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Imprecise global sensitivity analysis using bayesian multimodel inference and importance sampling

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ABSTRACT

Global Sensitivity Analysis (GSA) aims to understand the relative importance of uncertain input variables to model response. Conventional GSA involves calculating sensitivity (Sobol') indices for a model with known model parameter distributions. However, model parameters are affected by aleatory and epistemic uncertainty, with the latter often caused by lack of data. We propose a new framework to quantify uncertainty in probability model-form and model parameters resulting from small datasets and integrate these uncertainties into Sobol' index estimates. First, the process establishes, through Bayesian multimodel inference, a set of candidate probability models and their associated probabilities. Imprecise Sobol' indices are calculated from these probability models using an importance sampling reweighting approach. This results in probabilistic Sobol' indices, whose distribution characterizes uncertainty in the sensitivity resulting from small dataset size. The imprecise Sobol' indices thus provide a measure of confidence in the sensitivity estimate and, moreover, can be used to inform data collection efforts targeted to minimize the impact of uncertainties. Through an example studying the parameters of a Timoshenko beam, we show that these probabilistic Sobol' indices converge to the true/deterministic Sobol' indices as the dataset size increases and hence, distribution-form uncertainty reduces. The approach is then applied to assess the sensitivity of the out-of-plane properties of an E-glass fiber composite material to its constituent properties. This second example illustrates the approach for an important class of materials with wide-ranging applications when data may be lacking for some input parameters.

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1. Introduction

Computational simulation is widely used to better understand complex mathematical and physical systems. Typically these simulations aim to model the system response, specifically targeting some quantity of interest (QoI) and its dependence on some set of input model parameters. In many cases, these input parameters are not precisely known or deterministic because of inherent randomness in the system and/or a lack of knowledge/data. In traditional analyses, uncertainty is quantified probabilistically and propagated through the computational model. Consequently, the corresponding QoI is uncertain.

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Sensitivity analysis is the quantitative assessment of the influence of variations in input parameters on variations in the output QoI. Sensitivity analysis therefore enables the assessment of the relative importance of each model input to the specific QoI [1,2]. Generally speaking, there are two classes of sensitivity analysis: *Local Sensitivity Analysis* (LSA) and *Global Sensitivity Analysis* (GSA). LSA focuses on the influence of the small variations in the input parameters around some nominal values and are typically quantified by evaluating local gradients in the system solution with respect to the input parameters. GSA, on the other hand, examines the effect of variations in the input parameters across the entire range of the parameter space. We are specifically interested in GSA in this work. Two prominent methods have been developed for GSA. The first is the one-factor-at-a-time approach in which each parameter is perturbed in turn while keeping all other parameters fixed at their nominal value. This approach has been shown to break down when the model deviates from linearity [3] and cannot account for a probability density over the parameter domain. The second is based on the estimation of variance-based sensitivity indices (so-called Sobol' indices) [4] that prove more robust to model form and relies on each parameter having an associated probability measure.

A variety of methods have been proposed for variance-based GSA that employ, for example, Fourier analysis as in the FAST (Fourier Amplitude Sensitivity Test) algorithm [5,6], Monte Carlo methods [7,8], and surrogate modeling methods such as polynomial chaos [9,10], Gaussian processes/Kriging [11], and support vector machines [12] considering both independent and correlated input parameters [13]. Moreover, the range of recent applications for GSA spans across physical systems of all types from chemistry [14] to structural acoustics [15] and structural vibration of nuclear reactor assemblies [16]. In this work, we employ Monte Carlo estimates of global sensitivity indices because they are robust, simple to use, and couple conveniently with the multimodel uncertainty quantification methods for imprecise probabilities proposed herein. Extension of the concepts proposed herein to utilize more efficient GSA algorithms thus remains an important research objective.

Conventional GSA methods are built from a classical probabilistic framework in which input uncertainty is characterized through a known probability measure on the input parameters. Hence, the first step of GSA is to identify or assume a reasonable probability distribution for the input variables. However, as commonly occurs when data characterizing the input parameters are sparse, it may be impossible to identify the appropriate distribution. This can lead to assumptions that may seem reasonable but are nonetheless subjective and may yield sensitivity indices that are inaccurate, non-conservative, or even potentially unreasonable with no quantitative error metrics. These errors arise from so-called *epistemic uncertainty* – or uncertainty that arises from a lack of knowledge or data and can therefore be reduced with additional data collection [17]. The inclusion of epistemic uncertainty gives rise to two distinct objectives for *imprecise global sensitivity analysis*:

1. To assess confidence in estimates of conventional global sensitivity indices.
2. To specifically understand the influence of epistemic uncertainty on system response, and therefore inform data collection efforts such that they reduce the impact of uncertainty in system response.

To address both objectives in this work, we propose a method that infers a probability distribution for the Sobol' indices. Thus, toward the first object, the method provides a natural measure of confidence. Toward the second objective, the inferred distribution identifies parameters that may contribute significantly to system response and also have large uncertainty. Therefore, it is useful in identifying parameters that should be targeted for further data collection efforts. Generally speaking, several theories have been proposed to address the various forms of epistemic uncertainty. It has been argued that epistemic uncertainty requires a different mathematical treatment than *aleatory uncertainty* [18], which arises from irreducible randomness and is naturally treated probabilistically. However, no scientific consensus has been achieved in terms of what that treatment should be. The larger problem is that a unified mathematical treatment of epistemic uncertainty must be general enough to accommodate the many types of epistemic uncertainty – such as those that arise from vague, qualitative, or conflicting data, total or near-total ignorance, small datasets that give limited information about a probability measure, and the “unknown unknown” among others. Different mathematical theories have been developed which account for some of these epistemic uncertainties; typically by generalizing the measure used to quantify events in the algebra of possibilities. Specific examples include possibility theory which introduce the concepts of possibility and necessity measures [19], Dempster-Shafer/Evidence theory which introduces the concepts of belief and plausibility measures [20,21], Choquet capacities which introduce conjugate measures of lower and upper probability [22], fuzzy sets [23,24] and fuzzy measures [25], random sets and sets of probability measures [26,27], and interval methods [28] including interval probabilities and probability boxes (p-boxes) [18]. In the intervening years, efforts have been made to unify these theories under an over-arching theory of imprecise probabilities, most notably through the works of Walley [29,30].

Perhaps more relevant for our purposes, many recent efforts have been made in the engineering community to translate these theories of imprecise probabilities into the practice of uncertainty quantification and stochastic analysis in computational modeling. This includes efforts to: extend Monte Carlo simulations [31–33], develop non-intrusive stochastic simulation methods for imprecise probability models [34–37], construct p-boxes and Dempster-Shafer belief functions [38], understand the effects of imprecision on reliability/probability of failure [39–43], propagate p-boxes [44,45], and perform Bayesian model averaging [46] to name just a few. A concise review of imprecise probability methods in engineering can be found in [47]. Among the many studies of epistemic uncertainty in engineering, relatively few have considered the prob-

lem of imprecise global sensitivity analysis. To the authors' knowledge, such investigations date back a little more than a decade beginning with the work of Helton et al. who merged GSA with evidence theory to estimate imprecise sensitivity measures [48] and Hall who estimated the upper and lower bounds of sensitivity indices when the uncertainty in the model inputs are expressed as closed convex sets of probability measures [49]. Among the most comprehensive studies of imprecise GSA is that conducted by Oberguggenberger et al. [50] who compared classical GSA with GSA for problems with uncertainties defined by random sets, fuzzy sets, and intervals. Other recent works include those of Song et al. [51] who devised GSA for input uncertainties characterized by p-boxes and computed the imprecise sensitivity indices using extended Monte Carlo simulation [31] (EMCS). Li and Mahadevan [52] devised a scheme to estimate Sobol' indices when both aleatory and epistemic uncertainty are present in time series data. More recently, Wei et al. [53] proposed a probabilistic framework where epistemic input uncertainties are characterized by second-order probability models to compare the relative importance of influential and non-influential input variables using EMCS. Schöbi and Sudret [54] used polynomial chaos expansions to develop interval Sobol' indices when input uncertainties are characterized by p-boxes, and Hart and Germaud [55] provided a theoretical analysis for the robustness of the Sobol' indices to changes in the distribution of the uncertain variables.

In this study, we investigate imprecise GSA where epistemic uncertainty specifically results from sparse data sets, which may be compiled from disparate data sources. This focus is motivated by the difficulty of data collection under complex conditions in engineering practice. In many cases, experimental or validated simulation data for quantifying parameter uncertainties are strictly limited. As a result, it is impossible to assign an objective and accurate probability distribution for the input variables to a computational model and precisely estimate their impact on the response output. The specific contributions of this study can be summarized as follows:

- We derive a formulation for computing main effect and total sensitivity indices using importance sampling.
- We apply a Bayesian multimodel inference process in conjunction with the importance sampling-based GSA to estimate the distribution of imprecise Sobol' indices whose uncertainty results from lack of data quantifying input uncertainty.
- We demonstrate how to obtain the optimal sampling density to efficiently employ the proposed multimodel GSA for engineering systems.
- We illustrate how to use the results of the proposed imprecise GSA to assess confidence in computed sensitivity indices and inform future testing and data collection.

It is important to emphasize that the novelty of the work presented here lies in bringing the components of importance sampling based GSA and Bayesian multimodel inference together for a robust and efficient approach to imprecise GSA. The development of the individual components of the approach is not the primary intent. Indeed previous works have, for example, derived formulations for computing sensitivity indices using importance sampling (see e.g. [53]) – although the formulation provided here has some distinct differences and advantages that are discussed below.

The paper is structured as follows. We begin in Section 2 by presenting a brief review of GSA, particularly variance-based methods and Sobol' indices. Section 3 introduces the Bayesian multimodel inference methodology and its application for identifying imprecise probability models given limited data. An efficient importance sampling-based Monte Carlo method for imprecise global sensitivity analysis is then proposed in Section 4. The effectiveness of the proposed algorithm is illustrated by a closed-form numerical example in Section 5. Section 6 presents an application of the proposed method to predicting the sensitivity of composite material properties to the properties of its constituents. Finally, some concluding remarks are provided in Section 7.

2. Variance-based methods for GSA

Variance-based GSA decomposes the variance of the model output into fractions which can be attributed to input variables within a probabilistic framework. Variance-based measures of sensitivity are attractive as they are applicable over the whole space of input random variables, and they can also deal with nonlinear responses and measure the effect of interactions in nonadditive systems [8]. Here we review some of the basic principles of variance-based GSA.

2.1. Sobol' indices

Consider that $y = f(\mathbf{x})$ is an integrable function, where \mathbf{x} is a vector of d mutually independent random variables $\{x_1, \dots, x_d\}$ having probability density $p(\mathbf{x}) = \prod_{i=1}^d p_i(x_i)$. Sobol' [7] proved that $f(\mathbf{x})$ can be decomposed according to the high dimensional model representation (HDMR) in the following way:

$$y = f_0 + \sum_{i=1}^d f_i(x_i) + \sum_{1 \leq i < j \leq d} f_{ij}(x_i, x_j) + \dots + f_{1,2,\dots,d}(x_1, x_2, \dots, x_d) \quad (1)$$

where f_0 is a constant, $f_i(x_i)$ are univariate functions of x_i , $f_{ij}(x_j, x_i)$ are bivariate functions of (x_i, x_j) and $f_{1,2,\dots,d}(x_1, x_2, \dots, x_d)$ are multivariate functions of $\{x_1, \dots, x_d\}$. Assuming the input parameters are mutually independent random variables and the model function is square-integrable, the variance of the model is defined as

$$V = \text{Var}[f(\mathbf{x})] = \int f^2(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} - f_0^2 = \sum_{s=1}^d \sum_{1 \leq i_1 < \dots < i_s \leq d} \int f_{i_1, \dots, i_s}^2 p(x_{i_1}, \dots, x_{i_s}) dx_{i_1} \dots x_{i_s} \quad (2)$$

This leads to the following decomposition of the variance:

$$V = \sum_{i=1}^d V_i + \sum_{1 \leq i < j \leq d} V_{ij} + \dots + V_{1,2,\dots,d} \quad (3)$$

where the partial variances are calculated as follows:

$$V_{i_1, \dots, i_s} = \int f_{i_1, \dots, i_s}^2(x_{i_1}, \dots, x_{i_s}) p(x_{i_1}, \dots, x_{i_s}) dx_{i_1} \dots x_{i_s}, \quad s = 1, \dots, d \quad (4)$$

The Sobol' indices are defined as the relative contribution of the partial variances to the total variance following the decomposition in Eq. (3)

$$S_{i_1, \dots, i_s} = \frac{V_{i_1, \dots, i_s}}{V} = \frac{V_{i_1, \dots, i_s}}{\sum_{i=1}^d V_i + \sum_{1 \leq i < j \leq d} V_{ij} + \dots + V_{1,2,\dots,d}} \quad (5)$$

such that:

$$\sum_{i=1}^d S_i + \sum_{1 \leq i < j \leq d} S_{ij} + \dots + S_{1,2,\dots,d} = 1 \quad (6)$$

where the index S_i measures the contribution of each variable x_i to the variance of y taken separately without interacting with any other inputs, hence S_i is commonly referred to as the first-order index. Higher order indices in Eq. (6) measure the interactive contributions to the total variance. Using S_i , S_{ij} and higher order indices, one can therefore infer the impact of each input variable and the interaction of variables on the output variance. A measure of the total contribution of variable i follows as

$$S_i^T = \sum_{\{i\} \subset \{i_1, \dots, i_s\}} \frac{V_{i_1, \dots, i_s}}{V} \quad (7)$$

which measures the contributions of variable x_i and its interactions to the output variance. Unlike the first-order indices,

$$\sum_{i=1}^d S_i^T \geq 1 \quad (8)$$

because the interaction effect between, for example x_i and x_j , is contained in both S_i^T and S_j^T . The sum of the S_i^T is equal to 1 if and only if the model is purely additive without any interaction effects.

