Probability-space Surrogate Modeling for Sensitivity Analysis and Optimization

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ABSTRACT: This paper presents probability-space surrogate modeling approaches for global sensitivity analysis (GSA) and optimization under uncertainty. A probability model is learned first based on the available data to capture the nonlinear probabilistic relationships between the quantity of interest and input variables as well as among different input variables. Based on the learned probability model, approaches are then developed for design optimization under uncertainty and fast computation of the first order and total-effect sensitivity indices. This framework is applicable to not only GSA with correlated random variables and for sets of input variables, but also coupled multidisciplinary systems design under uncertainty with multiple objectives. The implementation of the proposed framework is investigated through two probability models, namely Gaussian copula model and Gaussian mixture model. One numerical example and one aircraft wing design problem demonstrate the effectiveness of the proposed method for GSA and multidisciplinary design under uncertainty.

1. INTRODUCTION

Problems in uncertainty quantification and decision-making often involve a large number of evaluations of the system model. When the system model is computationally expensive to evaluate, it is replaced with inexpensive surrogate models. The common practice is to build the surrogate model in the space of the input and output variables. This paper explores building the surrogate model in the space of probability distribution of the variables. Two types of analysis are explored with this approach, namely, multidisciplinary optimization and global sensitivity analysis.

Multidisciplinary optimization (MDO) under uncertainty aims at developing optimization ap-

proaches for systems modeled through computer simulations in individual disciplines that interact with each other. The fixed point iteration (FPI) approach developed by Kroo et al. (1994) is the commonly used for solving multidisciplinary problems where repeated runs of individual disciplines are carried out until convergence. The computational effort further increases with the consideration of uncertainty, which requires multiple evaluations of multidisciplinary analysis within each optimization iteration. Several approaches have been developed to reduce the large computational effort in MDO, such as an efficient decoupling approach proposed in Du and Chen (2005), and the likelihood-based approach proposed in Sankararaman and Mahadevan

(2012). However, these methods can become expensive and unaffordable in high-dimensional problems when physics-based computer simulation models (such as finite element analysis) are directly used. MDO under uncertainty results in a nested three-loop analysis, and is computationally very expensive.

Another important topic in uncertainty quantification is global sensitivity analysis (GSA), which quantifies the contributions of input random variables to the variability of an output quantity of interest (QoI) (Saltelli and Bolado (1998); Hu and Mahadevan (2018)). This analysis has been widely studied to rank the importance of input random variables and used in dimension reduction, uncertainty reduction, and resource allocation. Various approaches have been developed to perform GSA, such as the Fourier amplitude sensitivity test (FAST) methods proposed by McRae et al. (1982), methods based on correlation ratio developed by Xu and Gertner (2007), and Kullback-Leibler divergence based approaches presented in Da Veiga (2015). Among these GSA methods, variance decomposition-based Sobol indices are widely used. Two types of Sobol indices are usually computed, namely first-order Sobol indices and total-effect Sobol indices. A straightforward way of computing Sobol indices is to implement a double-loop Monte Carlo simulation (MCS). This double-loop procedure, however, requires a large number of evaluations of the prediction model and is unaffordable if the prediction model is expensive.

To overcome the computational effort challenge in MDO under uncertainty and GSA, various approaches have been proposed in recent years. In practical engineering applications, it is quite often that we may only have a group of numerical samples of input-output pairs, nothing more. The distributions, correlations, and interactions between different variables need to be learned purely based on the available numerical data. In that situation, current MDO under uncertainty and GSA methods cannot be adopted to perform MDO under uncertainty or rank the importance of variables for a given QoI due to the fact that the prediction model is not available. As a data-driven approach, surrogate model-based MDO or GSA is still applicable. However, this is

not always the case. In some situations, it is observed that the surrogate model-based MDO or GSA approaches may become inapplicable as well due to the reasons discussed in Li and Mahadevan (2016).

Also, note that when surrogate modeling is applied to MDO or GSA, especially for problems with correlated input variables, an algebraic model is built first. The probability distributions of the input variables are then learned from the data. Based on propagating the learned probability distributions through the constructed algebraic surrogate model, the Sobol indices and optimal design for MDO are computed. This introduces an extra step in MDO and GSA. Motivated by answering the question of how to effectively perform MDO and GSA purely based on a group of available data, several approaches have been proposed recently. For example, Liang and Mahadevan (2016) have used a Bayesian network surrogate with Gaussian copula for a single objective multidisciplinary optimization under uncertainty; Li and Mahadevan (2016) presented a modularized method to estimate the first-order Sobol indices based on stratification of available samples; Sparkman et al. (2016); DeCarlo et al. (2018) proposed an importance sampling approach to compute Sobol indices from available data by introducing weights to different data points.

