Information fusion and machine learning for sensitivity analysis using physics knowledge and experimental data

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Abstract

Sensitivity analysis is often performed using computational models of the physical phenomena; such models could be physics-based or data-driven, and the sensitivity estimate is affected by the accuracy and uncertainty of the physics model. If the physics-based computational model is expensive, an inexpensive surrogate model is built and used to compute the Sobol' indices in variance-based global sensitivity analysis (GSA), and the surrogate model introduces further approximation in the sensitivity estimate. This paper considers GSA for situations where both a physics-based model and a small number of experimental observations are available, and investigates strategies to effectively combine the two sources of information in order to maximize the accuracy and minimize the uncertainty of the sensitivity estimate. Physics-informed and hybrid machine learning strategies are proposed to achieve these objectives. Two machine learning (ML) techniques are considered, namely, deep neural networks (DNN) and Gaussian process (GP) modeling, and two strategies for incorporating physics knowledge within these ML techniques are investigated, namely: (i) incorporating loss functions in the ML models to enforce physics constraints, and (ii) pre-training and updating the ML model using simulation data and experimental data respectively. Four different models are built for each type (DNN and GP), and the uncertainties in these models are also included in the Sobol' indices computation. The DNN-based models, since they have many degrees of freedom in terms of model parameters, are found to result in smaller bounds on the sensitivity estimates when compared to the GP-based

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models. The proposed methods are illustrated for an additive manufacturing example.
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1. Introduction

Computational models are often used to predict the response of an engineering system since conducting experiments to directly measure the true response is often not feasible. However, the computational model is usually an incomplete representation of the complex physical system. In this case, the system response prediction is affected by the model uncertainty. The various sources of uncertainty are classified as (a) epistemic uncertainty due to lack of knowledge, and (b) aleatory uncertainty due to the inherent variability in the system or the external inputs. Global sensitivity analysis (GSA) [1] aims to provide a quantitative assessment of the relative contribution of each uncertainty source to the uncertainty in the model response [2–4].

Much of the GSA literature has focused on variability in the inputs and their effects on output variability; the extension of GSA to include epistemic uncertainty sources (data, model) is recent and sparse [5–7]. Model outputs can have uncertainty even for a fixed input when there exists model uncertainty. When the model is computationally expensive, it is often replaced with a surrogate model to facilitate the estimation of Sobol indices, since such computation requires many input-output samples from the model; the surrogate model introduces additional uncertainty. Several types of surrogate models are used in the literature, e.g., polynomial chaos expansion (PCE), Gaussian process regression, neural networks, etc., to train a parametric relationship between the inputs and the outputs. The quality and quantity of the training data affect the accuracy of these surrogate models, which directly affects the uncertainty in the model output [8–10]. Thus, it is important to also quantify the contribution of surrogate model uncertainty to the output uncertainty. In La Gratiet et al [8], the Gaussian process (GP) surrogate model uncertainty is included in the Sobol index estimates with a Monte Carlo procedure using multiple realizations of the GP model prediction, which helps to construct prediction intervals for the Sobol index estimates.

In high dimensional problems, the use of surrogate model-based GSA, which repeatedly executes the code by suppressing some variables and running through the range of other variables, may be an issue as the number of required number of executions of the code increases rapidly with the number of inputs [8, 11–13]. Expanding GSA to consider both aleatory and epistemic uncertainty is beneficial in supporting resource allocation decisions; if the contribution of epistemic uncertainty is found to be significant, then it may be valuable to collect more data or refine the physics model to reduce the epistemic uncertainty and thus its contribution to the output uncertainty. Several GSA studies have developed auxiliary variable-based approaches to include both aleatory and epistemic uncertainty sources at a single level instead of using nested simulations, thus achieving both computational efficiency and direct ranking of the different sources of uncertainty. The auxiliary variable is used to transform one-to-many mapping to one-to-one mapping, thus facilitating the computation of Sobol indices for both aleatory and epistemic sources [14]. This idea is expanded in [15] to include several epistemic sources, such as input statistical uncertainty, surrogate model error, physics model discrepancy, and numerical solution error, and to systems with time series inputs and outputs.

Three scenarios of model and data availability can be considered for GSA: (1) use of a physics-based computational model, (2) use of available input-output data, either from experiments or previous simulations, or (3) use of both physics model and available input-output data. A straightforward model-based approach to estimate Sobol indices is to use a double-loop Monte Carlo simulation (MCS) [16]. In order to reduce the cost associated with the double-loop MCS, analytical and various efficient sample-based methods have been developed. The methodology developed by Sudret, which approximates the original physics model by a PCE and estimated the Sobol indices by post-processing the PCE coefficients [17]. The improved FAST method [18] combines the classical FAST method [2] with random balanced design [19] for generating samples to evaluate Sobol indices. Chen et al. [20] proposed analytical ways to compute Sobol' indices for GP with input variables following normal or uniform distributions.

In some problems, input-output data may be already available instead of having to simulate a physics model expressly for the purpose of GSA. Such data may be available from

experiments, from real-world observations, from Markov Chain Monte Carlo (MCMC) sampling during Bayesian model calibration, from MC sampling for reliability analysis, etc. In such cases, data-driven methods have been proposed to directly compute the Sobol indices based on available input-output samples instead of simulation runs of the physics model [11, 21]. A GSA method based on ANOVA using factorial design of experiments is developed by Ginot et al. [22]. The proposed method results in same values as the Sobol index since the variance decomposition used in the Sobol index estimations is same as the one used in the classical ANOVA [23]. The computational cost of most sample-based methods is proportional to the number of model input. Li and Mahadevan [24] proposed a modularized method, which has a computational cost that is not proportional to the model input dimension, to estimate the first-order Sobol indices based on stratification of available input-output samples. DeCarlo et al. [21] proposed an importance sampling approach by introducing weights to different data points to estimate Sobol indices from available data using Sobol' sequences to reduce the number of simulations. Probability model-based GSA have been recently proposed by Hu and Mahadevan [11] to estimate Sobol indices by building joint distribution models.

The third scenario is of interest in this paper, where both a physics-based model and some experimental or real-world data are available. One option, if adequate data is available, is to simply build a regression or machine learning (ML) model based on the observation data, and use this model to perform GSA. Multiple recent studies have pursued data-driven machine learning (ML) models in situations where abundant experimental data or real-world observations are available due to advances in modern sensing techniques. Generally, the construction of data-driven ML models does not require in-depth knowledge of the complex physics inherent in the physical process. ML models can learn complex systems using available observations, but the accuracy of these models depends on the quality and quantity of the data. If the available data is limited, then the complexity of the process cannot be captured. Further, since purely data-driven ML models do not explicitly consider physical laws, they can produce physically inconsistent results. In such cases, incorporating physics knowledge within ML models may improve the accuracy and efficiency of GSA computations. The combined use of physics-based

and ML models has been shown to achieve more accurate and physically consistent predictions by leveraging the advantages of each method [25–27].