2.2. Estimating Sobol' indices using the Monte Carlo method

The first-order indices S_i in Eq. (6) and total indices S_i^T in Eq. (7) can be calculated by formulating the sensitivity indices as follows [4,56]:

$$S_i = \frac{V_i}{V} = \frac{\text{Var}_{x_i} [E_{x_{-i}}[y|x_i]]}{\text{Var}[y]} \quad (9)$$

$$S_i^T = \sum_{\{i\} \subset \{i_1, \dots, i_s\}} \frac{V_{i_1, \dots, i_s}}{V} = \frac{E_{x_{-i}} [\text{Var}_{x_i} [y|x_{-i}]]}{\text{Var}[y]} = 1 - \frac{\text{Var}_{x_{-i}} [E_{x_i} [y|x_{-i}]]}{\text{Var}[y]} \quad (10)$$

where $\text{Var}_{x_i}[\cdot]$ denotes the variance when only x_i is allowed to vary and $E_{x_{-i}} (\text{Var}_{x_{-i}}[\cdot])$ denotes the expectation (variance) when all variables except x_i are allowed to vary.

The calculation of the Sobol' indices in Eqs. (9) and (10) analytically is often nontrivial unless the model or system is analytically tractable in low dimension. More commonly, sampling-based methods are used to compute the Sobol' indices. Many

advanced algorithms have been developed to reduce the computational cost of estimating Sobol' indices. Using numerical methods, the original model is often approximated by a surrogate model which is inexpensive to computationally evaluate. Sudret [9] showed that if the original model can be replaced by a polynomial chaos expansion (PCE), the Sobol' indices can be computed directly from the PCE coefficients. Le Gratiet et al. [57], further proposed the Gaussian process (GP) based GSA method in which confidence intervals on sensitivity indices can be derived from the properties of GP.

Although they are not the most computationally efficient, Monte Carlo-based approaches are also commonly employed because of their simplicity in implementation. In this work, we use a Monte Carlo-based approach, not because of its simplicity, but because it allows us to directly propagate a multimodel set of probability distributions representing both the underlying aleatory uncertainty and the epistemic uncertainty associated with limited data. Sobol' [7] first proposed the following formula for calculation of V_i in the first-order Sobol' indices (see Eq. (9)):

$$V_i = \int f(\mathbf{x})f(x_i, \xi_{-i})p(\mathbf{x})p(\xi_{-i})d\mathbf{x}d\xi_{-i} - E^2[f(\mathbf{x})] \quad (11)$$

where ξ_{-i} denotes all the variables in ξ not including ξ_i . Using the Monte Carlo method, this integral can be estimated by:

$$V_i \approx \frac{1}{m} \sum_{k=1}^m f(\mathbf{x}^k) f(x_i^k, \xi_{-i}^k) - \left[\frac{1}{m} \sum_{k=1}^m f(\mathbf{x}^k) \right]^2 \quad (12)$$

where the subscript i is the index of the model inputs, superscript k is the index of the samples and m is the number of samples. Eq. (12) requires m samples of \mathbf{x} and m samples of ξ , both of which are independently drawn from the joint PDF $p(\mathbf{x})$ of the model inputs. The total number of model evaluations to compute all V_i using Eq. (12) is therefore m evaluations of $f(\mathbf{x}^k)$ and dm evaluation of $f(x_i^k, \xi_{-i}^k)$ for each variable i for a total of $(d+1)m$ model evaluations, which is much smaller than the m^2 evaluations required for direct Monte Carlo of the double-integral implied by Eq. (9). This number rises to $(d+2)m$ model evaluations if we also wish to estimate total indices S_i^T .

To improve the estimate accuracy, Homma and Saltelli [56] further proposed direct calculation of $E^2[f(\mathbf{x})]$ as

$$E^2[f(\mathbf{x})] = \int f(\mathbf{x})p(\mathbf{x})f(\xi)p(\xi)d\mathbf{x}d\xi \quad (13)$$

which yields a new integral representation for V_i obtained by substituting Eq. (13) into Eq. (11):

$$\begin{aligned} V_i &= \int f(\mathbf{x})p(\mathbf{x})f(x_i, \xi_{-i})p(\xi_{-i})d\mathbf{x}d\xi_{-i} - \int f(\mathbf{x})p(\mathbf{x})f(\xi)p(\xi)d\mathbf{x}d\xi \\ &= \int f(\mathbf{x})p(\mathbf{x})[f(x_i, \xi_{-i})p(\xi_{-i}) - f(\xi)p(\xi)]d\mathbf{x}d\xi \end{aligned} \quad (14)$$

The corresponding Monte Carlo approximation

$$V_i \approx \frac{1}{m} \sum_{k=1}^m f(\mathbf{x}^k) \left(f(x_i^k, \xi_{-i}^k) - f(\xi^k) \right) \quad (15)$$

is proven to be a more accurate estimator of first-order Sobol' indices but without introducing any additional model evaluation [58]. Saltelli [58] also provided the formula for estimation of total Sobol' indices as:

$$V_{T_i} \approx \frac{1}{2m} \sum_{k=1}^m \left(f(\xi^k) - f(x_i^k, \xi_{-i}^k) \right)^2 \quad (16)$$

Various sample-based approaches have been recently proposed to improve the accuracy or reduce the computational cost of estimating Sobol' indices. These approaches include improvements to the formulation of the Sobol' indices, such that more accurate estimates are obtained without introducing additional model evaluations [59–61]. Another way is to improve the efficiency of the estimator using, for example, low-discrepancy sequences (i.e. Sobol' sequence [62]) or Latin hypercube sampling [63,64]. Again, because efficiency in estimating the Sobol' indices themselves is not our first priority, we do not elaborate on these methods. However, in practice we employ Latin hypercube sampling of our importance sampling density in the applications because it is simple and does not require reformulation of the estimator.

3. Bayesian multimodel inference for imprecise probabilities from limited data

Methods for global sensitivity analysis, as presented above, employ samples that are drawn from a known probability density. However, identifying a probability density requires either a large data set characterizing the distribution or some assumptions. In engineering practice, however, it is common that only small/limited data are available such that a unique probability distribution cannot be identified without significant (and potentially problematic) assumptions. In this section, we review a Bayesian multimodel methodology developed previously by the authors [33,65], in which families of probabilistically weighted probability distributions are estimated to quantify uncertainties.

Multimodel inference, as introduced by Burnham and Anderson [66], involves two components: 1. model selection, and 2. parameter estimation. When selecting a probability distribution to represent a data set, the model selection problem is simply stated as follows. Given a collection of N_p candidate models (probability distributions) $\mathcal{M} = \{M_j\}_{j=1,\dots,N_p}$ and data \mathbf{d}_s , identify the model M_i that “best” fits the data. The notion of best fit varies depending on the user’s selected metric. In this work, we employ Bayesian posterior probabilities as the measure of best fit following from [65]. An alternative approach, presented in [33], employs information-theoretic criteria for model selection. In the multimodel setting, multiple candidate models may be selected because the data set does not provide sufficient evidence to conclusively select only a single model.

In the Bayesian setting employed here, we begin by assigning prior probabilities $\pi_j = p(M_j)$ with $\sum_{j=1}^{N_p} \pi_j = 1$ to each model in \mathcal{M} . Using Bayes’ rule, we can calculate the posterior probability, given the data \mathbf{d}_s as:

$$\hat{\pi}_j = p(M_j|\mathbf{d}_s) = \frac{p(\mathbf{d}_s|M_j)p(M_j)}{\sum_{j=1}^{N_p} p(\mathbf{d}_s|M_j)p(M_j)}, \quad j = 1, \dots, N_p \quad (17)$$

having $\sum_{j=1}^{N_p} \hat{\pi}_j = 1$ and where

$$p(\mathbf{d}_s|M_j) = \int_{\theta_j} p(\mathbf{d}_s|\theta_j, M_j)p(\theta_j|M_j)d\theta_j, \quad j = 1, \dots, N_p \quad (18)$$

is the marginal likelihood or evidence of model M_j .

Typically, the model $M_k \in \mathcal{M}$ with the highest posterior model probability $p(M_k|\mathbf{d}_s)$ is identified as the “best” model [67,68]. Rather than selecting the model with the highest probability, Bayesian multimodel inference ranks the candidate models according to their posterior model probabilities calculated by Eq. (17) retains all plausible models with non-negligible probability. Notice that the evidence $p(\mathbf{d}_s|M_j)$ is critical in Bayesian multimodel inference, as evident from Eq. (18), and consequently needs to be calculated with caution. Several methods have been proposed to estimate the evidence (e.g. [69,67,68,70–72]) and a detailed discussion of the evidence calculation can be found in [65].

The second step of Bayesian multimodel inference is parameter estimation. Once the set of plausible models and their associated model probabilities have been identified, additional uncertainties associated with model parameters also need to be considered given limited data. For each plausible model M_j , $j = 1, \dots, m$, we again assign a prior probability to the model parameters θ_j , denoted $p(\theta_j|M_j)$. Applying Bayes’ rule, we estimate the posterior parameter distribution by:

$$p(\theta_j|\mathbf{d}_s, M_j) = \frac{p(\mathbf{d}_s|\theta_j, M_j)p(\theta_j|M_j)}{p(\mathbf{d}_s|M_j)} \propto p(\mathbf{d}_s|\theta_j, M_j)p(\theta_j|M_j), \quad j = 1, \dots, m \quad (19)$$

where $p(\mathbf{d}_s|\theta_j, M_j)$ is the likelihood function and $p(\mathbf{d}_s|M_j)$ is the evidence. Here, the evidence calculation is not as critical because the posterior is identified implicitly through Markov Chain Monte Carlo (MCMC) sampling.

Standard practice in Bayesian inference is to select a unique set of parameters θ_j using, for example, the maximum a posteriori (MAP) estimator,

$$\hat{\theta}_j^{\text{MAP}}(\mathbf{d}_s, M) = \arg \max_{\theta_j} p(\theta_j|\mathbf{d}_s, M_j) = \arg \max_{\theta_j} p(\mathbf{d}_s|\theta_j, M_j)p(\theta_j|M_j) \quad (20)$$

In the limited data cases considered here, the posterior probability will likely possess large variance. For this reason, we retain the full posterior pdf $p(\theta_j|\mathbf{d}_s, M_j)$ (at least its MCMC samples) for evaluation of imprecise sensitivity indices. Note that the effect of the prior probabilities (for both model selection and parameter estimation) in this Bayesian multimodel inference has been carefully investigate in [65].

Summarizing, the Bayesian multimodel inference yields the following:

- A set of plausible probability models M_j , $j = 1, \dots, m$;
- The corresponding model probability $p(M_j)$ for each plausible probability model;
- The full joint posterior parameter probability density $p(\mathbf{d}_s|\theta_j, M_j)$ for each plausible model.

Theoretically, this process yields an infinite set of parametrized probability models (i.e. a finite set of probability models, each with continuous joint parameter distributions). For practical purposes, it is necessary to reduce this to a finite, but statistically representative, set of N_c probability models, denoted $\mathcal{P} = \{p(M_1, \theta_1), \dots, p(M_{N_c}, \theta_{N_c})\}$, from which we can perform imprecise GSA. This is achieved by Monte Carlo sampling from the infinite set of probability models. Each model, $p(M_i, \theta_i) \in \mathcal{P}$ is identified by randomly selecting a model family from \mathcal{M} with probabilities $p(M_i|\mathbf{d}_s), i = 1, \dots, m$ and randomly selecting its parameters from the joint parameter probability density $p(\theta_i|\mathbf{d}_s, M_i)$. It is important to emphasize that N_c can be selected arbitrarily large as it does not govern the cost of the GSA itself (i.e. selection of N_c does not influence

the number of required model evaluations), but instead only governs how many times each sensitivity index from the GSA must be reweighted according to the importance sampling procedure discussed next.

4. Imprecise global sensitivity analysis

If the conventional Monte Carlo method is used to estimate Sobol' indices for each model in \mathcal{P} , the total computational cost is

$$C_{MC} = \underbrace{N_c \times N_c \times \cdots \times N_c}_d \times (d+1) \times m = N_c^d \times (d+2) \times m \quad (21)$$

N_c must be sufficiently large number such that it can adequately represent the overall uncertainties in both model form and model parameters. In fact, as previously stated, we want to allow N_c to be arbitrarily large. This thus leads to a huge number of simulations, making estimation of Sobol' indices intractable and cost prohibitive.

Here, we propose an importance sampling approach that reduces the total cost of imprecise GSA from $\mathcal{O}(N_c^d dm)$ to $\mathcal{O}(N_c dm)$. First, let us briefly introduce importance sampling.

4.1. Importance sampling

Importance sampling is a variance reduction technique in which one can estimate statistical expectations with respect to a specified probability distribution, the target density $p(\mathbf{x})$, using samples drawn from a different distribution, the importance sampling density $q(\mathbf{x})$. Specifically, the desired expected value with respect to $p(\mathbf{x})$, $\mu = E_p[f(\mathbf{x})]$, can be expressed as:

$$\mu = E_p[f(\mathbf{x})] = \int f(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} = \int \frac{f(\mathbf{x}) p(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) d\mathbf{x} = E_q \left[\frac{f(\mathbf{x}) p(\mathbf{x})}{q(\mathbf{x})} \right] \quad (22)$$

where $E_q[\cdot]$ denotes expectation with respect to $q(\mathbf{x})$. Defining weights $w(\mathbf{x}) = p(\mathbf{x})/q(\mathbf{x})$ (referred to as the *importance weights* or *likelihood ratio*), the importance sampling estimator of $E_p[f(\mathbf{x})]$ is

$$\hat{\mu}_p = E_p[f(\mathbf{X})] \approx \frac{1}{N} \sum_{i=1}^N \frac{f(\mathbf{x}_i) p(\mathbf{x}_i)}{q(\mathbf{x}_i)} = \frac{1}{N} \sum_{i=1}^N f(\mathbf{x}_i) w(\mathbf{x}_i), \quad \mathbf{x}_i \sim q(\mathbf{x}). \quad (23)$$

The quality of an importance sampling estimator is determined by the variance of the weights or the related quantity, the effective sample size [73]. A related investigation on the effectiveness of importance sampling reweighting in the context of Bayesian updating can be found in [74]. For brevity, additional details are not provided herein.