The above reviewed data-driven MDO and GSA approaches, are all limited to low dimensional problems, and have difficulty in dealing with highdimensional MDO problems. This paper aims to overcome these drawbacks of current data-driven MDO and GSA methods by developing a generalized probability-space surrogate modeling framework, which is able to perform MDO and GSA computations purely based on data. In the proposed framework, a probability model is built first based on the available data to capture the joint probability distribution of the system inputs and outputs. Based on the learned probability model, approaches are developed to effectively perform MDO and compute different types of Sobol indices. Two approaches, namely Gaussian copula model and Gaussian mixture model, are explored in this paper to build the probability model for use in MDO under uncertainty and GSA.

The remainder of this paper is organized as follows. Section 2 reviews background concepts of probability-space surrogate modeling. Section 3 discusses how to perform GSA based on the probability-space surrogate model. Section 4 presents MDO based on probability-space surrogates. Section 5 uses two numerical examples to illustrate the proposed methods, and Section 6 provides the concluding remarks.

2. PROBABILITY-SPACE SURROGATE MODELING

We briefly introduce the probability-space surrogate modeling approaches. Two approaches, namely a Gaussian copula and a Gaussian mixture model, are employed to build probability-space models.

2.1. Gaussian copula model

A copula function describes the dependence between random variables by connecting the marginal cumulative distribution functions to the joint cumulative distribution function (Hu and Mahadevan (2017)). For a vector of random input variables \vec{X}_c and a output variable, Y, the joint CDF $F(\vec{X}, Y)$ is connected to the marginal CDFs through the copula function C as follows

$$F(\vec{X},Y) = C(\vec{F}(\vec{X}_c), F_Y(Y))|\vec{\theta}, \qquad (1)$$

where $\vec{F}(\vec{X}) = [F_{X_1}(X_1), \cdots F_{X_n}(X_n)]$ is a vector of marginal CDF functions, n is the number of variables in \vec{X} , and $\vec{\theta}$ is a vector of parameters of the copula function.

The copula functions are usually defined for bivariate problems. Only a few copula functions, such as Gaussian copula and student's t copula, are well-studied for the multi-variate high-dimensional case. Here, the Gaussian copula is used as an example to illustrate the application of a copula function to data-driven GSA. For Gaussian copula, we have $\vec{\theta} = \vec{R}$, where \vec{R} is the correlation matrix between variables and the PDF for the Gaussian copula case is given by Xue-Kun Song (2000)

$$f(\vec{X},Y) = \vec{f}(\vec{X})f_Y(Y)\frac{\partial \Phi^{-1}(\vec{F}(\vec{X}))}{\vec{F}(\vec{X})}$$
$$\frac{\partial \Phi^{-1}(F_Y(Y))}{F_Y(Y)}\phi(\Phi^{-1}(\vec{U}),\Phi^{-1}(U_Y))|\vec{R}, \quad (2)$$

in which $\Phi^{-1}(\cdot)$ is the inverse CDF function of a standard normal variable.

The above equation indicates that \vec{R} is the most important part for the modeling of a Gaussian copula. This correlation matrix can be solved using either optimization using the maximum likelihood estimate or empirical estimation from data.

2.2. Gaussian mixture model

The GMM represents an arbitrary probability distribution using mixtures of Gaussian components. For a random variable X_i , its PDF $f_{X_i}(x_i)$ is approximated using a Q component Gaussian distribution as follows (Rasmussen (2000))

$$f_{X_i}(x) = \sum_{i=1}^{Q} \lambda_i \phi(x, \mu_i, \sigma_i), \qquad (3)$$

where Q is the number of Gaussian components, λ_i , μ_i , and σ_i are the weight, mean, and standard deviation of the i-th Gaussian component.