In this work, we incorporate physics knowledge into the ML models to better capture the physics of the process by leveraging physical laws while improving the generalization performance of data-driven models. Two types of ML models are considered in this paper, namely, GP and DNN. Four different physics-informed machine learning (PIML) models are developed for each type (i.e., GP or DNN) to predict the output quantity of interest (QoI), through combinations of two strategies: (1) incorporating loss functions in the ML models to enforce physics constraints, and (2) pre-training the ML model with simulation data and then updating it with experimental data. The proposed methods can use multiple physics-based loss functions and enhance the data-driven ML models to obey the physics laws. The resulting GSA includes the effect of uncertainty in the ML or PIML model.

In summary, the contributions of this paper are as follows:

- Physics knowledge and experimental observations are fused in order to maximize the accuracy and minimize the uncertainty of sensitivity estimates.
- Two PIML strategies and their combinations are investigated for sensitivity analysis using both physics knowledge and experimental data.
- Four different models are built for both GP and DNN, and the uncertainties in these models are included in the Sobol indices computation.
- The accuracy, uncertainty and computational effort for different options for ML and PIML models are evaluated and compared.

The outline of the rest of this paper is as follows. Section 2 provides background information on related methods. Section 3 presents the proposed methodology. The proposed methodology is illustrated for a numerical example in Section 4. Concluding remarks are provided in Section 5.

2. Background

This section introduces each of the basic techniques used in developing the proposed methodology, namely variance-based GSA, Gaussian process surrogate modeling, and deep neural networks (DNN). These techniques are well established with extensive literature, therefore only a brief introduction is given here.

2.1. Probabilistic sensitivity analysis

Consider a deterministic real integrable one-to-one system response function $\mathrm{Y} = f(\mathbf{X})$, where $f(\cdot)$ is the computational model, $\mathbf{X} = \{\mathrm{X}_1, ..., \mathrm{X}_k\}$ are mutually independent model inputs, and Y is the model output. As shown by [16], the variance of Y can be decomposed as

$$V(\mathrm{Y}) = \sum_{i}^{k} V_i + \sum_{i_1}^{k} \sum_{i_2=i_1+1}^{k} V_{i_1 i_2} + \sum_{i_1}^{k} \sum_{i_2=i_1+1}^{k} \sum_{i_3=i_2+1}^{k} V_{i_1 i_2 i_3} + ... + V_{12...k} \tag{1}$$

where V_i is the variance of Y due to $\mathrm{X_i}$ alone, and $V_{i_1...i_p} (p \geq 2)$ indicates the variance of Y due to $\{\mathrm{X_{i_1}}, ..., \mathrm{X_{i_p}}\}$.

The Sobol indices are defined by dividing both sides of Eq. (1) with $V(\mathrm{Y})$

$$1 = \sum_{i}^{k} S_i + \sum_{i_1}^{k} \sum_{i_2=i_1+1}^{k} S_{i_1 i_2} + \sum_{i_1}^{k} \sum_{i_2=i_1+1}^{k} \sum_{i_3=i_2+1}^{k} S_{i_1 i_2 i_3} + ... + S_{12...k} \tag{2}$$

where S_i is the first-order or main effects index that assesses the contribution of $\mathrm{X_i}$ individually to the variance of the output Y without considering interactions with other inputs. The higher-order indices $S_{i_1...i_p} (p \geq 2)$ in Eq. (2) measure the contributions of the interactions among $\{\mathrm{X_{i_1}}, ..., \mathrm{X_{i_p}}\}$.

The evaluation of S_i is defined as follows:

$$S_i = \frac{V_i}{V(\mathrm{Y})} = \frac{V_{X_i}(E_{\mathbf{X}_{-i}}(\mathrm{Y}|\mathrm{X}_i))}{V(\mathrm{Y})} \tag{3}$$

where $\mathbf{X}_{-i}$ are all the model inputs other than X_i.

The overall contribution of $\mathrm{X_i}$ considering an individual input and its interactions with all other inputs is measured by the total effects index S_i^T:

$$S_i^T = 1 - \frac{V_{-i}}{V(\mathrm{Y})} = \frac{V_{\mathbf{X}_{-i}}(E_{\mathrm{x}_i}(\mathrm{Y}|\mathbf{X}_{-i}))}{V(\mathrm{Y})}. \tag{4}$$

The computation of S_i analytically is nontrivial since $E_{\mathbf{X}_{-i}}(\cdot)$ requires multi-dimensional integrals. A basic sampling-based approach is to use double-loop sampling [16]. One approach to reduce the computational cost is to replace the original computational model $f(\cdot)$ by a surrogate model and use this surrogate model in GSA with double-loop sampling [28–32]. A second approach is to use analytical solutions based on the coefficients of a polynomial chaos approximation [17]. A third approach is to pursue efficient single loop sampling techniques [24].

2.2. Gaussian process surrogate modeling

The GP surrogate model provides a prediction $G(\mathbf{u})$ at a given input $\mathbf{u}$ as

$$G(\mathbf{u}) = \mathbf{h}(\mathbf{u})^T\boldsymbol{\beta} + Z(\mathbf{u}) \tag{5}$$

where $\mathbf{h}(\cdot)$ is the trend function, $\boldsymbol{\beta}$ is the vector of trend coefficients, and $Z(\cdot)$ is a zero-mean stationary GP which describes the deviation of the model from the trend. The covariance between the outputs $Z(\cdot)$ of the GP surrogate at points $\mathbf{a}$ and $\mathbf{b}$ is defined as:

$$\mathrm{Cov}[Z(\mathbf{a}), Z(\mathbf{b})] = \sigma_Z^2 R(\mathbf{a}, \mathbf{b}) \tag{6}$$

where σ_Z^2 is the process variance and $R(\cdot,\cdot)$ is the correlation function. A squared exponential function with separated length scale parameters l_i for each input dimension has often been used in the literature:

$$R(\mathbf{a}, \mathbf{b}) = \exp\left[-\sum_{i=1}^{\mathrm{M}} \frac{(a_i - b_i)^2}{l_i}\right] \tag{7}$$