4.2. Importance Sampling for estimating Sobol' indices

The importance sampling idea is an attractive one for us because it allows us to estimate Sobol' indices with respect to one probability measure, and through a simple reweighting determine the corresponding Sobol' indices with respect to another measure. Therefore, given samples from a specified importance sampling density, we propose herein an approach to estimate Sobol' indices according to each of the candidate probability models in our plausible set \mathcal{P} .

Let us revisit the formula for calculating of first-order variance, shown in Eq. (14). Consider the finite set \mathcal{P} of candidate target probability models having densities $p_j(\mathbf{x}|\theta), j = 1, \dots, N_c$. The i -th partial variance given the specified probability model $p_j(\mathbf{x}|\theta_j)$ is calculated as

$$V_i^j = \int f(\mathbf{x}) p_j(\mathbf{x}|\theta_j) [f(x_i, \xi_{-i}) p_j(\xi_{-i}|\theta_j) - f(\xi) p_j(\xi|\theta_j)] d\mathbf{x} d\xi \quad (24)$$

Applying importance sampling, the partial variance in Eq. (24) can be rewritten in terms of an alternative probability model, $q(\mathbf{x})$, as:

$$V_i^j = \int f(\mathbf{x}) \frac{p_j(\mathbf{x}|\theta)}{q(\mathbf{x})} q(\mathbf{x}) \left[f(x_i, \xi_{-i}) \frac{p_j(\xi_{-i}|\theta)}{q(\xi_{-i})} q(\xi_{-i}) - f(\xi) \frac{p_j(\xi|\theta)}{q(\xi)} q(\xi) \right] d\mathbf{x} d\xi \quad (25)$$

The Monte Carlo estimator in Eq. (15) is then modified to account for the reweighting as follows:

$$\begin{aligned} \hat{V}_i^j &\approx \frac{1}{m} \sum_{k=1}^m f(\mathbf{x}^k) \frac{p_j(\mathbf{x}^k|\theta)}{q(\mathbf{x}^k)} \left[f(\mathbf{x}_i^k, \xi_{-i}^k) \frac{p_j(\xi_{-i}^k|\theta)}{q(\xi_{-i}^k)} - f(\xi^k) \frac{p_j(\xi^k|\theta)}{q(\xi^k)} \right] \\ &\approx \frac{1}{m} \sum_{k=1}^m f(\mathbf{x}^k) w_j(\mathbf{x}^k) \left[f(\mathbf{x}_i^k, \xi_{-i}^k) w_j(\xi_{-i}^k) - f(\xi^k) w_j(\xi^k) \right] \end{aligned} \quad (26)$$

Similarly, we can generalize this method to modify the total-order indices S_i^T formulation in Eq. (16) using importance sampling reweighting as:

$$\begin{aligned}\hat{V}_{T_i}^j &\approx \frac{1}{2m} \sum_{k=1}^m \left[f\left(\xi^k\right) \frac{p_j(\mathbf{x}^k|\boldsymbol{\theta})}{q(\mathbf{x}^k)} - f\left(\mathbf{x}_i^k, \xi_{-i}^k\right) \frac{p_j(\xi_{-i}^k|\boldsymbol{\theta})}{q(\xi_{-i}^k)} \right]^2 \\ &\approx \frac{1}{2m} \sum_{k=1}^m \left[f\left(\xi^k\right) w_j(\mathbf{x}^k) - f\left(\mathbf{x}_i^k, \xi_{-i}^k\right) w_j(\xi_{-i}^k) \right]^2\end{aligned}\quad (27)$$

Compared with the conventional Monte Carlo approach, Eqs. (26) and (27) allow us to estimate Sobol' indices using only a single Monte Carlo simulation with sampling density $q(\mathbf{x})$, then reweight the estimator for each candidate plausible model in \mathcal{P} . Although similar formulations for importance sampling-based GSA exist, it is worth mentioning that the formulation presented here is fully general in the sense that, unlike some other methods, there are no additional constraints placed on the sampling distribution. The method proposed in [53], for example, assumes that the sampling density belongs to the same family of distributions as the target density. Such a constraint is, by its nature, incompatible with the proposed multimodel formulation which aims to compute sensitivities from sets of distributions composed of multiple distribution types.

The fundamental challenge then is how to identify a *single optimal sampling density* $\hat{q}(\mathbf{x})$ that is most representative of all potential target densities $p_j(\mathbf{x}|\boldsymbol{\theta}), j = 1, \dots, N_c^d \in \mathcal{P}$. This issue has been resolved in a previous work [33] and is recalled briefly in the following.

4.3. Optimal importance sampling

Zhang and Shields [33] provide an explicit analytical derivation for the optimal importance sampling density given an ensemble of candidate target densities. The approach firstly introduces a widely used metric, the mean square difference (MSD), to quantify the difference between one importance sampling density and one target density, which is given by:

$$\mathcal{M}(P||Q) = \frac{1}{2} \int (p(\mathbf{x}|\boldsymbol{\theta}) - q(\mathbf{x}))^2 d\mathbf{x} \quad (28)$$

The corresponding total expected mean squared difference between a single sampling density $q(\mathbf{x})$ and the ensemble of N_c probability models $p_j(\mathbf{x}|\boldsymbol{\theta}_j), j = 1, \dots, N_c$ can be formulated as:

$$\mathcal{E} = \sum_{j=1}^{N_c} E[\mathcal{M}(\mathcal{P}_j||Q)] = E_\theta \left[\int \sum_{j=1}^{N_p} \frac{1}{2} (p_j(\mathbf{x}|\boldsymbol{\theta}_j) - q(\mathbf{x}))^2 d\mathbf{x} \right] \quad (29)$$

To ensure the sampling density $q(\mathbf{x})$ is as close as possible to the multiple target densities $p_j(\mathbf{x}|\boldsymbol{\theta}_j), j = 1, \dots, N_c$, an overall optimization problem is solved to minimize the total expected mean squared difference expressed as a functional $\mathcal{L}(q)$ given isoperimetric constraint $\mathcal{I}(q)$

$$\begin{aligned}&\underset{q}{\text{minimize}} \quad \mathcal{L}(q) = E_\theta \left[\int \mathcal{F}(\mathbf{x}, \boldsymbol{\theta}, q(\mathbf{x})) d\mathbf{x} \right] \\ &\text{subject to} \quad \mathcal{I}(q) = \int q(\mathbf{x}) d\mathbf{x} - 1 = 0\end{aligned}\quad (30)$$

where the action functional $\mathcal{F}(\cdot)$ is the total square differences:

$$\mathcal{F}(\mathbf{x}, \boldsymbol{\theta}, q(\mathbf{x})) = \frac{1}{2} \sum_{j=1}^{N_p} (p_j(\mathbf{x}|\boldsymbol{\theta}_j) - q(\mathbf{x}))^2 \quad (31)$$

and E_θ is the expectation with respect to the posterior probability of the model parameters $\boldsymbol{\theta}$. $\mathcal{I}(q)$ ensures that $q(\mathbf{x})$ is a valid probability density function. Notice that the optimization problem in Eq. (30) has closed-form solution given by the convex mixture model [33]

$$q^*(\mathbf{x}) = \frac{1}{N_p} \sum_{j=1}^{N_p} E_\theta [p_j(\mathbf{x}|\boldsymbol{\theta})] \quad (32)$$

and this solution can be generalized to combine the posterior model probabilities as

$$q^*(\mathbf{x}) = \sum_{j=1}^{N_p} \hat{\pi}_j E_\theta [p_j(\mathbf{x}|\boldsymbol{\theta})] \quad (33)$$

where $\hat{\pi}_j$ is the posterior model probability for model M_j , computed by Eq. (17). It is straightforward to apply this optimal sampling density to estimate Sobol' indices for imprecise GSA. As the random variables are assumed to be independent, the optimal sampling density can be identified for each random variable and then multiplied to obtain the joint sampling density.

Again, it is important to highlight the advantages of the optimal sampling density proposed in Eqs. (32) and (33) as compared to comparable methods in the literature. The optimal density given herein is both analytically derived (provably opti-

mal) and fully general for a set of arbitrarily weighted probability distributions of arbitrary type. Other methodologies for estimating the optimal sampling density require some constraining assumptions as well as additional model evaluations. For example, the method proposed in [53], requires that the optimal sampling density belong to the same family of distributions as the target and then uses a simulation-based procedure involving an additional set of model evaluations in order to estimate the optimal parameters of the assumed distribution form.

4.4. Proposed methodology for imprecise GSA

Algorithm 1 summarizes the proposed step-by-step approach for estimating imprecise sensitivity indices. The algorithm starts from initial data collection. This is followed by the Bayesian multimodel methodology to quantify the uncertainties associated with probability model-form and model parameters. In particular, this involves first defining the set of candidate probability models \mathcal{M} , assigning a prior probability to each of these models, and applying Bayes' rule to obtain posterior model probabilities $\hat{\pi}_j$ using Eq. (17). Next, Bayesian inference is again applied to each model $M_j \in \mathcal{M}$ to obtain the posterior joint parameter distributions. Again, priors must be assigned.

Next, a finite set of N_c probability models is established to represent the imprecise probabilities resulting from the small dataset. This step involves a straightforward Monte Carlo sampling from the model set \mathcal{M} where the model is selected according to its posterior probability $\hat{\pi}_j$ and then, for the selected model, a random sampling from the joint posterior parameter density. The result is a set of N_c probability distributions, each with equal probability of occurrence.

The optimal sampling density is then determined by solving the constrained optimization problem in Eq. (30), the solution of which is given by Eq. (33). Practically, Eq. (33) is implemented using the following Monte Carlo estimator to incorporate the expectation over θ :

$$\frac{1}{N_c} \sum_{j=1}^{N_c} p_j(\mathbf{x}|\theta_j) \quad (34)$$

and recognizing that the model probabilities $\hat{\pi}_j$ are accounted for in the sampling of p_j .

Finally, random samples are drawn from the optimal sampling density and the model is evaluated at these points. Importance weights are calculated for each random variable and it is only necessary to reweight each of the model evaluations according to the joint importance weights to calculate the sensitivity indices based on Eq. (26). It is also worth noting that high dimensional cases may lead to a huge number of total combined models N_c^d . Thus, a representative number $N_r \ll N_c^d$ of models are drawn using Latin hypercube sampling in this work.

This proposed methodology is also easily updated to accommodate new information if additional data are collected. The importance weights can be updated directly to account for the new data, but this comes at the cost of a loss of optimality in the importance sampling density because the potential target densities have changed. This issue is discussed in [33]. In a recent work [74], an efficient Monte Carlo resampling method is developed to accommodate a probability measure change from Bayesian updating that minimizes the impact on the sample set and computational cost.

Algorithm 1: Efficient algorithm for imprecise GSA

- 1: Collect initial data \mathbf{d}_s for random model inputs
 - 2: **for** $t \leftarrow 1$ to d
 - 3: Select candidate probability models $\mathcal{M}^t = \{M_j^t\}, j = 1, 2, \dots, N_p$ with prior probabilities $\pi_j^t = p_t(M_j)$
 - 4: Compute the posterior model probabilities $\hat{\pi}_j^t$ according to Eq. (17)
 - 5: Assign an informative/noninformative parameter prior $p_t(\theta_j|M_j)$
 - 6: Estimate the posterior parameter distribution $p_t(\theta_j|\mathbf{d}_s, M_j)$ according to Eq. (19)
 - 7: Establish a finite model set $\mathcal{P}^t = \{\mathcal{P}_i^t\}, i = 1, 2, \dots, N_c$ using random sampling
 - 8: Determine the optimal sampling density $q_t^*(\mathbf{x})$ according to Eq. (33)
 - 9: Generate random samples $\mathbf{x}_t \sim q_t^*(\mathbf{x})$
 - 10: Calculate the importance weights $w_t^k(\mathbf{x}_t) = p_t^k(\mathbf{x}_t)/q_t^*(\mathbf{x}_t), k = 1, 2, \dots, N_c$
 - 11: **end for**
 - 12: Evaluate the computational model $f(\mathbf{x}), \mathbf{x} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_d\}$
 - 13: Calculate the joint importance weights $w(\mathbf{x}) = w(\mathbf{x}_1) \cdot w(\mathbf{x}_2) \cdots w(\mathbf{x}_d)$
 - 14: **for** $l \leftarrow 1$ to N_c^d
 - 15: Reweight the random samples \mathbf{x} according to the joint importance weights $w(\mathbf{x})$
 - 16: Calculate the first-order Sobol' Indices $S_i^j = V_i^j/V^j, i = 1, \dots, d; j = 1, \dots, N_c$ according to Eq. (26)
 - 17: **end for**
 - 18: **if** additional data \mathbf{d}^* are collected
 - 19: $\mathbf{d}_s = \mathbf{d}_s + \mathbf{d}^*$ and **goto** step 1
 - 20: **end if**
-

4.5. Performance & limitations

Because the proposed method brings together several components from previously developed theories and integrates them into a new framework for GSA, its performance depends on the combined performance of each of its constituents. In other words, in order to achieve accurate results in the proposed imprecise GSA, we must demonstrate accuracy in model selection, Bayesian parameter inference, importance sampling, and Sobol' index estimation. Fortunately, each of these components have been studied extensively on their own and the method to combine them here leverages the state-of-the-art in each facet. Nonetheless, the proposed method may be hindered by some challenges in each of the constituents, which are discussed herein.