For $\vec{Z} = [\vec{X}, Y]$, the joint PDF $f(\vec{x}, y)$ is approximated using a multi-variate GMM as

$$f(\vec{z}) = \sum_{i=1}^{Q} \lambda_i \phi(\vec{z}, \vec{\mu}_i, \vec{\Sigma}_i), \tag{4}$$

where $\vec{z} = [\vec{x}, y]^T$, $\vec{\mu}_i = [\vec{\mu}_{i,\vec{x}}, \vec{\mu}_{i,y}]^T$, and

$$\vec{\Sigma}_{i} = \begin{bmatrix} \vec{\Sigma}_{i,xx} & \vec{\Sigma}_{i,xy} \\ \vec{\Sigma}_{i,yx} & \sigma_{i,y}^{2} \end{bmatrix}.$$
 (5)

The expectation maximization (EM) method as discussed in Moon (1996) is commonly used to estimate the parameters of the GMM model. Next, we discuss how to perform GSA and MDO using probability-space surrogate models.

3. GSA USING A PROBABILITY-SPACE SURROGATE MODEL

3.1. Global sensitivity analysis

Defining Y as a QoI and its prediction model given by $Y = g(\vec{X})$, where $\vec{X} = [X_1, X_2, \dots, X_n]$ is a vector of random input variables, the variance Var(Y) of Ycan be decomposed as follows:

$$Var(Y) = \sum_{i=1}^{n} V_i + \sum_{1 \le i < j}^{n} V_{ij} + \dots + V_{12...n}, \quad (6)$$

where $V_i = Var_{X_i}(E_{\vec{X}_{\sim i}}(Y|X_i))$ is the variance of Y estimate $Var_{\vec{X}_c}(E_{\vec{X}_r}(Y|\vec{X}_c = \vec{x}_c))$ as caused by X_i without considering its interactions with other input variables (i.e. $\vec{X}_{\sim i}$) and $V_{12...k}, \forall k =$ $3, \dots, n$ represents the proportion of Var(Y) caused by variables $[X_1, X_2, \dots, X_k]$.

Based on the above variance decomposition, the commonly used first-order and total effect Sobol' indices are defined as (Sudret (2008))

$$S_i = \frac{Var_{X_i}(E_{\vec{X}_{\sim_i}}(Y|X_i))}{Var(Y)},\tag{7}$$

$$S_{T_i} = 1 - \frac{Var_{\vec{X}_{\sim i}}(E_{X_i}(Y|\vec{X}_{\sim i}))}{Var(Y)}, \tag{8}$$

where S_i and S_{T_i} are the first-order and total-effect Sobol' indices of X_i , respectively.

3.2. GSA with probability surrogate models

Next, we discuss how to compute Sobol indices where using probability surrogate models.

3.2.1. GSA with Gaussian copula model

Define the input variables of interest in GSA as \vec{X}_c and the remaining input random variables as \vec{x}_r , we have

$$E_{\vec{X}_r}(Y|\vec{x}_c) = \frac{1}{c(\vec{u}_c)|\vec{R}_{cc}} \int_0^1 F_Y^{-1}(u_Y)c(\vec{u}_c, u_Y)|\vec{R}du_Y,$$

For the purpose of generalization, here, an MCSbased method is adopted to estimate Eq. (9) as below

$$E_{\vec{X}_r}(Y|\vec{X}_c = \vec{x}_c) \approx \frac{1}{N_{MCS}c(\vec{u}_c)|\vec{R}_{cc}}$$

$$\sum_{k=1}^{N_{MCS}} F_Y^{-1}(u_Y^{(k)})c(\vec{u}_c, u_Y^{(k)})|\vec{R}, \quad (10)$$

where $u_Y^{(k)}$ is the k-th sample of U_Y and N_{MCS} is the number of MCS samples used for integration.

estimate
$$Var_{\vec{X}_c}(E_{\vec{X}_c}(Y|\vec{X}_c = \vec{x}_c))$$
 as

$$Var_{\vec{X}_{c}}(E_{\vec{X}_{r}}(Y|\vec{X}_{c}=\vec{x}_{c})) \approx \frac{1}{2N_{MCS}s^{2}} \sum_{i=1}^{s} \frac{1}{2N_{MCS}s^{2}} \sum_{i=1}^{s} \frac{1}{c(\vec{u}_{c}^{(i)})|\vec{R}_{cc}} \sum_{k=1}^{N_{MCS}} F_{Y}^{-1}(u_{Y}^{(k)})c(\vec{u}_{c}^{(i)}, u_{Y}^{(k)})|\vec{R}| - \frac{1}{c(\vec{u}_{c}^{(j)})|\vec{R}_{cc}} \sum_{k=1}^{N_{MCS}} F_{Y}^{-1}(u_{Y}^{(k)})c(\vec{u}_{c}^{(j)}, u_{Y}^{(k)})|\vec{R}|^{2}, \quad (11)$$

Once we are able to compute $Var_{\vec{X}_c}(E_{\vec{X}_c}(Y|\vec{x}_c))$, various Sobol' indices can be computed using Eqs. (7) and (8).