The hyperparameters of the GP model, i.e., $\boldsymbol{\Theta} = \{l, \sigma_Z, \sigma_{obs}\}$, where σ_{obs} is the observation error, are inferred from the training data. A common method is to maximize the log marginal

likelihood function, which is defined as

$$\log\, p(\mathbf{Y}|\mathbf{X};\boldsymbol{\Theta}) = -\frac{1}{2}\mathbf{Y}(\mathbf{K}_{TT} + \sigma^2_{obs}\mathbf{I})^{-1}\mathbf{Y} - \frac{1}{2}\log|\mathbf{K}_{TT} + \sigma^2_{obs}\mathbf{I}| + \frac{n}{2}\log 2\pi. \tag{8}$$

The outputs of the GP model are the mean prediction $\mu_G(\cdot)$ and the variance of the prediction $\sigma^2_G(\cdot)$, defined as:

$$\mu_G(\mathbf{u}) = \mathbf{h}(\mathbf{u})^T\boldsymbol{\beta} + \mathbf{r}(\mathbf{u})^T\mathbf{R}^{-1}(\mathbf{g} - \mathbf{F}\boldsymbol{\beta}) \tag{9}$$

$$\sigma^2_G(\mathbf{u}) = \sigma^2_Z - \mathbf{A}\begin{bmatrix} \mathbf{0} & \mathbf{F}^T \\ \mathbf{F} & \mathbf{R} \end{bmatrix}^{-1}\mathbf{A}^T \tag{10}$$

where $\mathbf{r}(\mathbf{u})$ is a vector containing the covariance between $\mathbf{u}$ and each of the training points $\{x_1, x_2, ..., x_n\}$, $i \in \{1, ..., n\}$, $\mathbf{R}$ is an $n \times n$ matrix containing the correlation between each pair of training points, $\mathbf{R}(x_i,\ x_j) = \mathrm{Cov}[Z(x_i), Z(x_j)]$; $\mathbf{g}$ is the vector of original physics model outputs at each of the training points, $\mathbf{F}$ is a $n \times q$ matrix with rows $\mathbf{h}(\mathbf{u}_i)^T$, and $\mathbf{A} = \begin{bmatrix}\mathbf{h}(\mathbf{u})^T & \mathbf{r}(\mathbf{u})^T\end{bmatrix}$.

2.3. Deep neural networks

In recent years, due to the confluence of advanced sensing and imaging techniques, big data processing techniques, and enormous computational power, rapid advances are being made in developing sophisticated data-driven machine learning models, particularly neural networks. A deep neural network (DNN) is composed of multiple hidden layers and has four major components: neuron, activation function, cost function, and optimization. Figure 1 shows a neural network consisting of three inputs, two hidden layers, each having four neurons, and two output neurons. The values of various input variables of a particular neuron are multiplied by their associated weights, then the sum of the products of the neuron weights and the inputs are calculated at each neuron. The summed value is passed through an activation function that maps the summed value to a fixed range before passing these signals on to the next layer of neurons.

The predictions of the DNN after a forward propagation, $\hat{\mathbf{Y}}$, are compared against the true response of the system, $\mathbf{Y}$, by defining a loss function (e.g., root mean squared error (RMSE); $\mathcal{L}_{\mathrm{RMSE}}(\mathbf{Y}, \hat{\mathbf{Y}}) = \sqrt{\sum_{i=1}^{n}(\mathrm{y}_i - \hat{\mathrm{y}}_i)^2/n}$), which measures how far off the predictions are from the

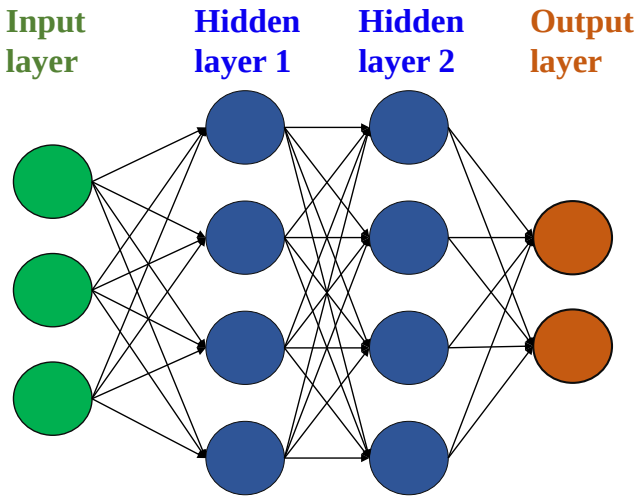

Fig. 1. A deep neural network with two hidden layers.

observations for the n training samples. After the forward propagation, backpropagation algorithms are employed to keep track of small perturbations to the weights that affect the error in the output and to distribute this error back through the network layers by computing gradients for each layer using the chain rule. In order to minimize the value of the loss function, necessary adjustments are applied at each iteration to the neuron weights in each layer of the network. These procedures are performed at each iteration until the loss function converges to a stable value.

3. Proposed methodology

The proposed methodology for sensitivity analysis using both physics knowledge and experimental data consists of the following steps:

1. PIML strategies
2. Implementation of PIML in GP
3. Implementation of PIML in DNN
4. Model uncertainty quantification in GP and DNN
5. Sobol indices computation with model uncertainty

The following subsections describe these steps in detail.

3.1. PIML strategies

PIML models seek to incorporate physics knowledge or constraints within the data-driven ML models. When a mechanistic, physics-based model is also available, complementary strengths of both mechanistic and ML models can be leveraged in a synergistic manner [27]. The aim is to improve the predictions beyond that of physics-based models or ML models alone by coupling physics-based models with ML models. Thus two different strategies to combine physics knowledge and ML models can be considered: (1) incorporate physics constraints in the ML models, and (2) pre-train and update the ML models using physics model input-output and experimental data, respectively.

3.1.1. Strategy 1: Enforcing physics constraints

A direct strategy to enforce physics constraints in ML model predictions is by including the constraints in the loss functions used in training the ML model [25]. Consider a PIML model with inputs $\boldsymbol{X}$ and outputs $\hat{\boldsymbol{Y}}$ trained using physical laws that are incorporated as constraints into the loss function:

$$\mathcal{L} = \mathcal{L}_{\text{ML}} + \lambda_{\text{phy}} \mathcal{L}_{\text{phy}}(\hat{\boldsymbol{Y}}), \tag{11}$$

where $\mathcal{L}_{\text{ML}}$ is the log marginal likelihood of the data for a GP model:

$$\mathcal{L}_{\text{GP}} = \log\, p(\mathbf{Y}|\mathbf{X};\boldsymbol{\Theta}) \tag{12}$$

and regular training loss function for a DNN that evaluates a supervised error, e.g., root mean squared error (RMSE):

$$\mathcal{L}_{\text{DNN}}(\boldsymbol{Y}, \hat{\boldsymbol{Y}}) = \sqrt{\sum_{i=1}^{n} \frac{(Y_i - \hat{Y}_i)^2}{n}} \tag{13}$$

which measures the accuracy of predictions $\hat{\boldsymbol{Y}}$ for n training samples. The physics-based loss function $\mathcal{L}_{\text{phy}}$ in the second term of Eq. 11 is weighted by a hyperparameter λ_{phy}; the value of λ_{phy} controls the strength of the physics constraint enforcement. The inclusion of the second

term ensures physically consistent model predictions and helps to reduce the generalization error, which is a measure of how accurately a model is able to predict the output QoI for previously unseen data, even when there is a small amount of training data [25].