The proposed approach involves a two-level Bayesian inference (model selection and parameter estimation). The main drawback of the Bayesian approach for model selection is that it relies on the estimation of the model evidence for each model. The integral in Eq. (18) is rarely straightforward to evaluate. Several simplifications have been proposed in the literature [67–72]. To avoid evidence calculation, one may consider the information-theoretic approach detailed in [66], that also has a Bayesian interpretation, and which has been previously applied by the authors [33]. In the authors' experience, only small differences in model probabilities are observed when applying the information-theoretic and Bayesian approaches when Bayesian priors are non-informative. In the second level, a conventional MCMC approach is used to infer the parameter distributions. We specifically use the affine invariant ensemble sampler of Goodman and Weare [75], but note that any validated MCMC sampler can be used here.

More important to the two-level Bayesian inference are the assignment of the priors. We have written extensively on this topic in [65] and note that, because we are dealing with small data sets, the prior will dominate in Bayes' rule in both model selection and parameter estimation. Consequently, the use of informative priors at any point in the methodology must be justified by strong evidence as the data set will be too small to overcome any bias that an incorrectly assigned informative prior would introduce.

In addition, the assumption of the probability distribution for input variables may have a critical impact on the resulting sensitivity indices. This study assumes the input dataset that follow standard parameterized distribution such as commonly used Normal, Lognormal, Gamma, and Weibull distribution. However, in theory, the proposed method is capable of handling data that follow irregular distributions but learning irregular distributions is a much more challenging problem than estimating standard parameterized distributions, especially from small datasets. This is because the model selection requires a careful balance between goodness-of-fit and parsimony of the model. In small data cases, it is easy to fit irregular models (e.g. kernel density estimates, KDEs) but these have the severe drawback of overfitting. Typically, KDEs have a potentially very large number of parameters (a location and scale parameter for each kernel) that will be almost certain to overfit a small dataset. Given the large number of parameters, the proposed approach will work for these models but (correctly) assign very high uncertainty to these parameters. In other words, Bayesian inference cannot effectively learn a large number of parameters from a small data set. For this reason, we mainly focus on the standard probability distribution types and do not attempt to learn irregular distributions such as KDEs or Gaussian mixture models.

Another issue that may arise in the inference process is undersampling the identified model set. More specifically, if N_c is chosen to be too small, the sampled probability distributions will not be fully representative of the underlying model set and the solution will underestimate the uncertainty. Fortunately, this is easily overcome because the expense of the proposed approach depends only weakly on N_c , so in practice it can be set arbitrarily large. With an increase in N_c , the only associated increase in computational cost is the cost of importance sampling reweighting. It is important to emphasize that N_c is independent of the number of model evaluations necessary to apply the methodology.

Finally, the quality of the solution depends most strongly on the quality of the importance sampling reweighting scheme. This is typically assessed by studying the variance of the importance sampling weights, or equivalently through the Effective Sample Size (ESS). In some cases, particularly in very small data cases where there is a large degree of variability in the set of models, the ESS may become small for some candidate distributions particularly those that deviate considerably from the optimal. To investigate the effectiveness of the method for very small datasets, two case studies were considered. In Section 5, the well-known Timoshenko equation for beam deflection is solved to explore the effects of varying the amount of data for the input parameters to demonstrate the accuracy of imprecise GSA on small datasets. This study is highly controlled and involves synthetically generated data from known probability distributions such that accuracy and convergence can be carefully tracked. The second case study presented in Section 6 investigates out-of-plane properties of a composite material and relies on data from a comprehensive literature survey that provides only sparse data on the constituent material properties. This problem represents a practical application of the proposed method under "real world" conditions of limited data and illustrates how the proposed approach can be used to assess confidence in model based sensitivities and inform targeted testing efforts to minimize the influence of uncertainties.

5. Numerical example

In this section, we use a thick cantilever beam example [60] shown in Fig. 1 to illustrate the proposed methodology for the estimation of imprecise sensitivity indices. This example computes the beam's deflection δ analytically using the Timoshenko beam theory [76]

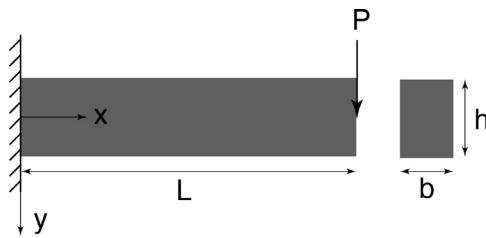


Fig. 1. Thick cantilever beam illustration.

$$\delta = \frac{P}{6EI} \left[(4 + 5\nu) \frac{h^2 L}{4} + 2L^3 \right] \quad (35)$$

where $I = bh^3/12$. The statistical information of these model inputs in Eq. (35) are listed in Table 1 [60].

Table 1 provides a distribution for each random variables of model inputs provided by [60]. We assume that these distributions are the “true” distributions for each variable, but are a priori unknown. Data sets of increasing size are drawn from these distributions and the multimodel sensitivity analysis approach proposed herein is applied at various points to observe the uncertainty in the estimated Sobol’ indices and their convergence to the “true” values given in [60].

To define the initial data set, we randomly generate 50 data for each model input according to the corresponding true distribution with mean and coefficient of variation (COV) given in Table 1. Fig. 2 shows histograms of the initial 50 data for each model input. Clearly, a single probability model cannot be precisely identified from these data.

Given the limited data, Bayesian multimodel inference is implemented to quantify the uncertainties associated with the probability model-form and model parameters. Table 2 shows the candidate probability models with the corresponding posterior model probabilities for all six model inputs. It is clear that a single probability model cannot even be precisely identified from the data for any of the six random inputs.

Next, the Bayesian inference is employed to estimate the parameter uncertainty for each specified model form. A noninformative prior is assumed herein such that the estimate is totally determined by the small data set. Again, effects of priors have been investigated in [65]. Then, using Monte Carlo sampling, the five models and their joint parameter densities are discretized to obtain a finite set of $N_c = 500$ models for each parameter. To draw each sample, the probability model is randomly selected according to the posterior model probabilities in Table 2 and model parameters are then randomly generated from the joint posterior parameter distribution. Fig. 3 shows the $N_c = 500$ candidate distributions for each parameter drawn from the model set accompanied by the computed optimal importance sampling density. Epistemic uncertainty resulting from the small dataset size is represented by the width of the “cloud” of distributions. If all of the combinations of probability models for these six variables are considered, the total model input set would be of size $500^6 = 1.5625^{16}$, which is obviously prohibitive. Therefore, a representative set of $N_r = 5000$ joint probability models is generated by Latin hypercube sampling instead. Note, the selection of $N_c = 500$ and $N_r = 5000$ is arbitrary. These numbers can be assigned to be as large as is desirable without requiring any additional model evaluations.

A total of 100,000 random samples drawn from the optimal sampling density are employed for the estimation of the beam’s deflection δ according to Eq. (35). Using the efficient algorithm for imprecise GSA shown in Algorithm 1, the Sobol’ indices with respect to the 5000 candidate joint probability densities are estimated by only reweighting these random samples and without requiring additional model evaluations. Fig. 4 shows histograms of the imprecise Sobol’ indices for each parameter given 50 data. The corresponding empirical cumulative density functions (CDF) are shown in Fig. 5. A kernel density estimate is used to estimate a smooth probability density function from the 5000 Sobol’ indices estimates (black curves

Table 1

Statistical summary of model inputs for the thick cantilever beam [60].

Input Symbol/Unit	Load P/kN	Young’s modulus E/GPa	Poisson’s ratio ν	Width b/mm	Height h/mm	Length L/mm
Mean	2.5	200	0.225	1	3	3.5
COV	10%	5%	5%	5%	5%	5%
Distribution type	Normal	Lognormal	Lognormal	Lognormal	Lognormal	Lognormal

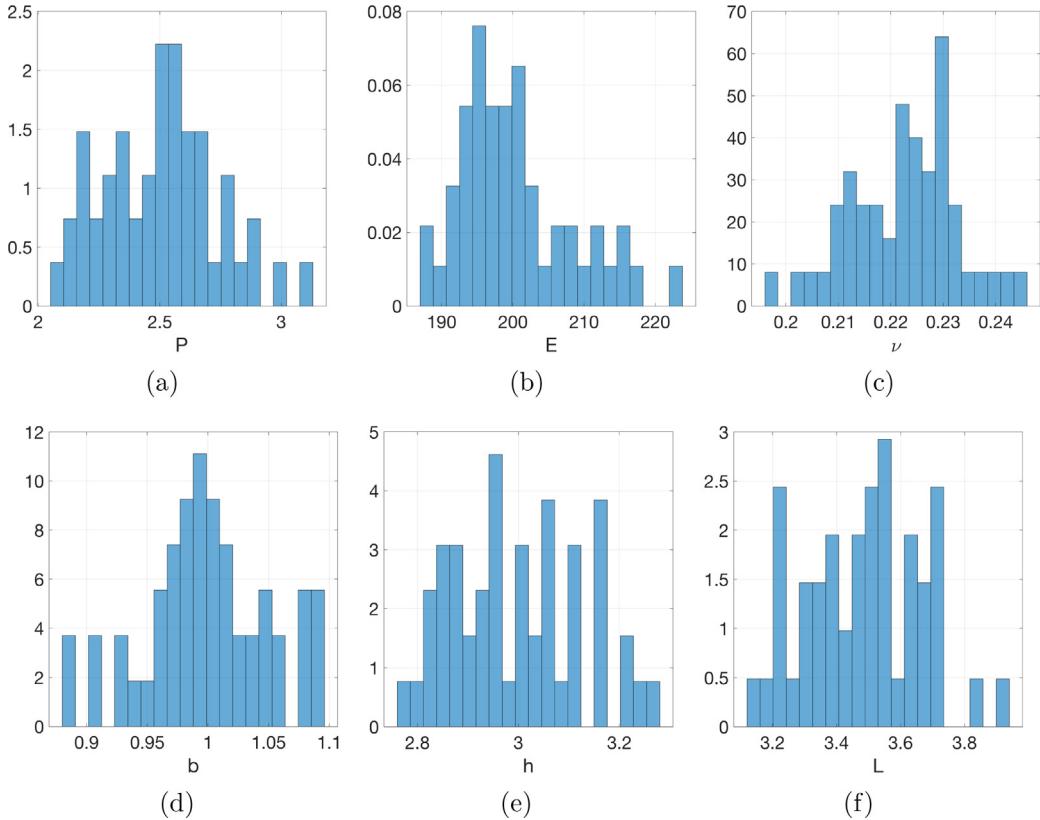


Fig. 2. Initial data set: 50 randomly generated data for each model input (a) Load (b) Young's modulus (c) Poisson's ratio (d) Width (e) Height and (f) Length.

Table 2

Model probabilities from the given initial 50 data for each model input

Distribution	$\hat{\pi}_P$	$\hat{\pi}_E$	$\hat{\pi}_\nu$	$\hat{\pi}_b$	$\hat{\pi}_h$	$\hat{\pi}_L$
Gamma	0.3141	0.2781	0.2283	0.2505	0.3216	0.3077
Logistic	0.1214	0.2035	0.137	0.1597	0.0542	0.0841
Lognormal	0.344	0.3594	0.1972	0.2242	0.3405	0.3092
Normal	0.2147	0.1589	0.2877	0.2901	0.2737	0.2845
Weibull	0.0058	0.0001	0.1497	0.0754	0.01	0.0145

in Fig. 4). The true Sobol' indices, obtained using the true probability densities for each parameter are shown by a red line in Figs. 4 and 5.

Notice that, instead of a single deterministic value, imprecise GSA results in a probabilistic description of the Sobol' indices. Around the true value, the imprecise Sobol' indices show significant variation caused by uncertainties associated with sparse data from which to quantify the model input. Each variable shows a relatively large range such that it is not easy to identify which variable is the most or least sensitive one. Instead, the variable sensitivity can be probabilistically estimated with a confidence interval. For example, there is a 95% probability that the sensitivity of L is in the range [0.2, 0.6]. In this case, L seems to be the most sensitive variable, but based on the data we cannot say so conclusively.

