance, we first get the component-wise variance $W_\ell^c(m)$ based on the posterior $p(\boldsymbol{\phi}|\mathscr{X}_m)$. Then, we generate Δm additional data from the true input model F_ℓ^c. Denote the updated dataset and posterior as $\mathscr{X}_{m+\Delta m}$ and $p(\boldsymbol{\phi}|\mathscr{X}_{m+\Delta m})$. Then, we can estimate the new component-wise variance $W_\ell^c(m+\Delta m)$. Thus, $\Delta W_\ell^c(\Delta m) = W_\ell^c(m) - W_\ell^c(m+\Delta m)$ measures the value of additional Δm data. We record the average absolute error of $|\Delta\widehat{W}_\ell(\Delta m) - \Delta W^c_\ell(\Delta m)|$ obtained from 100 macro-replications in Table 4. We set $\Delta m = 10, 50$ when $m = 50, 100$ and $\Delta m = 50, 100$ when $m = 500$. Our method provides more accurate estimate for the value of additional data.

Table 4: Estimation error of value of additional Δm data.

Error of $\Delta\widehat{W}_1(\Delta m)$ (Arrival)		Our Method	Ng (2006)	Song (2015)
$m = 50$	$\Delta m = 10$	0.016	0.025	0.033
	$\Delta m = 50$	0.079	0.104	0.137
$m = 100$	$\Delta m = 10$	5.9E-03	6.6E-03	7.4E-03
	$\Delta m = 50$	0.041	0.05	0.066
$m = 500$	$\Delta m = 50$	3.8E-03	4.8E-03	5.7E-03
	$\Delta m = 100$	0.011	0.014	0.021
Error of $\Delta\widehat{W}_2(\Delta m)$ (Service)		**Our Method**	**Ng (2006)**	**Song (2015)**
$m = 50$	$\Delta m = 10$	0.023	0.034	0.041
	$\Delta m = 50$	0.087	0.116	0.150
$m = 100$	$\Delta m = 10$	6.4E-3	7.1E-3	7.7E-3
	$\Delta m = 50$	0.055	0.064	0.078
$m = 500$	$\Delta m = 50$	5.1E-3	5.8E-3	6.2E-3
	$\Delta m = 100$	0.018	0.025	0.032

6.2 A Biopharmaceutical Inventory Example

Here, we use the bio-pharmaceutical inventory control example to evaluate the performance of our approach. Suppose there are 3 drugs. For each drug, the inventory is kept to meet the customer demand and we use the (R, Q) ordering policy. If the inventory position is less than the reorder point R, Q units of drugs are ordered. Both customer demand and delivery lead time from supplier for each drug are random. There are $L = 5$ input models with $d = 10$ parameters.

The demands for drugs 1 and 2 are dependent, following a multivariate normal distribution $\mathscr{N}((\mu_1, \mu_2)^\top, \boldsymbol{V})$ with $\mu_1 = 50, \mu_2 = 100$, $v_{11} = 20, v_{12} = v_{21} = 10, v_{22} = 40$. The demand for drug 3 follows $\mathscr{N}(\mu_3, v_3)$ with $\mu_3 = 100$ and $v_3 = 10$. The lead time for drug i follow by $\text{Pois}(\lambda_i)$ with $\lambda_1 = 0.5, \lambda_2 = 1, \lambda_3 = 2$. The parameters are estimated from finite "real-world data." Based on Gelman et al. (2004), for the multivariate normal, we use the conjugate Normal-Inverse-Wishart prior with $\boldsymbol{V} \sim \text{Inverse-Wishart}(v_0, \Lambda_0^{-1})$ and $(\mu_1, \mu_2)|\boldsymbol{V} \sim \mathscr{N}(\boldsymbol{\mu}_0, \boldsymbol{V}/\kappa_0)$, where $v_0 = 1, \kappa_0 = 0.01, \boldsymbol{\mu}_0 = (0, 0)^\top$ and Λ_0 is a 2×2 diagonal matrix with the diagonal term to be 0.01. For the normal distribution, we use the conjugate Normal-Inverse-Gamma prior with $v_3 \sim \text{Inverse-Gamma}(1/2, 1/2)$ and $\mu_3|v_3 \sim \mathscr{N}(0, v_3/\kappa_0)$ where $\kappa_0 = 0.01$. For Poisson distributions, we use the conjugate Gamma prior $\lambda_i \sim \text{Gamma}(1, 1)$ for $i = 1, 2, 3$.

The inventory policy for the 3 drugs is $R = (100, 100, 150)$ and $Q = (200, 200, 300)$ respectively. We are interested in the expected total inventory for the 3 drugs. According to Jensen and Bard (2003), suppose R_i and Q_i are the reorder point and order quantity for drug i, then the expected inventory level $\text{I}_i = \frac{Q_i}{2} + R_i - \mu_i T_i$ where μ_i is the average demand of drug i during each time period and T_i is the expected delivery delay. Thus, in our problem, the expected total inventory is a nonlinear function of input parameters. We presume it to be unknown and estimate from simulations. We use $m = 50, 100, 500$ data for each input model F_ℓ with $\ell = 1, \ldots, L$ to obtain the posterior distribution for the input parameters, select $k = 50, 100$ design points, and run $n = 10, 100$ replications at each design point. At each replication, the run length is 100 and the warm up period is also 100. We report average ratio of $\widehat{\sigma}_I^2/\widehat{\sigma}_M^2$ from 100 macro-replications in Table 5. The input uncertainty dominates the metamodel uncertainty.