(8) 3.2.2. GSA with Gaussian mixture model After $f(\vec{x}_c, y)$ is approximated using GMM, for given $\vec{X}_c = \vec{x}_c$, the conditional PDF $f(y|\vec{x}_c)$ is given

$$f(y|\vec{x}_c) = \sum_{i=1}^{Q} \lambda_i(\vec{x}_c) \phi(y, \vec{\mu}_{i,y|\vec{x}_c}, \sigma_{i,y|\vec{x}_c}^2), \quad (12)$$

$$\vec{\mu}_{i,y|\vec{x}_c} = \mu_{i,y} + \vec{\Sigma}_{i,yc} \vec{\Sigma}_{i,cc}^{-1} (\vec{x}_c - \vec{\mu}_{i,\vec{x}_c}), \tag{13}$$

$$\sigma_{i,y}^2 = \sigma_{i,y}^2 - \vec{\Sigma}_{i,yc} \vec{\Sigma}_{i,cc}^{-1} \vec{\Sigma}_{i,yc}^T, \tag{14}$$

$$\lambda_i(\vec{x}_c) = \frac{\lambda_i \phi(\vec{x}_c, \vec{\mu}_{i,\vec{x}_c}, \vec{\Sigma}_{i,\vec{x}_c})}{\sum_{k=1}^{Q} \lambda_k \phi(\vec{x}_c, \vec{\mu}_{k,\vec{x}_c}, \vec{\Sigma}_{k,\vec{x}_c})}.$$
 (15)

Based on Eq. (12), $E_{\vec{X}_c}(Y|\vec{X}_c = \vec{x}_c)$ can be computed as

$$E_{\vec{X}_r}(Y|\vec{X}_c = \vec{x}_c) = \sum_{i=1}^{Q} \lambda_i(\vec{x}_c) \mu_{i,y|\vec{x}_c},$$
 (16)

With the available data, we have

$$Var_{\vec{X}_{c}}(E_{\vec{X}_{r}}(Y|\vec{X}_{c} = \vec{x}_{c}))$$

$$\approx \frac{1}{2s^{2}} \sum_{i=1}^{s} \sum_{j=1}^{s} (\sum_{k=1}^{Q} \lambda_{k}(\vec{x}_{c}^{(i)}) \mu_{k,y|\vec{x}_{c}^{(i)}} - \sum_{k=1}^{Q} \lambda_{k}(\vec{x}_{c}^{(j)}) \mu_{k,y|\vec{x}_{c}^{(j)}})^{2}. \quad (17)$$

With Eq. (17) and Eqs. (7) and (8), the first-order Using Eq. (10) and the available data, we then and total-effect Sobol' indices can be computed.

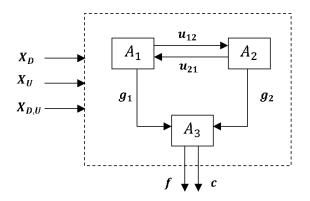


Figure 1: A conceptual two-way multi-physics system

4. MULTIDISCIPLINARY DESIGN OPTI-MIZATION USING A PROBABILITY-SPACE SURROGATE MODEL

4.1. Multidisciplinary optimization under uncertainty (MDOUU)

Consider a conceptual two-way coupled multiphysics system, as shown in Figure 1. Let X_D , X_U and $X_{D,U}$ represent the set of deterministic design variables, uncertain but non-design variables, and design variables associated with uncertainty respectively. Let g_1 and g_2 represent the outputs of the individual disciplinary systems, which are propagated through a third discipline A_3 to obtain the objective functions f and constraint functions c. The coupling variables between the coupled disciplines, i.e., A_1 and A_2 , are represented as u_{12} and u_{21} respectively. Due to the presence of uncertainty, the objective and constraint functions are stochastic for a given realization of the design variables. For illustration, an reliability-based design optimization formulation (a form of MDOUU), where the mean of the objective functions are optimized can be written as