Next, we investigate the convergence of the imprecise sensitivity indices with increasing data set size. We consider cases of 100, 250, 500, 1000, 5000, and 10000 data collected for each variable and observe the histograms of their sensitivities in Tables 3 and 4. With increasing data set size, uncertainties associated with the model inputs gradually diminish and the imprecise Sobol' indices narrow around the true value as expected. Note that the true value is always included in the range of the Sobol' indices probability distribution. It is critical to investigate the dependence of the confidence level of the estimated Sobol' indices on the number of data. We therefore define a sim-

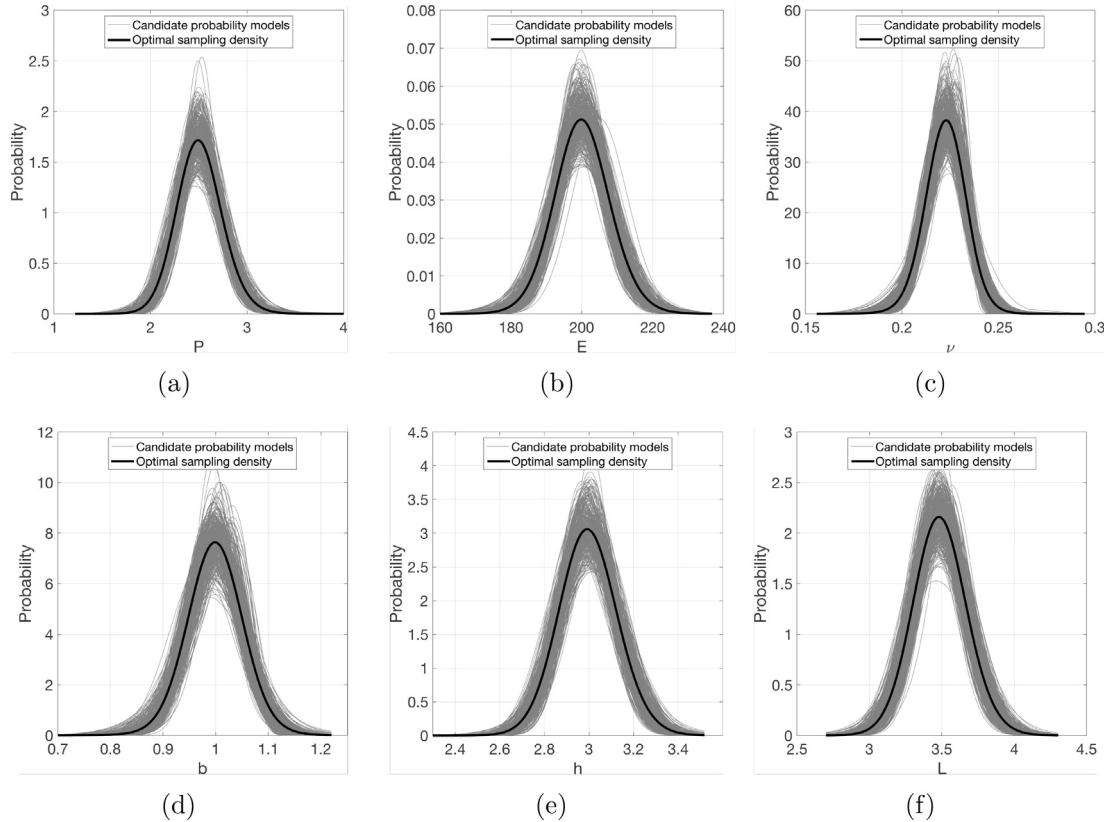


Fig. 3. Candidate probability models obtained from Bayesian multimodel inference for each model input (a) Load (b) Young's modulus (c) Poisson's ratio (d) Width (e) Height and (f) Length.

ple confidence metric using the range of upper and lower quantiles of 0.025 for the estimated Sobol' indices S given n data as follows:

$$\chi_S^{(n)} = 1 - \left(Q_{0.975}(S^{(n)}) - Q_{0.025}(S^{(n)}) \right) \quad (36)$$

such that total confidence in Sobol' indices corresponds to a vanishing range and a confidence level of $\chi_S^{(n)} = 1$. Fig. 6 shows the confidence level relative to dataset size. Plots of this type are helpful for decision makers since they provide guidance to aid in determining the number data to collect, where to concentrate data collection efforts, and the confidence that can be achieved. Likewise, Fig. 7 shows the CDFs of imprecise first-order Sobol' indices as a function of dataset size from 100 to 10000. Again, it is easy to observe that the imprecise Sobol' indices gradually converge to the true values.

From the convergence figures, if we compare convergence of the variables that are less sensitive with those that are more sensitive we observe some interesting trends. Notice that the less sensitive variables (E , v , and b) have wide ranges of sensitivity for very small data sets (< 100 samples) – even producing some erroneous negative sensitivities. However, for data set sizes larger than 100, the sensitivities converge rather quickly. In other words, with relatively small data sets (< 250), we can identify variables that do not have high sensitivity. Meanwhile, for the variables that exhibit the highest sensitivity (P , h , and L), the convergence to a precise sensitivity is more gradual. While, for these variables, we can identify early that they will be influential, it takes a very large data set to determine which variables are the most sensitive. This leads to a potentially important conclusion. The investigation indicates that small data sets (< 250) may be sufficient for broadly identifying which variables will have high (low) sensitivity, but large data sets (> 1000) are necessary to identify precisely how sensitive the model is to each variable.

Finally, it is worth noting that no additional model evaluations were required to estimate these imprecise sensitivity indices as additional data were collected. We only needed to reweight the 100,000 samples drawn from the original optimal

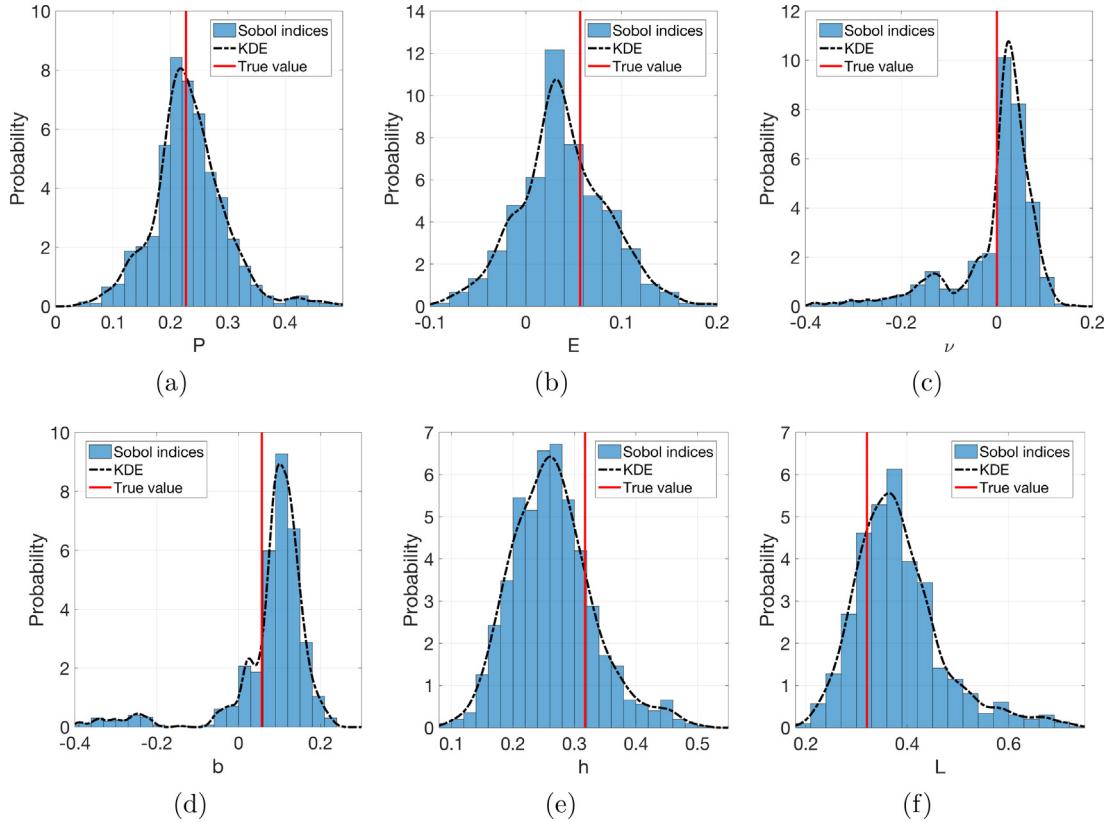


Fig. 4. Histogram of imprecise first-order Sobol' indices for each model input given 50 data: (a) Load (b) Young's modulus (c) Poisson's ratio (d) Width (e) Height and (f) Length.

sampling density identified from 50 data to reflect the updated candidate probability densities for random model inputs. Note that the updated candidate probability densities are estimated by efficient Bayesian updating that requires no additional model evaluations.

6. Application: IGSA for out-of-plane composite lamina properties

Here, we explore the influence of the constituent (fiber and matrix) material properties on the out-of-plane elastic properties of a unidirectional composite lamina.

6.1. Problem description

Given their attractive properties such as high specific strength and stiffness, fiber reinforced composites are widely used in many industrial domains including automotive, naval/marine, aerospace, and infrastructure. To evaluate the structural performance of a composite part, the accurate determination of each lamina's mechanical properties in the layup is critical for the safe use of the part - especially for structures such as aircraft where reliability is essential. Various analytical and numerical methods have been developed to determine the mechanical properties of unidirectional lamina based on the elastic properties of the constituent materials (matrix and fibers) [77], providing the capability to rapidly explore constituent combinations for optimized composite designs.

Analytical micromechanical models can be roughly categorized as homogenization models, elasticity models, semi-empirical models and phenomenological models. The analytical approach is computationally efficient but may not provide accurate predictions under certain conditions. Therefore, the technique chosen for this example problem is finite element analysis (FEA) using a representative volume element (RVE). FEA was chosen given its versatility to investigate user defined configurations and to avoid many of the assumptions and limitations of the theoretical models [78]. The computational

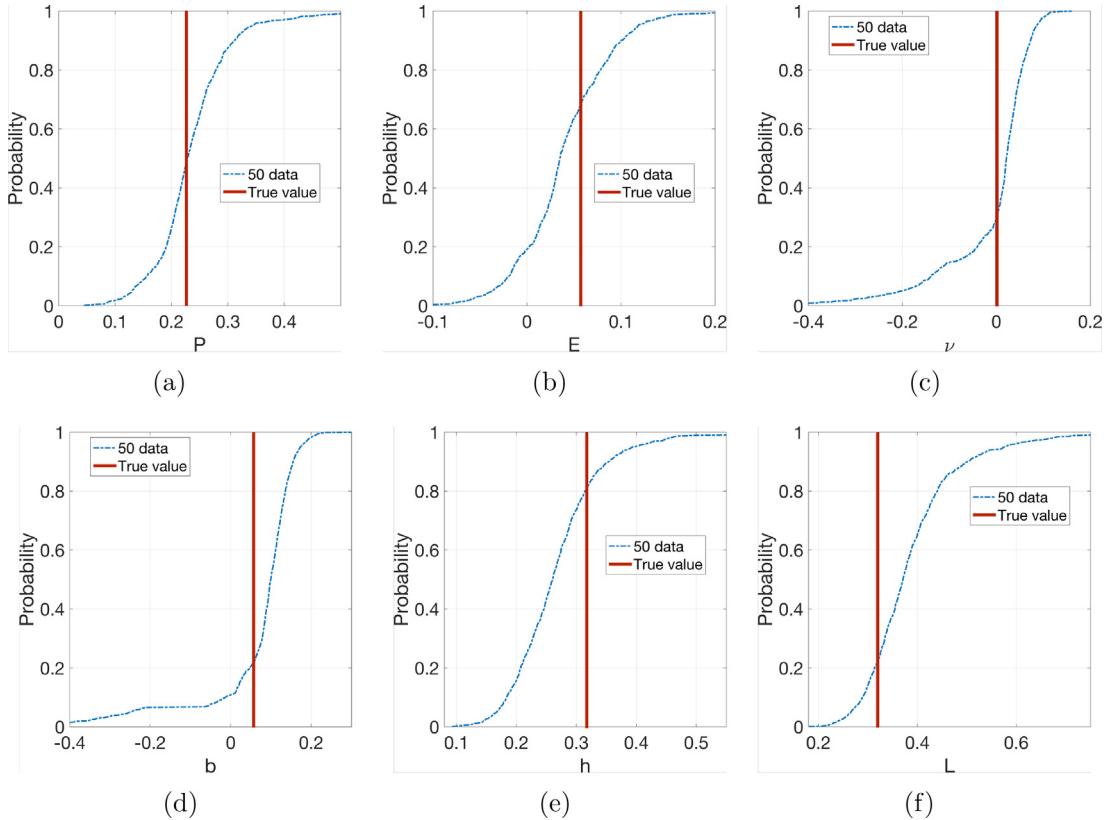


Fig. 5. CDF of imprecise first-order Sobol' indices for each model input given 50 data: (a) Load (b) Young's modulus (c) Poisson's ratio (d) Width (e) Height and (f) Length.

demand of FEA historically limited its use, but today's high performance computing capabilities now enable comprehensive non-deterministic investigation of RVE's in a feasible amount of time, as we will demonstrate.

Unidirectional composites are typically considered as transversely isotropic materials composed of two phases: a matrix phase and a fiber reinforcement phase, as shown in Fig. 8 for a hexagonal packing configuration. Generally speaking, the matrix phase is composed of an isotropic material (e.g. epoxy) and the reinforcement phase for most traditional materials is modeled as isotropic (e.g. glass fibers) or transversely isotropic (e.g. carbon fibers). The overall mechanical properties of a transversely isotropic unidirectional fiber reinforced lamina with a hexagonal packing geometry are defined by five independent engineering constants which are presented in the following compliance matrix:

$$C = \begin{bmatrix} 1/E_{11} & -v_{12}/E_{11} & -v_{12}/E_{11} & 0 & 0 & 0 \\ -v_{12}/E_{11} & 1/E_{22} & -v_{23}/E_{22} & 0 & 0 & 0 \\ -v_{12}/E_{11} & -v_{23}/E_{22} & 1/E_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{12} \end{bmatrix} \quad (37)$$

where E_{11} and E_{22} are the longitudinal and transverse Young's moduli respectively, G_{12} and G_{23} are the longitudinal and transverse shear moduli, v_{12} is the major Poisson's ratio and v_{23} is the minor Poisson's ratio. The transverse shear modulus is determined from the transverse Young's modulus and minor Poisson's ratio [79] as

$$G_{23} = \frac{E_{22}}{2(1 + v_{23})} \quad (38)$$

Table 3

Histograms of imprecise first-order Sobol' indices (three highest sensitivities) as a function of data set size from 100, 250, 500, 1000, 5000 to 10000.