Table 5: Ratio of input and metamodel uncertainties.

$\widehat{\sigma}_I^2/\widehat{\sigma}_M^2$		$m=50$	$m=100$	$m=500$
$n=10$	$k=50$	16.653	8.280	2.954
	$k=100$	29.702	13.498	6.623
$n=100$	$k=50$	19.625	8.591	3.162
	$k=100$	36.735	14.293	7.440

Similar with Table 2, we report the approximation error of the total input variance, with $\mathrm{Err}_1 = \frac{|\widehat{\sigma}_I^2 - \sum_{\ell=1}^{L} W_\ell|}{\widehat{\sigma}_I^2}$, for the bio-pharmaceutical inventory control example. We use $n=100$ and $k=100$. The results in Table 6 are obtained based on 100 macro-replications. Our method can better approximate the total input variance.

Table 6: Approximation error of the input variance.

Err_1	Our Method	Ng (2006)	Song (2015)
$m=50$	0.315	0.394	0.470
$m=100$	0.247	0.296	0.331
$m=500$	0.120	0.148	0.166

We evaluate the estimation accuracy of the impact from the ℓ-th input model, $\widehat{W}_\ell(m)$ for $\ell=1,\ldots,5$. Since there are 5 components, we consider the average estimation error $\mathrm{Err}_2 = \frac{1}{L}\sum_{\ell=1}^{L} \frac{|\widehat{W}_\ell(m) - W_\ell^c(m)|}{W_\ell^c(m)}$. We estimate the mean response by side experiment. We record the results of Err_2 obtained from 100 macro-replications in Table 7. Our method can provide the better estimation of the impact from each input uncertainty. In addition, we evaluate the value of collecting additional Δm data and record the average absolute error of $|\Delta\widehat{W}_\ell(\Delta m) - \Delta W_\ell^c(\Delta m)|$ in Table 8 for $\ell=1,\ldots,5$.

Table 7: Average error of estimated component-wise input variance.

Err_2	Our Method	Ng (2006)	Song (2015)
$m=50$	0.208	0.257	0.314
$m=100$	0.173	0.202	0.238
$m=500$	0.149	0.164	0.173

7 CONCLUSIONS

Built on the functional ANOVA introduced by Oakley and O'Hagan (2004), we extend the metamodel-assisted Bayesian framework proposed in Xie et al. (2014) for global sensitivity analysis that can quantify the impact of each input model estimation uncertainty. Then, we estimate the value of collecting additional data from each input model, which could be used to guide the data collection and efficiently improve the system performance estimation accuracy. The empirical study on an $M/M/1/K$ queue and a biopharma inventory example demonstrates the efficiency and efficacy of proposed approach.

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Table 8: Estimation error of value from collecting additional Δm input data.

Error of $\Delta\widehat{W}_1(\Delta m)$ (Drug 1,2 Demand)		Our Method	Ng (2006)	Song (2015)
$m = 50$	$\Delta m = 10$	0.429	0.548	0.637
	$\Delta m = 50$	1.872	2.470	3.105
$m = 100$	$\Delta m = 10$	0.157	0.193	0.248
	$\Delta m = 50$	0.790	0.922	1.145
$m = 500$	$\Delta m = 50$	0.104	0.119	0.136
	$\Delta m = 100$	0.413	0.458	0.504
Error of $\Delta\widehat{W}_2(\Delta m)$ (Drug 3 Demand)		**Our Method**	**Ng (2006)**	**Song (2015)**
$m = 50$	$\Delta m = 10$	0.315	0.384	0.471
	$\Delta m = 50$	1.396	1.728	2.159
$m = 100$	$\Delta m = 10$	0.106	0.143	0.188
	$\Delta m = 50$	0.495	0.550	0.631
$m = 500$	$\Delta m = 50$	0.091	0.104	0.122
	$\Delta m = 100$	0.389	0.417	0.484
Error of $\Delta\widehat{W}_3(\Delta m)$ (Drug 1 Lead Time)		**Our Method**	**Ng (2006)**	**Song (2015)**
$m = 50$	$\Delta m = 10$	0.259	0.320	0.383
	$\Delta m = 50$	1.162	1.557	1.898
$m = 100$	$\Delta m = 10$	0.082	0.103	0.117
	$\Delta m = 50$	0.376	0.429	0.510
$m = 500$	$\Delta m = 50$	0.068	0.094	0.105
	$\Delta m = 100$	0.252	0.323	0.419
Error of $\Delta\widehat{W}_4(\Delta m)$ (Drug 2 Lead Time)		**Our Method**	**Ng (2006)**	**Song (2015)**
$m = 50$	$\Delta m = 10$	0.330	0.385	0.446
	$\Delta m = 50$	1.493	1.837	2.294
$m = 100$	$\Delta m = 10$	0.109	0.132	0.158
	$\Delta m = 50$	0.460	0.538	0.606
$m = 500$	$\Delta m = 50$	0.089	0.105	0.123
	$\Delta m = 100$	0.327	0.388	0.451
Error of $\Delta\widehat{W}_5(\Delta m)$ (Drug 3 Lead Time)		**Our Method**	**Ng (2006)**	**Song (2015)**
$m = 50$	$\Delta m = 10$	0.481	0.553	0.630
	$\Delta m = 50$	2.175	2.763	3.406
$m = 100$	$\Delta m = 10$	0.175	0.198	0.216
	$\Delta m = 50$	0.602	0.683	0.775
$m = 500$	$\Delta m = 50$	0.124	0.145	0.168
	$\Delta m = 100$	0.500	0.595	0.643

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