Min
$$\mu[f_i(X_D, X_U, X_{D,U})]$$

 $Pr(c_j(X_D, X_U, X_{D,U}, u_{12}, u_{21}) < 0) > \gamma_j$
 $lb_d \le X_D \le ub_d$ (18)
 $Pr(X_{D,U} \ge lb_{X_{D,U}}) \ge p_{lb}$
 $Pr(X_{D,U} \le ub_{X_{D,U}}) \ge p_{ub}$

In the above formulation, $f_i(i=1,2...k)$ and $c_j(j=1,2,..m)$ represent the objective and constraint functions respectively. $c_j < 0$ represents the safe region and γ_j represents the reliability threshold

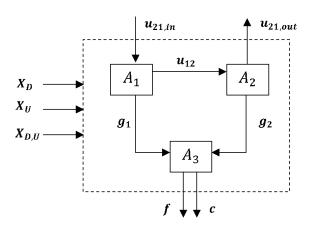


Figure 2: One-pass analysis approach in a two-way coupled multi-physics system

for the j^{th} constraint. p_{lb} and p_{ub} represent the probability thresholds for $X_{D,U}$ that they are in between their lower and upper bounds ($lb_{X_{D,U}}$ and $ub_{X_{D,U}}$). Similar formulation is available in Zaman and Mahadevan (2013).

4.2. MDOUU using a probability-space surrogate model

The first step in constructing a surrogate is the generation of training points. In multidisciplinary problems, the training points are generated through one pass analysis. To reach compatibility among individual disciplines, the one-pass analysis need to be carried out multiple times with the outputs of previous one-pass analysis as the inputs for the following one-pass analysis. A possible path for a one-pass analysis is shown in Figure 2.

In Figure 2, $u_{21,in}$ and $u_{21,out}$ are the same set of coupling variables but before and after carrying out a one-pass analysis through the disciplines A_1 and A_2 . Compatibility is assumed to be achieved when $u_{21,in} = u_{21,out}$. To achieve compatibility, multiple iterations of the coupled analysis are necessary. However, instead of multiple iterations to convergence, we build a probability-space surrogate using one-pass analysis data, and then impose the multidisciplinary compatibility condition. This saves tremendous computational expense, and the three-loop nested analysis can be transformed into a double loop analysis.

5. NUMERICAL EXAMPLES

In this section, two numerical examples with one featuring GSA and one featuring MDO are used to demonstrate the effectiveness of the proposed methods.

5.1. A mathematical example

A nonlinear model with nonlinear dependence given in Ref. Mara et al. (2015) is employed as our first example to illustrate the effectiveness of the proposed methods in performing GSA using probability models. The nonlinear function is given by

$$Y = f(\vec{X}) = X_1 X_2 + X_3 X_4, \tag{19}$$

where $(X_1, X_2) \in [0, 1]^2$ is uniformly distributed within the triangle $X_1 + X_2 \le 1$, $(X_3, X_4) \in [0, 1]^2$ is uniformly distributed within the triangle $X_3 + X_4 \ge 1$, X_1 and X_2 are dependent due to the shared hidden variable L_1 , and X_3 and X_4 are dependent due to the shared hidden variable L_3 . More details about this example is available in Ref. Mara et al. (2015).

We assume that the nonlinear function and the nonlinear dependence are unknown, and perform GSA purely based on given samples. We generate 1024 MCS samples of X_i , i = 1, 2, 3, 4 and Y. Using the generated MCS samples, we then compute various Sobol' indices.

We first compute the first-order and total-effect Sobol' indices of individual dependent random variables. Fig. 3 gives the first-order indices obtained from different methods. The Gaussian copulabased GSA methods cannot accurately estimate the first-order Sobol' indices whereas the GMM-based method can accurately estimate the first-order Sobol' indices for dependent variables.

Fig. 4 gives the results comparison of the total-effect Sobol' indices obtained from different methods. The results show that GMM-based method can effectively estimate the total-effect Sobol' indices.

5.2. Aircraft wing example

The design of a cantilever wing with a NACA 0012 airfoil is considered. We consider two competing objective functions to perform Reliability-based Robust Design Optimization: (1) Maximize the expected value of Lift, and (2) Minmize the standard deviation of Lift. The design is performed under the