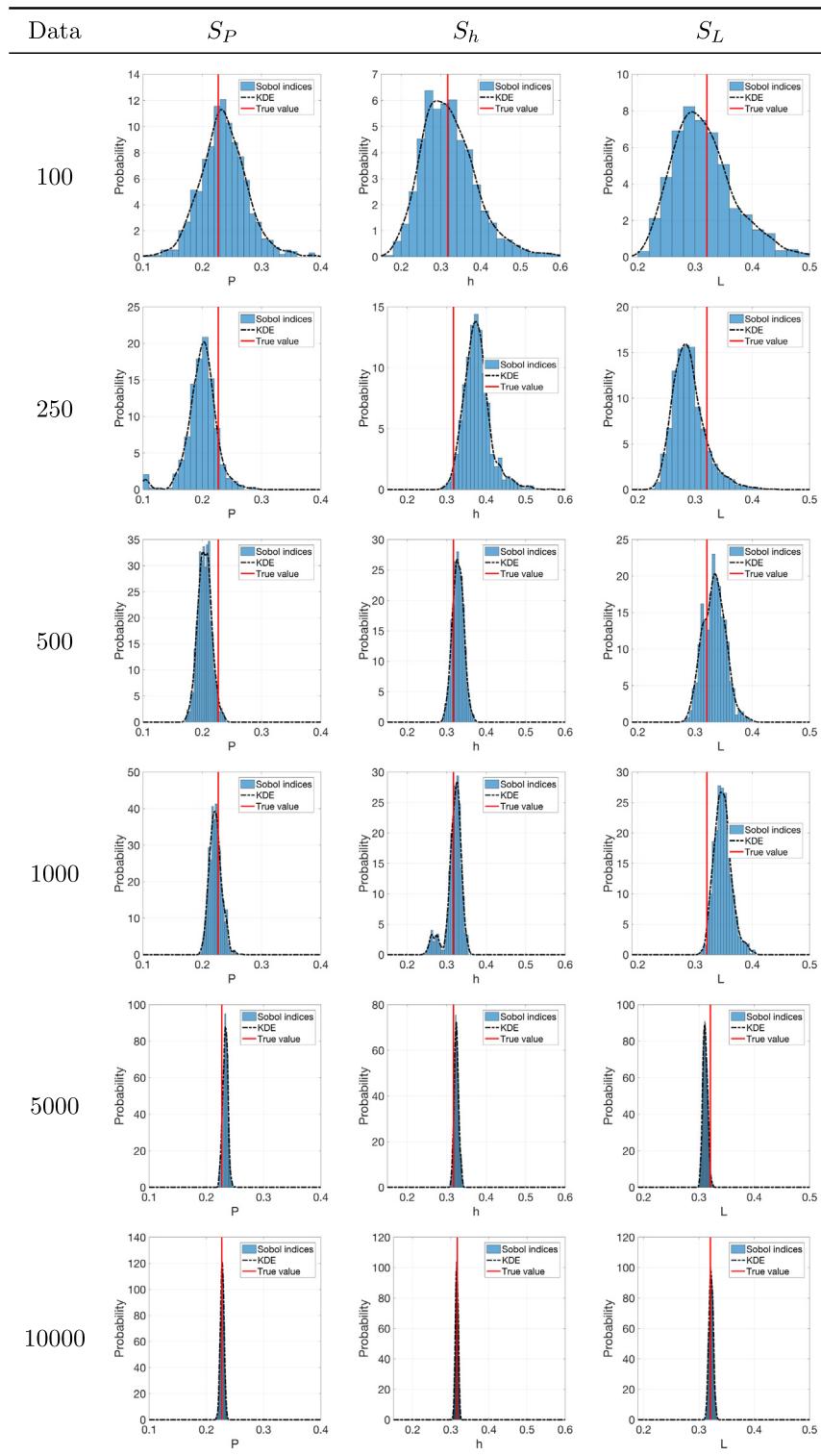
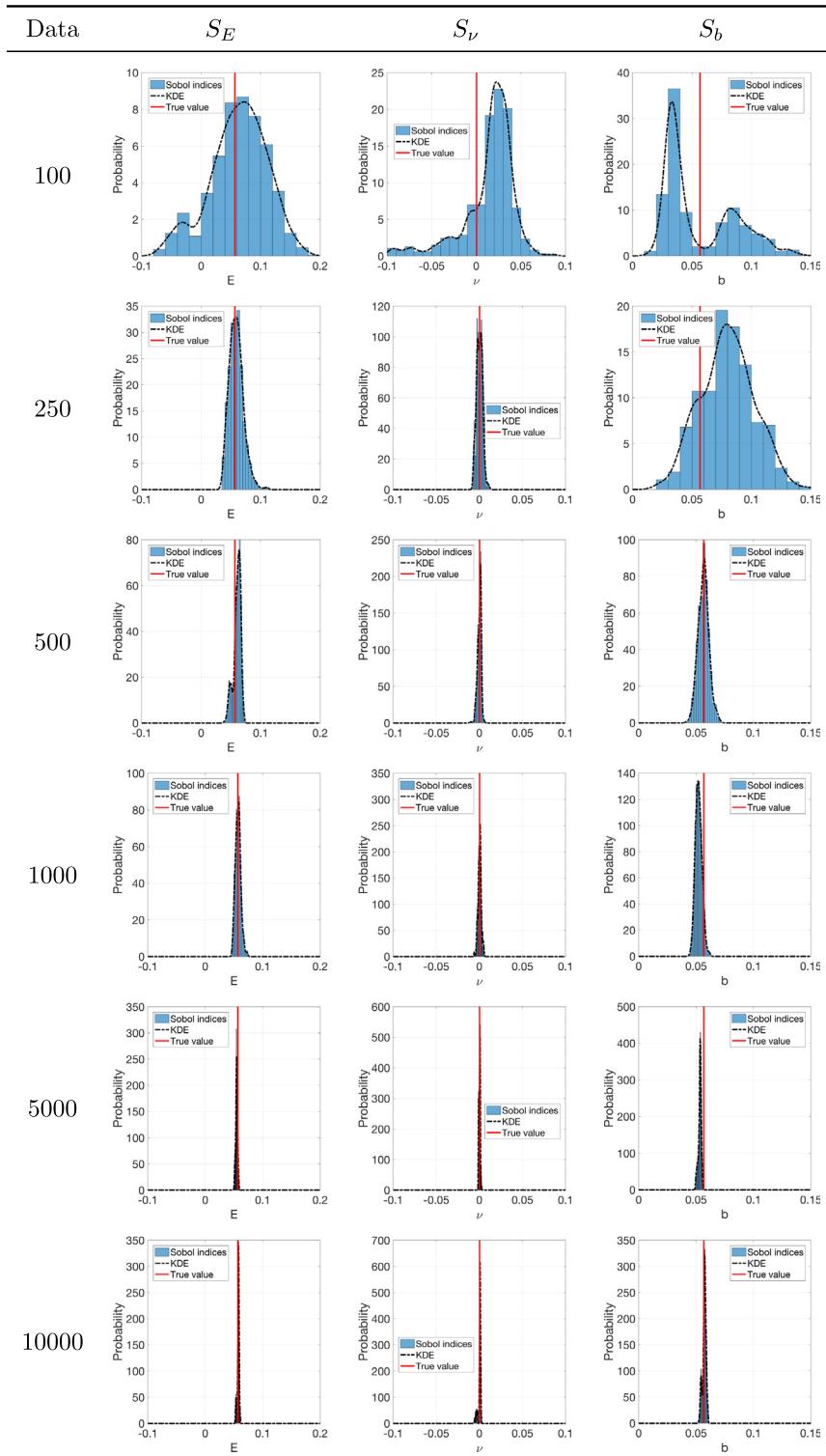


Table 4

Histograms of imprecise first-order Sobol' indices (three lowest sensitivities) as a function of dataset size from 100, 250, 500, 1000, 5000 to 10000.



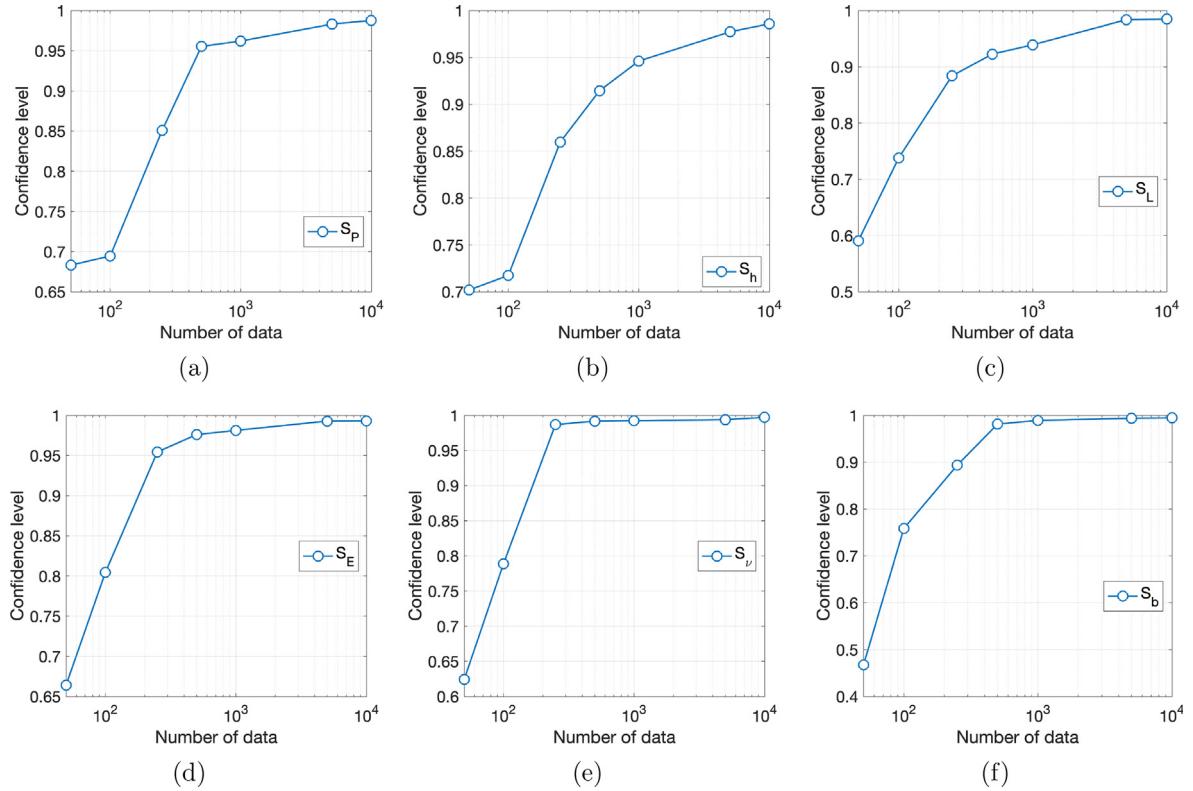


Fig. 6. Confidence level of the estimated Sobol' indices for (a) Load (b) Young's modulus (c) Poisson's ratio (d) Width (e) Height and (f) Length..

Numerical prediction and experimental determination of the in-plane lamina properties are typically straightforward and generally provide accurate values for these properties. The out-of-plane lamina properties, however, are difficult to obtain experimentally [80–83], and numerical prediction is an attractive alternative to rapidly predict these lamina properties. Therefore, determination of the two independent out-of-plane lamina properties (E_{22} and ν_{23}) is the focus of this example.

The lamina properties in Eq. (37) are a function of the constituent properties (matrix and fibers). The four independent constituent material properties and the fiber volume fraction as defined in Table 5 are needed to determine the lamina properties for the case of isotropic resin and fiber materials. The shear modulus for an isotropic material is determined from the Young's modulus and Poisson's ratio and is given by

$$G = \frac{E}{2(1 + \nu)} \quad (39)$$

In this example, we investigate a common composite lamina fabricated from Eglass fibers and LY556 polyester resin matrix. The FEA model is constructed as a 3D RVE with two symmetry planes in the $x - z$ and $x - y$ directions and periodic boundary conditions [84], as shown in Fig. 9. This FE model has 22750 nodes and 20448 C3D8R elements and was analyzed in Abaqus. A parametric input file provides the capability to rapidly investigate varying constituent properties and fiber volume for non-deterministic evaluation [85,86].

6.2. Identification of model input distributions

The multimodel imprecise GSA approach is particularly applicable to this problem given the lack of data characterizing the constituent material properties. Although used extensively in many applications, statistical data of this nature are scarce (typically only nominal design values are provided by suppliers and little guidance is provided in terms of variability). It is therefore essential to understand the sensitivity of the lamina properties to each of the individual constituent properties as

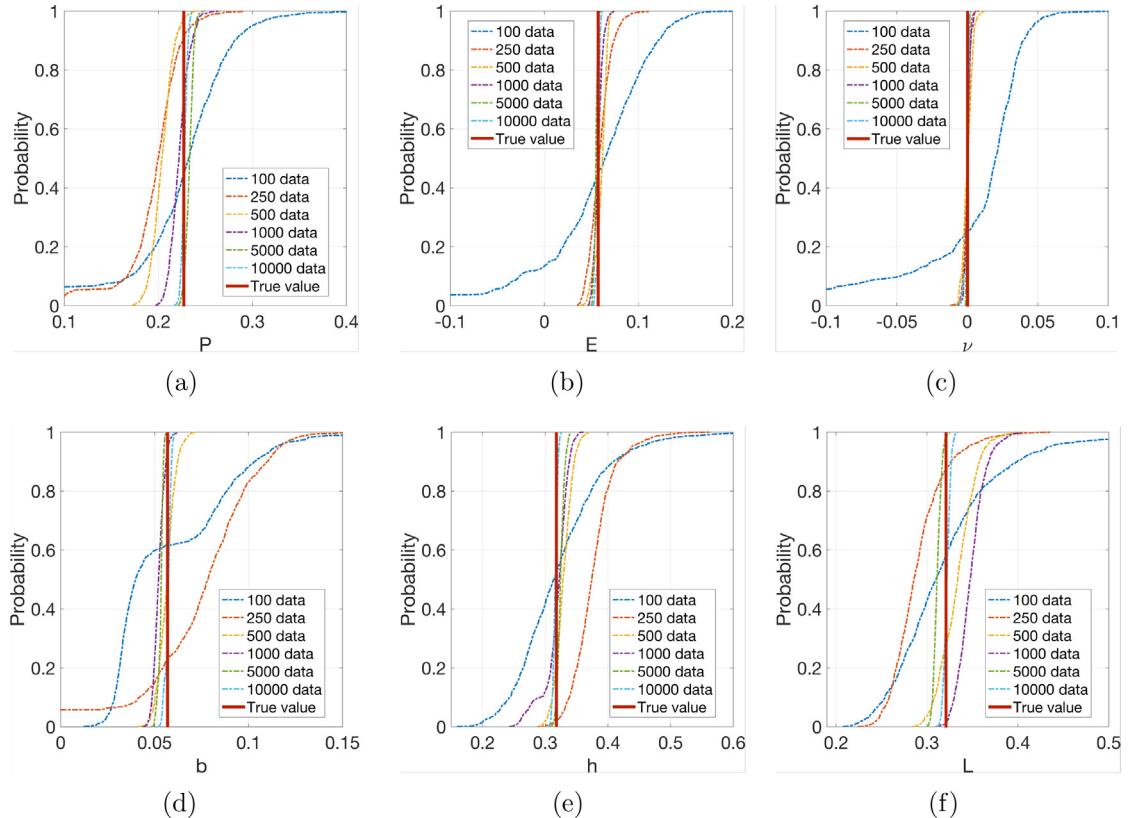


Fig. 7. CDF of imprecise first-order Sobol' indices as a function of data set size from 100, 250, 500, 1000, 5000 to 10000.