The physical inconsistencies in the model predictions are evaluated using the physics-based loss functions. The generic forms of these physical relationships can be expressed using the following constraints:

$$\mathcal{F}_1(\hat{\boldsymbol{Y}}, \boldsymbol{\Gamma}) = 0, \tag{14}$$
$$\mathcal{F}_2(\hat{\boldsymbol{Y}}, \boldsymbol{\Gamma}) \leq 0.$$

where Γ denotes model parameters and physical variables. These equations can involve algebraic relationships or partial differentials of $\hat{\boldsymbol{Y}}$ and $\boldsymbol{\Gamma}$. The physics-based loss functions for these equations can be defined as:

$$\mathcal{L}_{\text{phy}}(\hat{\boldsymbol{Y}}) = ||\mathcal{F}_1(\hat{\boldsymbol{Y}}, \boldsymbol{\Gamma})||^2 + \text{ReLU}(\mathcal{F}_2(\hat{\boldsymbol{Y}}, \boldsymbol{\Gamma})), \tag{15}$$

where $\text{ReLU(x)} = \max(0, \text{x})$ represents the rectified linear unit function and it is used here to specify a quantitative range of operation, which penalizes when the difference between the predicted and target values are larger than the threshold, or to formulate a monotonic relationship for the QoI $\hat{\boldsymbol{Y}}$ [33].

3.1.2. Strategy 2: Pre-training and Updating

The model output accuracy and uncertainty are dependent on the quality and quantity of the available data. In some systems, the high cost associated with conducting experiments makes it infeasible to have adequate amount of training data to build purely data-driven models. Thus, it is important to effectively combine the physics-based model and a small amount of available experimental data in order to maximize the accuracy and minimize the uncertainty of the sensitivity estimate. When the experiments are expensive, they could only be conducted for a few values of the inputs, whereas it might be possible to run the physics-based model for

multiple combinations of input values. In that case, the simulation data can be used to pre-train an ML model, which is used as the initial model to be updated with experimental observations. Further, training of ML models requires the choice of initial values of the model parameters. The transfer of physical knowledge using a pre-trained ML model can prevent poor initialization due to lack of knowledge of initial choice of ML model parameters prior to training.

Since the pre-training based on the mechanistic model can use a large amount of training data (with multiple input parameter combinations) over a wide range of values, the pre-training may help the eventual ML model to have wider generalization beyond experimental data. In the numerical example in Section 4, the pre-training strategy exercises the physics model over 1310 input combinations, whereas only 39 experiments are available. However, if the physics model is computationally expensive, then the advantage of the pre-training strategy in using a larger input data set (from physics model runs) compared to the experiments becomes limited.

The two proposed strategies to predict the QoI are shown in Fig. 2. Figure 2(a) shows the first method, where the physical knowledge is included through constraints within the loss function of an ML trained with experimental data. Figure 2(b) shows the second method, where an ML model is first trained with data generated using the physics-based model and then updated using experimental data. The proposed PIML strategies can be applied to physical process by leveraging the related physical constraints or physics-based models.

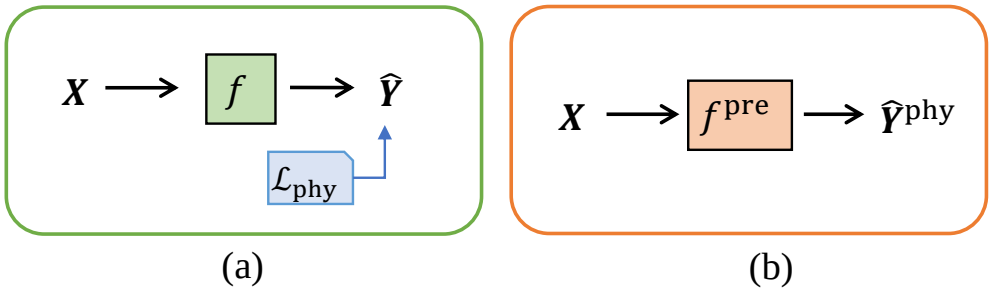

Fig. 2. PIML strategies: (a) incorporating physics-based loss functions in the ML models to enforce physics constraints, (b) pre-training an ML model with physics model input-output and updating it with experimental data.

3.2. Implementation of PIML strategies in GP and DNN

Based on the proposed two strategies to incorporate physics knowledge into the ML model, four separate ML models can be constructed for each type of surrogate model (GP and DNN):

1. GP
2. GP$^{\mathcal{L}_{\text{phy}}}$
3. GP$^{\text{upd}}$
4. GP$^{\text{upd},\mathcal{L}_{\text{phy}}}$
5. DNN
6. DNN$^{\mathcal{L}_{\text{phy}}}$
7. DNN$^{\text{upd}}$
8. DNN$^{\text{upd},\mathcal{L}_{\text{phy}}}$

The following subsections describe the implementation of these models in detail.

3.2.1. Implementation of PIML in GP

In the first model, GP, only experimental observations are used for training. The hyper-parameters are optimized during training by minimizing the error between the observations $\mathbf{Y}_{\text{obs}}$ and GP model predictions $\mathbf{Y_m}$. The difference between the true response of the system $\mathbf{Y}_{\text{true}}$ and observations $\mathbf{Y}_{\text{obs}}$ is attributed to observation error ϵ_{obs}, which is often treated as a zero-mean Gaussian random variable with variance σ^2_{obs}.