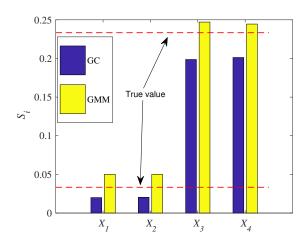


Figure 3: First-order Sobol' indices of dependent variables

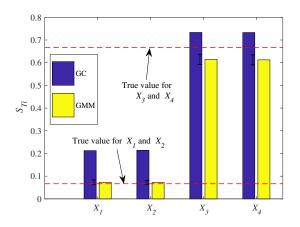


Figure 4: Total-effect indices of dependent variables

stress constraint with backsweep angle as the design variable, which is assumed to be associated with aleatory uncertainty represented through a Gaussian distribution with parameters 0 and 0.04 respectively. Since, the variability in the backsweep angle is known, we consider the mean of the backsweep angle as the design variable. Overall, the mathematical formulation of the design can be written as

Max
$$E[L(\mu_{bw})]$$
 and Min $Std[L(\mu_{bw})]$
 $Pr(s > 3 \times 10^5) \le 0.001$ (20)
 $0 \le \mu_{bw} \le 0.5$

In Equation (20), E[.] and Std[.] represent the expectation and standard deviation operators respectively. L, μ_{bw} and s represent the lift, mean of back-

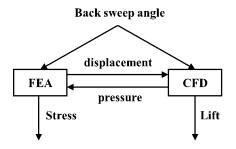


Figure 5: Coupling in aircraft wing analysis

sweep angle and maximum stress respectively. The individual disciplines along with the coupling variables is illustrated in Figure 5.

The multi-objective optimization is converted to a set of single-objective optimizations using the weighted-sum approach as

Min
$$\beta \times \frac{Std[L]}{S_{bl}} - (1 - \beta) \times \frac{E[L]}{E_{bl}}$$
 (21)

In Equation (21), β represents the weight factor for combining the two objective functions. E_{bl} and S_{bl} represent the normalization factors (1666.7 and 113) since the two objectives are in different order of magnitude. 200 training points are obtained through ANSYS fluid-structure interaction simulations for probability surrogate construction. he coupling between CFD and FEA is decoupled through severing the arrow from CFD to FEA. In this analysis, we have 258 coupling variables. Due to the large number of coupling variables, the Principal Component Analysis (PCA) is performed to reduce the number of coupling variables from 258 to 6. The first 6 PCs are chosen as they explain 95% variance in the data. Please refer to Liang and Mahadevan (2016) regarding the use of PCA for reducing model complexity in multidisciplinary analysis. We have 16 variables in the probability-space surrogate: mean of backsweep angle, backsweep angle (after considering aleatory uncertainty), 6 'in' nodal pressures, 6 difference values of nodal pressures, 1 maximum stress and 1 lift variable. Both Gaussian Copula and Gaussian Mixture Model are fit on these 16 variables using 200 training points. In the case of a GMM, a twocomponent model is used as it has the lowest BIC score. Using the surrogates, the multidisciplinary optimization is performed by conditionalising the 6

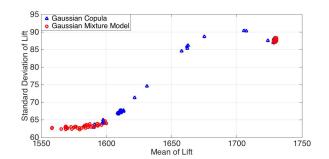


Figure 6: Comparison of Pareto Surfaces obtained using Gaussian Copula and a Gaussian Mixture Model

'difference' variables at zero and the design variable at a different value in each iteration of the optimization analysis. DIRECT global optimizer (Finkel et al. (2005)) is used to carry out each single objective optimization. For comparison of Pareto surfaces, the optimum design points obtained from optimization analysis using the two surrogates are evaluated using the GMM and plotted against each other in Figure 6.

In Figure 6, the points in upper right corner correspond to $\beta=0$ (maximization of the expected value of lift) and correspondingly, the lower left corner correspond to $\beta=1$, i.e., minimization of the standard deviation of lift. It can be seen that both the surrogates obtain the similar solution for optimization of expected value of lift, whereas the GMM is able to capture well the standard deviation of lift compared to the other two surrogates.

6. CONCLUSION

This paper presents methods for computing various Sobol' indices and performing multidisciplinary optimization under uncertainty, purely based on available input-output data. The data may be available from computational simulations, physical experiments, field observations, etc. In the proposed methods, probability-space surrogate models are built to approximate the joint PDF of the variables of interest. With the probability models learned from the data, various types of Sobol' indices are computed and multidisciplinary optimization under uncertainty is performed. The proposed framework is investigated using the Gaussian copula and Gaussian mixture models. The results of two numerical examples show that the Gaussian mixture models-

based GSA and MDO methods are able to accurately compute Sobol' indices and perform MDO based on an available data. This allows us to perform GSA and MDO for problems, where we can only collect a limited number of data points due to constraints of either computational or experimental resources.

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