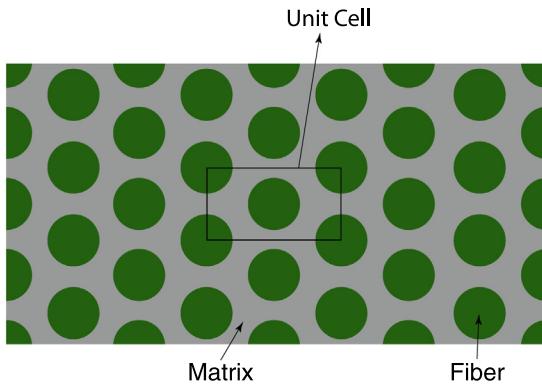


Fig. 8. Hexagonal unit cell in unidirectional composite.

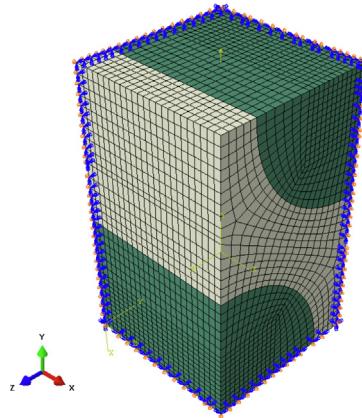
well as the effects of poorly defined probability distribution functions representing the input data. To generate a representative data set, relevant data was compiled from the literature for each constituent property (Table 5 and Table 6) and candidate probability distributions were identified for each property. Note that the references for $E_f = 71.5$ and $E_f = 76$ in Table 6 are listed as unavailable, because although each data value was confirmed using a credible reference before entry into the dataset, the source of the data is no longer available.

The available data are classified as extremely sparse. For Bayesian modeling from such sparse data, we must first assign priors to each material parameter. We therefore provide an upper and lower bound for the mean and coefficient of variation

Table 5

LY556 matrix material properties.

E_m	v_m	References
3.5	0.35	Karadeniz and Kumlutas, 2007 [87]
3.35	0.35	Soden et al., 2004 [83]
3.4	0.35	Chati and Mitra, 1998 [88]
3.2	0.35	Ciba Specialty Chemicals, 1998 [89]
3.45	0.35	Huang, 2001 [90]
3.35	0.35	Wongsto and Li, 2005 [91]

**Fig. 9.** Hexagonal unit cell FE model.**Table 6**

Eglass fiber material properties. *Data no longer publicly available.

E_f	v_f	References
75.79	0.22	Letto and Bradley, 1990 [92]
74	0.2	Soden et al., 2004 [83]
76		Bunsell, 2009 [93]
72		Lamb et al., 2003 [94]
72	0.2	Karadeniz and Kumlutas, 2007 [87]
72.4		Peters, 2013 [95]
70		Cheremisinoff, 1990 [96]
72.3	0.25	Lubin, 2013 [97]
74	0.25	Gay et al., 2007 [98]
72.4		American Society for Metals, 1965 [99]
72		Grayson, 1983 [100]
72.2		Broutman and Krock, 1967 [101]
72	0.3	Mallick, 1997 [102]
72.4		Jang, 1994 [103]
71.7		Balaguru and Shah, 1992 [104]
73.1	0.22	Huang, 2001 [90]
72.35	0.22	Barbero, 2017 [105]
76	0.22	Hull and Clyne, 1996 [106]
73	0.23	Daniel and Ishai, 1994 [78]
71.5		Unavailable*
76		Unavailable*
72		Jones and Bert, 1975 [107]
73.1	0.22	Shan and Chou, 1995 [108]
74	0.2	Wongsto and Li, 2005 [91]

Table 7

E-Glass fiber/LY556 Polyester Resin composite material model.

Material Property	Physical meaning	Number of data	Mean bound	COV bound
v_m	Matrix Poisson's ratio	6	[0.3, 0.4]	[5%, 10%]
V_f	Fiber volume fraction	1	[0.55, 0.65]	[5%, 10%]
E_m (GPa)	Matrix Young's modules	6	[3, 4]	[5%, 10%]
v_f	Fiber Poisson's ratio along 1-2 direction	12	[0.15, 0.35]	[5%, 10%]
E_f (GPa)	Fiber Young's modules along 1 direction	24	[70, 80]	[5%, 10%]

Table 8

Model probabilities from the given data for each material property.

Distribution	$\hat{\pi}_{v_m}$	$\hat{\pi}_{V_f}$	$\hat{\pi}_{E_m}$	$\hat{\pi}_{V_f}$	$\hat{\pi}_{E_f}$
Normal	0.200	0.200	0.203	0.104	0.180
Lognormal	0.200	0.200	0.193	0.249	0.214
Gamma	0.200	0.200	0.205	0.194	0.205
Inverse Gaussian	0.200	0.200	0.202	0.253	0.217
Logistic	0.200	0.200	0.197	0.199	0.185

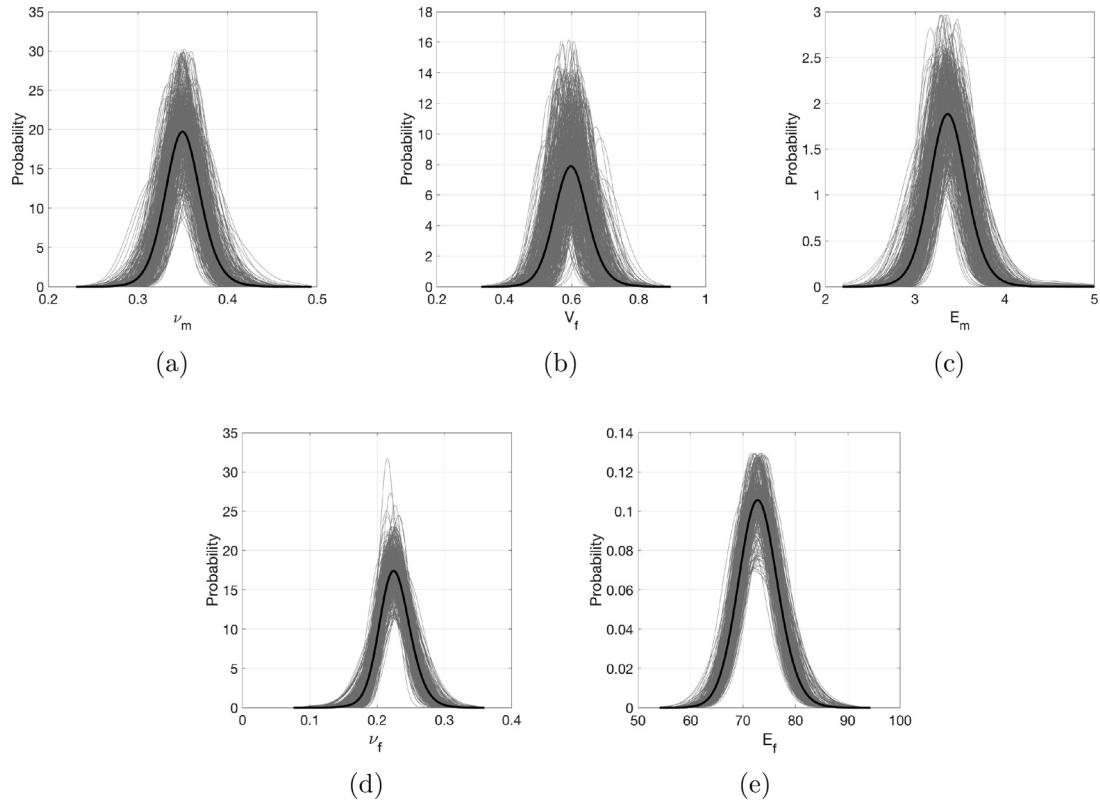


Fig. 10. 500 candidate probability distributions from multimodel Bayesian inference for (a) v_m , (b) V_f (c) E_m , (d) v_f and (e) E_f .

(COV) of each material property according to the authors' experience and literature review and assume these parameters are uniformly distributed within those bounds ([Table 7](#)).

In the multimodel inference approach, the following candidate probability models are considered: Normal, Lognormal, Gamma, Inverse Gaussian, and Logistic. Considering equal prior model probabilities ($\pi_j = 0.2, \forall j$), the first step is to determine the posterior model probabilities, $\hat{\pi}_j$ using Bayesian multimodel inference ([Section 3](#)). These posterior model probabilities are provided in [Table 8](#). Clearly the limited data has very little effect on the model probabilities, which remain largely unchanged. We do not have nearly enough data to identify a unique probability model for any of the parameters.

We then estimate the posterior joint density of model parameters using Bayesian inference. Finally, a finite set of probability models is established by randomly selecting the model family with model probabilities from [Table 8](#) and the associated parameter values from the posterior joint densities. Based on the ensemble of target probability models, the optimal sampling density is determined for importance sampling reweighting. [Fig. 10](#) shows the ensemble of candidate probability models for each material property. The gray curves represent the cloud of 500 candidate distributions and the thick black curve is the optimal sampling density. It can be observed that the cloud thickness is related to the data set size. The variables with extremely sparse data (v_m, V_f , and E_m) exhibit wide bands of candidate distributions. But the bands for v_f and E_f , which have more data, are narrower – as expected.

6.3. Estimating imprecise Sobol' indices

In the multimodel inference, we identify 500 candidate densities for each material property. The total number of combinations of these distributions is $500^5 = 3.125^{13}$, which is obviously prohibitive. Even though reweighting does not require model evaluation, this huge number is still unacceptable. Instead, a representative 5000 joint distributions are compiled using Latin hypercube sampling. For evaluation of the Sobol' indices, 50,000 random samples are drawn from the optimal

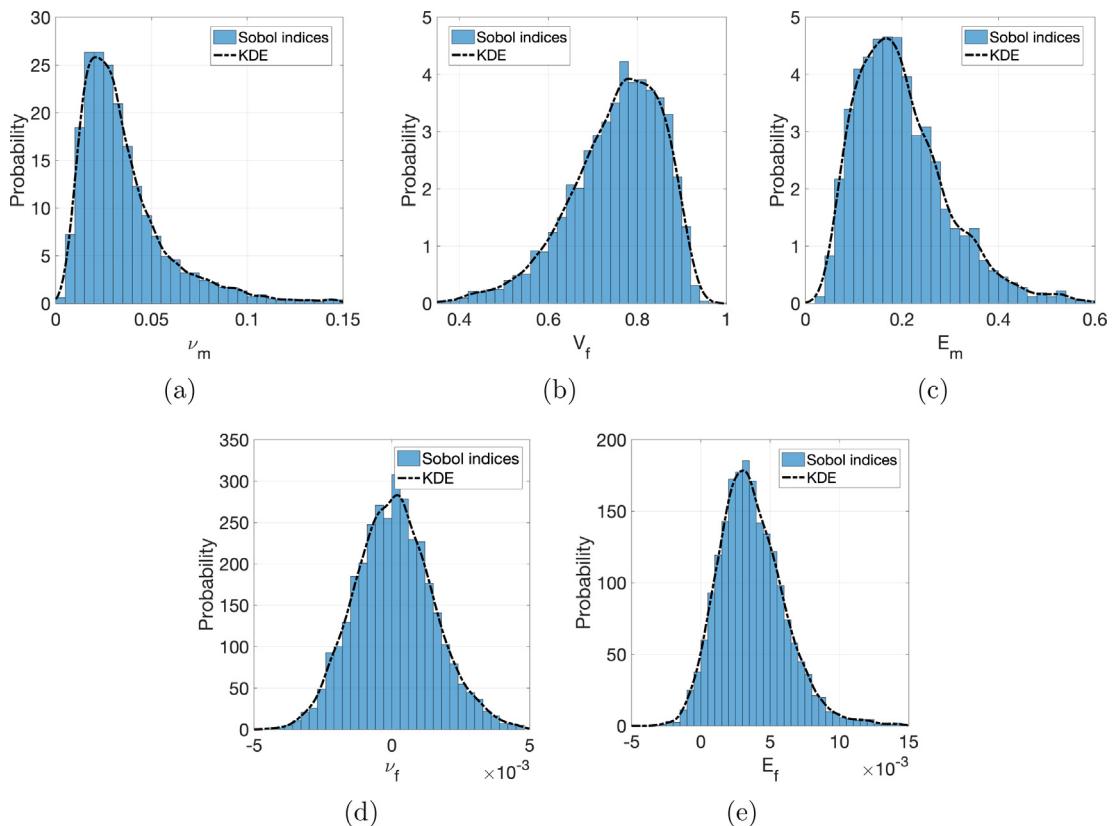


Fig. 11. Histogram of first-order Sobol' indices for E_2 : (a) v_m , (b) V_f (c) E_m , (d) v_f and (e) E_f .