Model 2 GP$^{\mathcal{L}_{\text{phy}}}$ incorporates the first strategy by enforcing physics constraints within the optimization of GP hyperparameters. More specifically, the physics constraints are incorporated into the maximization of the log marginal likelihood function (Eq. (8)) while inferring the hyperparameters of the GP model. Thus, the training of the second model is achieved by maximizing the following function:

$$\mathcal{L}_{\text{GP}} = \log\, p(\mathbf{Y}|\mathbf{X};\boldsymbol{\Theta}) - \lambda_{\text{phy}}\mathcal{L}_{\text{phy}}(\hat{\boldsymbol{Y}}), \tag{16}$$

Model 3, GP$^{\text{upd}}$, where the second PIML strategy is pursued, pre-trains a GP surrogate model with data generated from the physics model, then improves the surrogate using experimental data. Consider a physics model f^{phy} that maps input variables $\mathbf{X}$ and model parameters $\boldsymbol{\theta_m}$ to

the numerical model output $\mathbf{Y}_m$:

$$\mathbf{Y}_m = \mathbf{G}\big(\mathbf{X};\, \boldsymbol{\theta}_m(\mathbf{X})\big). \tag{17}$$

Let n_D be the number of collected observation data $\mathbf{Y}_{\text{obs}}$ from experiments with input variables $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(n_D)}$, where $\mathbf{x}^{(i)}$ are the input variables for the ith experiment. There exists uncertainty in the model prediction due to missing physics or approximations as discussed in Section 1. Thus, a model discrepancy term $\boldsymbol{\delta}(\mathbf{X})$ as a function of model inputs is introduced to capture the missing information between $\mathbf{Y}_{\text{true}}$ and $\mathbf{Y}_m$ [34]. Thus, the true system response can be described as

$$\mathbf{Y}_{\text{true}}(\mathbf{X}) = \mathbf{Y}_{\text{obs}}(\mathbf{X}) + \epsilon_{\text{obs}}(\mathbf{X}) = \mathbf{Y}_m(\mathbf{X}) + \boldsymbol{\delta}(\mathbf{X}) = \mathbf{G}\big(\mathbf{X};\, \boldsymbol{\theta}_m(\mathbf{X})\big) + \boldsymbol{\delta}(\mathbf{X}). \tag{18}$$

When the physics model $f^{\text{phy}}(\mathbf{X}) = \mathbf{Y}_m$ is computationally expensive, it is replaced by a cheaper surrogate model. In Model 3, a GP surrogate model $\text{GP}^{\text{phy}}(\mathbf{X}) = \hat{\mathbf{Y}}_m$ is used to approximate the physics-based simulation model. The accuracy of the surrogate model prediction depends on the quality and quantity of the training data generated by the original physics model. The surrogate model error (ϵ_δ) can be incorporated as follows:

$$\mathbf{Y}_m(\mathbf{X}) = \hat{\mathbf{Y}}_m(\mathbf{X}) + \epsilon_\delta. \tag{19}$$

A common approach to estimate the discrepancy term is the one formulated by Kennedy and O'Hagan [34], which is applicable in the context of Bayesian calibration. In that case, physics model parameters are sought to be calibrated, and a discrepancy term is added in the calibration equation. The discrepancy term can be expressed in multiple ways, such as constant, Gaussian random variable with unknown parameters (either input-dependent or not), or Gaussian process (either stationary or non-stationary) [35]. The hyperparameters of the discrepancy term are then estimated along with the physics model parameters using Bayesian calibration. However, the situation considered here is much simpler. There is no calibration of physics model parameters

here; only the discrepancy term is needed. (In other words, the physics model parameters are already established). In that case, the model discrepancy can be evaluated for different input values of experimental tests and realizations of observation errors as follows:

$$\overline{\boldsymbol{\delta}}(\mathbf{X}) = \mathbf{Y}_{\text{obs}}(\mathbf{X}) + \epsilon_{\text{obs}}(\mathbf{X}) - \hat{\mathbf{Y}}_m(\mathbf{X}). \tag{20}$$

where $\overline{\boldsymbol{\delta}}(\mathbf{X}) = \boldsymbol{\delta}(\mathbf{X}) + \epsilon_\delta$. In this work, a simplified approach is pursued by quantifying the overall model error instead of quantifying these error terms individually.

Following this, a GP model can be trained for the discrepancy term in terms of the inputs. Thus in model 3, two GP models are trained; (i) the first GP model ($\text{GP}^{\text{phy}}(\mathbf{X})$) replaces the physics model to predict the QoI; and (ii) the second GP model ($\text{GP}^{\text{exp}}(\mathbf{X})$) is constructed for the discrepancy term (i.e., the difference between the surrogate model prediction and real system) using experimental data.

The GP model for the model discrepancy ($\text{GP}^{\text{exp}}(\mathbf{X}) = \hat{\boldsymbol{\delta}}$) captures the combined contribution of measurement error, physics and surrogate model errors for a given prediction. Thus, the predictions of the first GP model (pre-trained) are corrected/updated with the second GP model representing the model discrepancy term and can be written as

$$\hat{\mathbf{Y}}_{corr}(\mathbf{x}) = \hat{\mathbf{Y}}_m(\mathbf{X}) + \hat{\boldsymbol{\delta}}. \tag{21}$$

Model 4 is a combination of the two strategies, in which both the pre-trained model is corrected with $\hat{\boldsymbol{\delta}}$ and physics constraints are enforced.

3.2.2. Implementation of PIML in DNN

In model 5, a DNN is trained using only experimental data. In order to train the model, an optimization algorithm is used to find a set of model parameters (weights and biases) that best map inputs to outputs. Model 6 extends model by implementing the first strategy: physical knowledge related to the physical process is enforced through constraints within the loss function of the DNN, $\text{DNN}^{\mathcal{L}_{\text{phy}}}$ as shown in Eq. 11. The physics-based loss functions are evaluated for

given physics inputs at every optimization iteration of $\text{DNN}^{\mathcal{L}_{\text{phy}}}$.

Model 7 pursues the second strategy: where a DNN model is pre-trained using the coupled multi-physics model input-output DNN^{phy} and then updated with experimental data. The pre-trained model, f^{pre}, is first trained with physics model input-output data consisting of input parameter combinations over a range of experimental values. Then, the weights and biases of the pre-trained network, which are chosen as initial points in the optimization, are updated for different combinations of the proposed strategies using experimental data. Note that here the model parameters are updated in a least squares sense, whereas in GP (in model 3 GP^{upd} and 4 $\text{GP}^{\text{upd},\mathcal{L}_{\text{phy}}}$) a discrepancy term is assumed and updated using the experimental data.

Model 8 is a combination of the two strategies for DNN, where the initialization of the model parameters are obtained using the physics model input-output DNN^{phy}. These model parameters are updated during the training phase by minimizing the regular training loss function shown in Eq. 13 together with the physics-based loss functions that are given in Eq. 25.