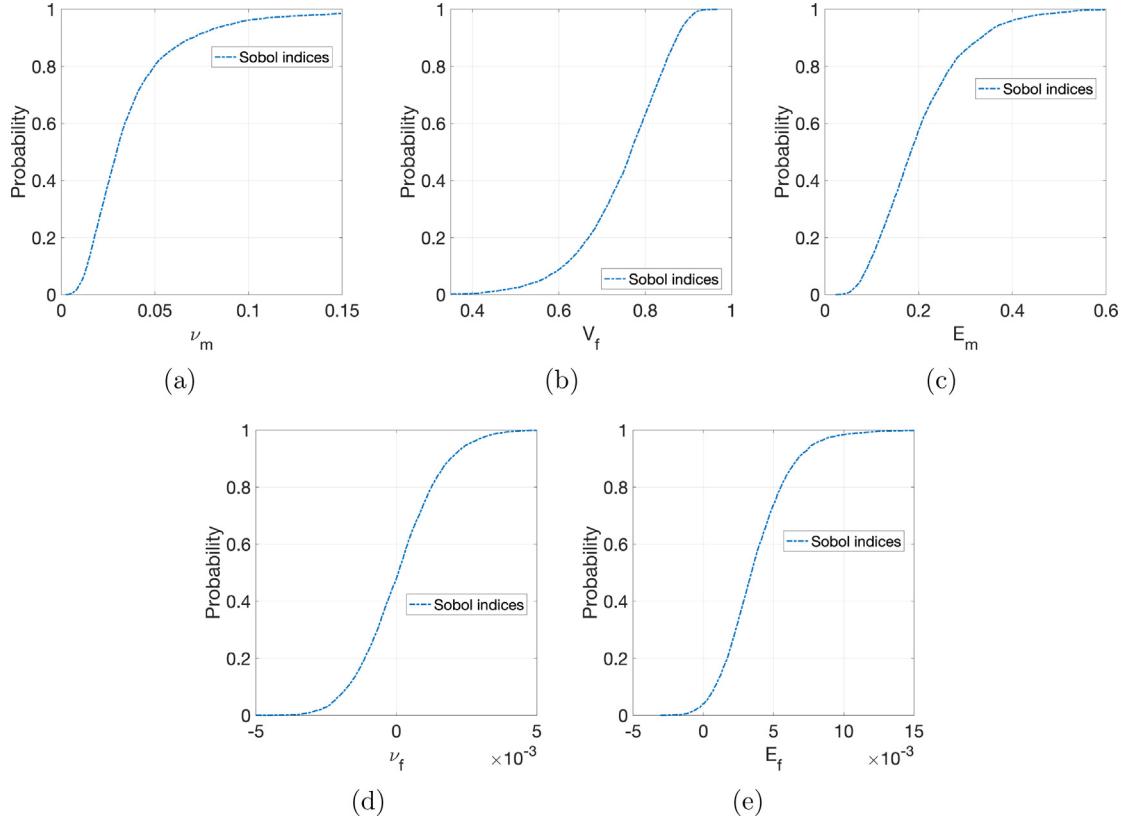


Fig. 12. CDF of first-order Sobol' indices indices for E_2 : (a) v_m , (b) V_f (c) E_m , (d) v_f and (e) E_f .

sampling density of each material property and computational model evaluations are performed using the finite element method.

We are specifically interested in the sensitivity of two resulting composite properties: 1. the Young's modulus along the 2 direction, E_2 (transverse to the fibers); and 2. the Poisson's ratio in the 2–3 direction v_{23} . Fig. 11 presents histograms of the first-order Sobol' indices for E_2 . Note that, even with very limited data, we can see that the overall influence of V_f is almost certainly the most significant although it has quite a large range from approximately 0.4 to 0.95. The second most significant variable is E_m which shows a variation from 0 to 0.6. Poisson's ratio of the matrix, v_m , with a variation range between 0 to 0.1, shows only moderate impact on E_2 . The fiber properties, v_f and E_f , meanwhile, play almost no role in determining E_2 . The corresponding empirical CDFs are shown in Fig. 12.

Figs. 13 and 14 show the histograms and empirical cdfs of the Sobol' indices for v_{23} . Note that v_m clearly becomes the most significant variable with Sobol' indices ranging from 0.8 to 1. The volume fraction, V_f , accounts for almost all of the remaining sensitivity of v_{23} . Even with such a small dataset, we can see that the other three variables, E_m , v_f and E_f have such a minor impact that their influence can be effectively ignored.

7. Conclusion

This work investigates the effect of uncertainties associated with small data sets for quantifying model inputs on the global sensitivity analysis of engineering systems. An effective method is presented to estimate imprecise first-order Sobol' indices. These imprecise Sobol' indices take a probabilistic form, such that instead of yielding known Sobol' indices for a given problem, the method produces distributions for the Sobol' indices reflecting the underlying epistemic uncertainty associated with a lack of data to quantify input probability distributions.

The approach for estimating imprecise Sobol' indices is set in a Bayesian multimodel framework, where first the probability model-form uncertainty is assessed using Bayesian inference and next the model parameter uncertainty is quan-

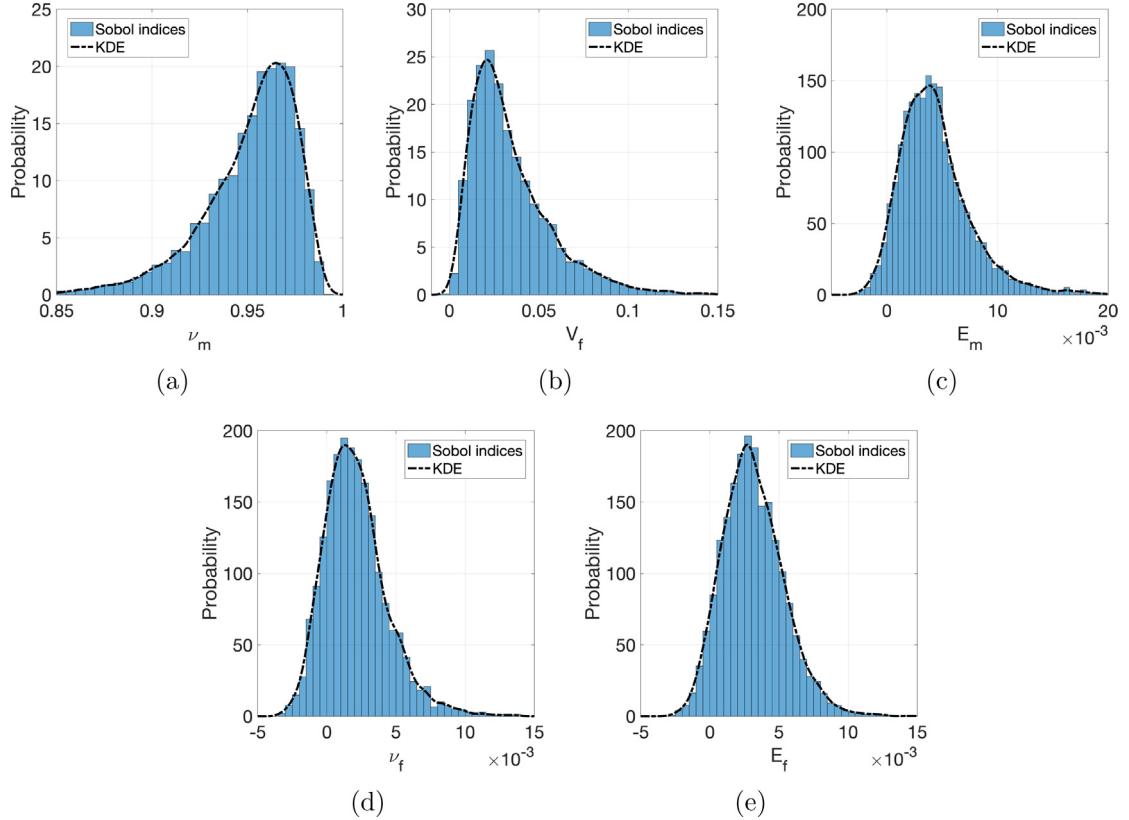


Fig. 13. Histogram of first-order Sobol' indices in terms of v_{23} : (a) ν_m , (b) V_f (c) E_m , (d) ν_f and (e) E_f .

tified (for each candidate probability model). The result is an ensemble of probability models that represents the imprecise probabilities in the assignment of model inputs. Based on the Monte Carlo method for Sobol' index calculation, a novel importance sampling-based formulation is derived to efficiently quantify imprecision in the Sobol' indices. The proposed algorithm therefore achieves simultaneous estimates of the Sobol' indices given multiple candidate inputs distribution at a low computational cost, when compared to a conventional approach that would require multi-loop Monte Carlo.

Through an analytical Timoshenko beam example, we systematically investigate the performance of the approach for estimating the imprecise sensitivity indices for increasing data set sizes. It is shown that a fully probabilistic description of the sensitivity indices is obtained and while the Sobol' indices have large variation (uncertainty) given initially small data sets, they gradually converge to the true (deterministic) estimates when a large number of data are collected. We also observe that Sobol' indices for the less sensitive variables appear to converge more quickly. That may allow rapid identification of less important variables for dimensionality reduction, even from small data sets.

Finally, the proposed method is applied to understand the influence of constituent properties on the overall out-of-plane properties of a transversely isotropic E-Glass fiber matrix composite. Considering data quantifying the constituent properties from the literature are extremely sparse, the method allows for probabilistically bounded sensitivity indices that can be used to probabilistically assess the importance of each constituent property. In particular, it is shown that out-of-plane elastic modulus depends most strongly on the fiber volume fraction and matrix elastic modulus, with some minor influence from the matrix Poisson's ratio. There is essentially no influence of the fiber properties. However, the precise degree of importance of each of the constitutive properties cannot be established and therefore, subsequent data collection efforts aimed at precisely understanding these quantities should focus on these properties. A similar investigation of the out-of-plane Poisson's ratio indicates that the matrix Poisson's ratio and volume fraction account for nearly all variability.

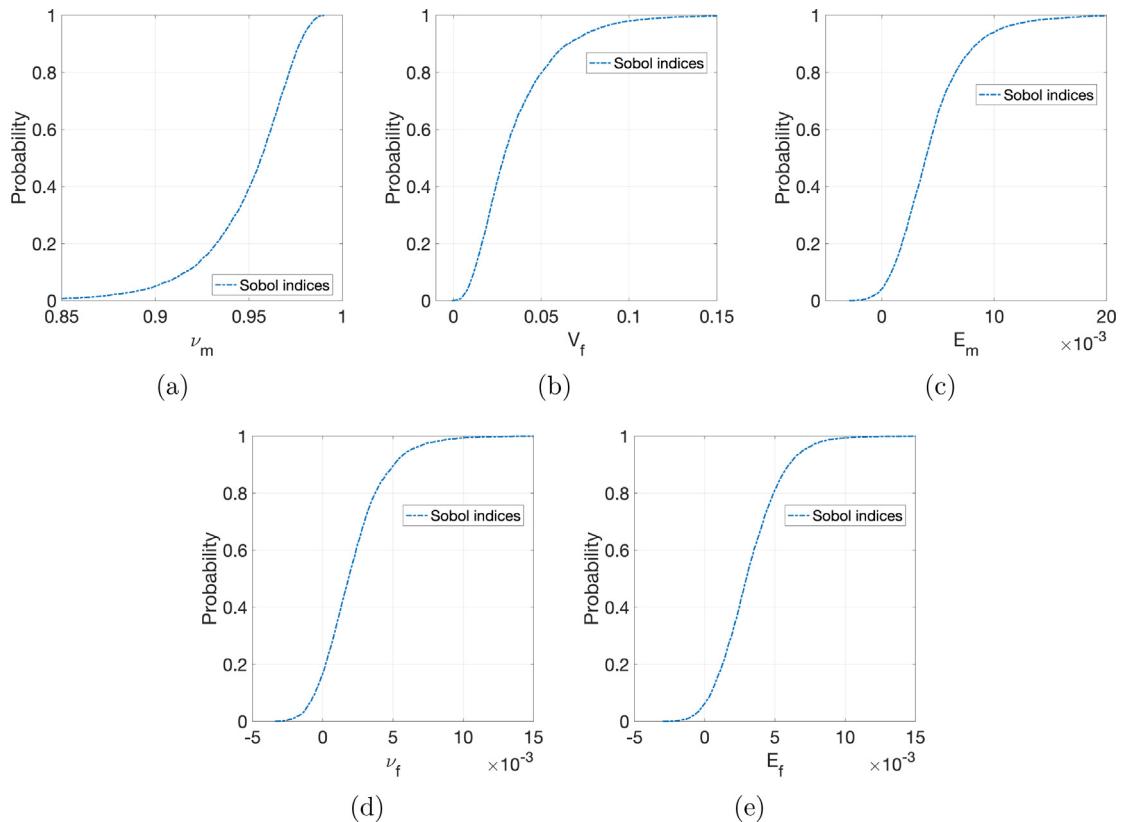


Fig. 14. CDF of first-order Sobol' indices indices in terms of v_{23} : (a) v_m , (b) V_f (c) E_m , (d) v_f and (e) E_f .

CRediT authorship contribution statement

Jiaxin Zhang: Conceptualization, Formal analysis, Investigation, Methodology, Software, Writing - original draft, Writing - review & editing, Validation, Visualization. **Stephanie TerMaath:** Data curation, Investigation, Validation, Writing - review & editing. **Michael D. Shields:** Conceptualization, Methodology, Writing - review & editing, Funding acquisition, Project administration, Supervision, Validation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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