3.3. Bayesian neural network

The estimates of the neural network model parameters (neuron weights $\mathbf{w}$) have uncertainty, and this uncertainty depends on the available training data. When the network's parameters are represented using distributions (to reflect the epistemic uncertainty) instead of deterministic values, the model is referred to as a Bayesian neural network (BNN) [36–38]. In this Bayesian context, the model parameter uncertainty is first described using a prior distribution $p(\mathbf{w})$, and the likelihood function is $p(\mathbf{Y}|\mathbf{X},\mathbf{w})$. (A commonly used prior distribution is Gaussian, i.e., $p(\mathbf{w} = \mathcal{N}(0,\mathcal{I}))$). Following Bayes' theorem, a posterior distribution over the model parameters given the training set $\{\mathbf{X},\mathbf{Y}\} = \{\{\mathbf{x}_1,...,\mathbf{x}_N\},\{\{\mathbf{y}_1,...,\mathbf{y}_N\}\}$ is defined by

$$p(\mathbf{w}|\mathbf{X},\mathbf{Y}) = \frac{p(\mathbf{Y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{p(\mathbf{Y}|\mathbf{X})}. \tag{22}$$

The Bayesian inference of the model outputs for a new input $\mathbf{x}^*$ is given by the predictive

distribution as follows:

$$p(\mathbf{y}^*|\mathbf{x}^*, \mathbf{X}, \mathbf{Y}) = \int_{\Omega} p(\mathbf{y}^*|\mathbf{x}^*, \mathbf{w}) p(\mathbf{w}|\mathbf{X}, \mathbf{Y}) d\mathbf{w}. \tag{23}$$

The posterior distribution of model parameters $p(\mathbf{w}|\mathbf{X}, \mathbf{Y})$ is challenging to evaluate over the entire parameter space Ω due to the high dimensionality of Ω, and the highly non-linear behavior in the neural network caused by the non-linear activation functions and their combinations across multiple hidden layers.

Therefore, different approximate inference techniques can be considered to infer the posterior distribution $p(\mathbf{w}|\mathbf{X}, \mathbf{Y})$ [39–42]. One such approximation is variational inference, which fits a simple and tractable distribution $q_\theta(\mathbf{w})$ to the posterior, parametrized by a variational parameter θ [39]. This approximates the intractable problem by optimizing the parameters of $q_\theta(\mathbf{w})$. The closeness of the variational distribution is often measured by the Kullback-Leibler (KL) divergence between the approximate distribution $q_\theta(\mathbf{w})$ and the true model posterior $p(\mathbf{w}|\mathbf{X}, \mathbf{Y})$.

Dropout is a regularization approach which helps reducing interdependent learning amongst the neurons; thus prevents over-fitting. The term *dropout* refers to randomly dropping out neurons with a given dropout rate during the training phase in a neural network. A Monte Carlo (MC) dropout technique has been developed in recent years [43] which is equivalent to performing approximate variational inference. In MC dropout, dropout is not only applied while training a model but also during prediction. Randomly chosen neurons are temporarily removed from the network along with their connections. Next, the gradients of neurons weights are calculated on a sub-neural network for each training data and these gradients are then averaged over the training sets to obtain the weights of overall network. The optimization of Bayesian neural networks to find the optimal model parameters with the MC dropout is equivalent to using dropout (only during training) as regularization—modification made to the model in order to reduce its generalization error—on neural networks. However, in contrast to standard neural networks, the MC dropout performs dropout and generates random samples following a Bernoulli distribution for each neuron in the input and hidden layers during testing.

The neuron that takes the value 0 is dropped out with a given dropout probability p_d. The outputs of the network are predicted using the collection of generated random samples from the posterior predictive distribution and the uncertainty in the prediction of a new data is quantified with the trained network.

The MC dropout strategy provides an efficient way of Bayesian inference to quantify the model prediction uncertainty, and can be applied to a variety of neural networks, such as feed-forward neural networks, convolutional neural networks, and recurrent neural networks [44].

3.4. Sobol indices computation with model uncertainty

As discussed earlier, often in physics-based and data-driven models it is necessary to quantify the model uncertainty and its contribution to the Sobol index estimates. In this section, we present the inclusion of model uncertainty in the Sobol index estimates.

Every surrogate model has uncertainty in the prediction. In a noise free model, the GP predictions at the training points have zero variance and at any other points the variance is non-zero. The prediction at any point is given by a normal distribution with a mean and variance. The uncertainty inherent in these predictions can be captured by sampling, which can be then used in GSA. The model uncertainty pertaining to the GP model is propagated to the Sobol index estimations using the following estimator (see [8]):

$$S_{m,n}^{X_{d_1}} = \frac{V_{m,n}^{X_{d_1}}}{V_{m,n}} = \frac{\frac{1}{m}\sum_k^m Z_n(X_k)Z_n(\overline{X}_k) - \frac{1}{m}\sum_k^m Z_n(X_k)\sum_k^m Z_n(\overline{X}_k)}{\frac{1}{m}\sum_k^m Z_n(X_k)^2 - (\frac{1}{m}\sum_k^m Z_n(X_k))^2}, \tag{24}$$

where Z is the Gaussian process and $(X, \overline{X})$ are the random vectors.

The distribution of $S_{m,n}^{X_{d_1}}$ can be obtained as follows:

I WILL COMPLETER THIS ALGORITHM TOMORROW.

Algorithm 1: Estimation of the distribut

1. Build $Z_n(x)$

Result: Write here the result

initialization;

while *While condition* **do**

    instructions;

    if *condition* **then**

        instructions1;

        instructions2;

    else

        instructions3;

    end

end

A similar approach is implemented to the DNN models with the use of MC dropout (with a given dropout rate). However, in contrast to GP models, the samplings are different in DNN models. In DNN models, we randomly set units of the network to zero and generate posteriors using MC dropout. Whereas, we sample from a multivariate normal distribution in GP models to quantify the uncertainty in the Sobol index estimates with prediction intervals.

Two types of ML models were considered, namely, GP and DNN models, for GSA by effectively fusing physics knowledge and experimental data to maximize the accuracy and minimize the uncertainty of the sensitivity estimates. Eight different PIML models were developed by leveraging the two strategies described above. The effect of ML model uncertainty on the Sobol index estimates is quantified using the algorithm described above.

4. Numerical illustration

An additive manufacturing application is used to illustrate the proposed PIML models for GSA and compare their performance. A commercial material Ultimaker Black Acrylonitrile butadiene styrene (ABS) was extruded from an Ultimaker 2 Extended+ 3D printer to manu-

facture fused filament fabrication (FFF) parts with unidirectionally aligned filaments and then measured with appropriate diagnostic techniques. FFF is a widely used additive manufacturing (AM) process due to its easy operation, low cost and suitability for complex geometries. As the molten filament is deposited layer upon layer through a nozzle, it cools down, solidifies and bonds with the surrounding filaments. Rectangular ABS amorphous polymer specimens of length 35 mm, width 12 mm, and thickness 4.2 mm are manufactured with constant filament height, width and length (0.7, 0.8, and 35 mm, respectively).

The output quantity of interest is porosity of the printed part, and the inputs are two process parameters, namely nozzle temperature and speed. The porosity of an FFF part is dependent on the temperature history at the interfaces between filaments. Thus, it is important to predict the temperature evolution of filaments for estimating the final mesostructure of the printed part. The analytical solution proposed by Costa et al. [45] for transient heat transfer during the printing process in FFF is used to predict the temperature evolution of filaments. A physics-based sintering model is developed, which considers realistic filament geometry, and allows the filament geometry to change during the printing process. This model is used to predict the porosity of the FFF part using the temperature evolution of filaments, material properties, part geometry, and process parameters as inputs. Thus the mapping from input to output is a multi-physics model, i.e., models of two physical phenomena (heat transfer and sintering) are combined to predict the porosity given the extrusion temperature and extrusion speed.

The statistical properties of the QoI are observed to have negligible variability along the length of the specimens; thus the porosity measurements were taken at the midpoint of each part with the use of microscopy images processed through the ImageJ software [46]. Filaments were extruded through a nozzle with 0.8 mm diameter. The build plate temperature was constant and set to 110°C. Using Latin hypercube sampling, 39 sets of process parameters $\boldsymbol{X}$ were generated. The ranges considered for the two process variables were: printer extrusion temperature T: ($210°C$ - $260°C$), and extrusion speed S: (15 mm/s - 46 mm/s).

The basic ML models, namely Model 1 (for GP) and Model 5 (for DNN) are simply trained with the 39 sets of process inputs (temperature and speed) and output (porosity). In the training

of Model 2 $\text{GP}^{\mathcal{L}_{\text{phy}}}$ and Model 6 $\text{DNN}^{\mathcal{L}_{\text{phy}}}$, we impose two physics-based loss functions (i.e., two separate physics relationships, $\mathcal{L}_{\text{phy},k}(\hat{\boldsymbol{Y}})$, where $k = \{1, 2\}$ and $\hat{\boldsymbol{Y}}$ is the porosity prediction). The physical inconsistencies in the model predictions are evaluated using the physics-based loss functions defined as follows:

$$\mathcal{L}_{\text{phy},1}(\hat{\boldsymbol{Y}}) = \frac{1}{N}\sum_{i=1}^{N} \text{ReLU}(-\hat{Y}_{\text{i}}),$$
$$\mathcal{L}_{\text{phy},2}(\hat{\boldsymbol{Y}}) = \frac{1}{N}\sum_{i=1}^{N} \text{ReLU}(\hat{Y}_{\text{i}} - \phi_{0,\text{i}}), \tag{25}$$

where these loss functions consider the physical violations related to the porosity across N samples. In the first loss function, negative values of porosity are treated as physical violations. The second loss function penalizes the model when the predicted final porosity $\hat{Y}_i$ is greater than the initial porosity $\phi_{0,i}$ of ith part. This is based on the physics knowledge that the total void area decreases as the bond formation takes place. Thus, the porosity predictions are ensured to be physically meaningful with the inclusion of these physics-based penalty functions.

In Model 3 GP^{upd} and Model 7 DNN^{upd}, the ML models are pre-trained using the multi-physics model input-output. The pre-trained ML models are then updated using the experimental data. The training data for pre-training consists of 1310 input parameter combinations over a range of experimental values, i.e., ($210°C \leq T \leq 260°C$, 15 mm/s $\leq S \leq$ 46 mm/s). (Note that there are only 39 physical experiments are available; this is one of the advantages of this pre-training/updating strategy, where the pre-training can be over a much larger set of input combinations, thus improving the generalization performance of the updated model). The input data are normalized prior to the training of the ML models (the output quantity porosity is dimensionless and between 0 and 1),

Model 4 $\text{GP}^{\text{upd},\mathcal{L}_{\text{phy}}}$, which is a combination of the two strategies for DNN and uses the model parameters obtained through the physics model input-output as the initial values. Then, during the training of the updating phase these parameters are updated by minimizing the following loss function:

Following this, a GP model can be trained for the discrepancy term in terms of the inputs.

Thus in model 3, two GP models are trained; (i) the first GP model ($\text{GP}^{\text{phy}}(\mathbf{X})$) replaces the physics model to predict the QoI; and (ii) the second GP model ($\text{GP}^{\text{exp}}(\mathbf{X})$) is constructed for the discrepancy term (i.e., the difference between the surrogate model prediction and real system) using experimental data.

Model 4 is a combination of the two strategies for GP, in which two GP models are trained; (i) the first GP model ($\text{GP}^{\text{phy}}(\mathbf{X})$) trained using the physics model input-output samples; and (ii) the second GP model ($\text{GP}^{\text{exp}}(\mathbf{X})$) is built for the discrepancy term using the experimental data while maximizing the following function to optimize the hyperparameters of $\text{GP}^{\text{exp}}(\mathbf{X})$:

$$\mathcal{L}_{\overline{\text{GP}}} = \mathcal{L}_{\text{GP}} + \lambda_{\text{phy}}^{\text{GP}} \mathcal{L}_{\text{phy}}(\hat{\boldsymbol{Y}}). \tag{26}$$

Model 8 $\text{DNN}^{\text{upd},\mathcal{L}_{\text{phy}}}$, which is a combination of the two strategies for DNN, uses the model parameters obtained through the physics model input-output as the initial values. Then, during the training of the updating phase these parameters are updated by minimizing the following loss function:

$$\mathcal{L}_{\overline{\text{DNN}}} = \mathcal{L}_{\text{DNN}} + \lambda_{\text{phy}}^{\text{DNN}} \mathcal{L}_{\text{phy}}(\hat{\boldsymbol{Y}}). \tag{27}$$

The computational cost of different models for training and estimation of Sobol indices based on 5000 MC samples with a fixed number of experimental data ($n = 39$) is given in Table. 1. The time it takes for training and computation of Sobol indices using GP models 2-4 is significantly greater than model 1, i.e., 2-5 minutes. The difference becomes even greater when the number of observations increase. The reason for the difference between the training time of GP and GP^{upd} is the pre-training phase, where a large amount of physics input-output samples used. Whereas, the difference between the training time of GP and $\text{GP}^{\mathcal{L}_{\text{phy}}}$ due to the inclusion of physics constraints, which makes it harder for the optimization to find optimal hyperparameters. Whereas, the computation time for training of each DNN model is on average 15 sec using a desktop computer (Intel® Xeon® CPU E5-1660 v4@3.20GHz with 32 GB RAM and GPU NVIDIA Quadro K620 with 2 GB) and the Sobol index estimations based on 5000

samples take approximately 1-2 minutes for DNN models (models 5-8).

Table 1
Computational effort of eight models for training and estimation of first-order and total-effect Sobol indices using 5000 MC samples with $n = 39$ number of observations.

Models	Training time [in minutes]	Evaluation of the distribution of $S_{m,n}^{X_{d_1}}$ [in minutes]
GP	< 1	3
$\text{GP}^{\mathcal{L}_{\text{phy}}}$	2	5
GP^{upd}	3	7
$\text{GP}^{\text{upd},\mathcal{L}_{\text{phy}}}$	4	8
DNN	< 1	1
$\text{DNN}^{\mathcal{L}_{\text{phy}}}$	< 1	2
DNN^{upd}	< 1	2
$\text{DNN}^{\text{upd},\mathcal{L}_{\text{phy}}}$	1	2

4.1. GSA using GP models

The Sobol index computations with the GP models (1-4) are based on 5000 MC samples and 100 realizations of the Gaussian process. The hyperparameters of models 2 ($\text{GP}^{\mathcal{L}_{\text{phy}}}$) and 4 ($\text{GP}^{\text{upd},\mathcal{L}_{\text{phy}}}$) are assumed to be ($\lambda_{\text{phy}}^{\text{GP}} = 50, 50$). The standard deviation of the observation error is assumed to be 0.001.

The effect of number of observations in the first-order Sobol index estimates of temperature for the first four models are illustrated in Fig. **??**. The mean values of $S_{m,n}^{X_{d_1}}$ based on the GP model predictions are denoted with solid dots at given number of observations n. The 95% prediction intervals are represented with bars above and below the solid dots for the corresponding model.

The prediction intervals decrease as more number of experimental data used to train the models. Further, all four models converge to similar first-order and total-effect sensitivity estimates for both printer extrusion temperature and speed. The relative contribution of printer extrusion speed to the variability of the porosity (≈ 0.65) is greater than printer extrusion temperature (≈ 0.25).

4.2. GSA using DNN models

The four DNN models (Models 5 to 8) were implemented using the Keras package [47] with Tensorflow in the backend. The hyperparameters of models 6 ($\text{DNN}^{\mathcal{L}_{\text{phy}}}$) and 8 ($\text{DNN}^{\text{upd},\mathcal{L}_{\text{phy}}}$)

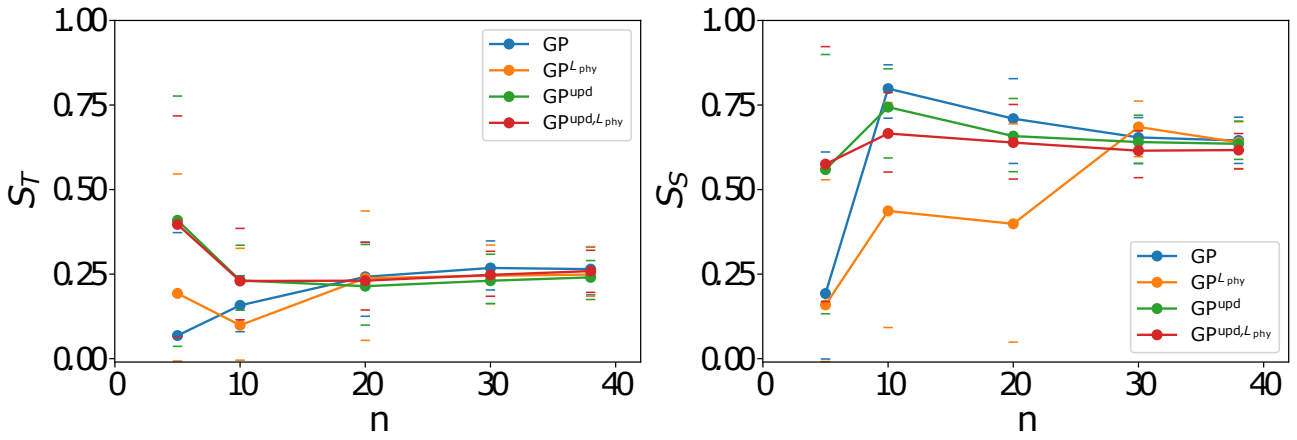

Fig. 3. First-order sensitivity index estimators for: (a) printer extrusion temperature, and (b) speed using GP models.

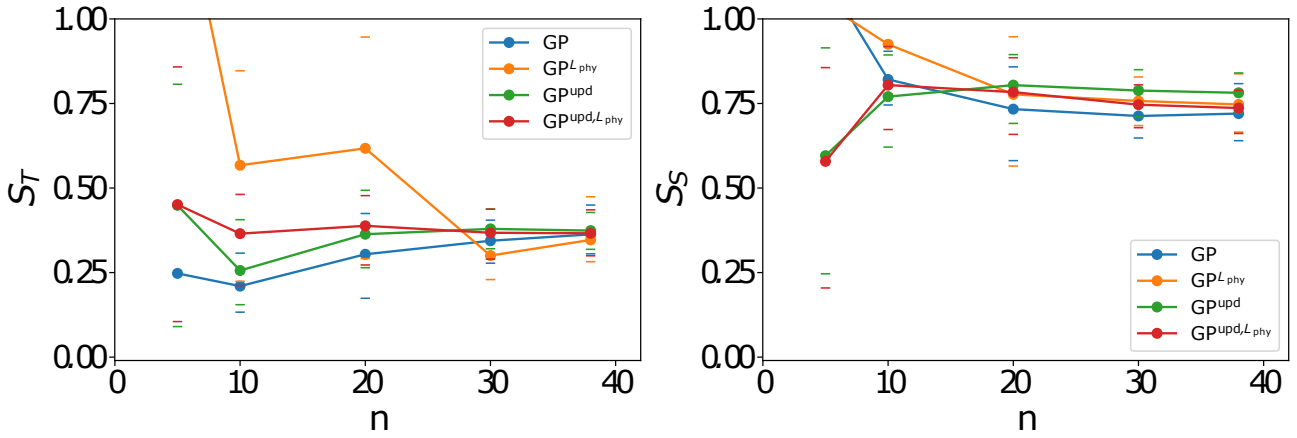

Fig. 4. Total-effect sensitivity index estimates for: (a) printer extrusion temperature, and (b) speed using GP models.

are tuned with grid search ($\lambda_{\text{phy}}^{\text{DNN}} = 0.15, 0.15$). Fully-connected DNN models with 2 hidden layers and 5 neurons in each hidden layer are constructed. The Rectified Linear Unit (ReLU) activation function and Adam optimizer are used to perform stochastic gradient descent in learning the model parameters.

4.2.1. GSA using DNN models without MC dropout

The DNN models without MC dropout maps deterministic inputs to a deterministic output. Therefore, unique Sobol index values are obtained. These unique values based on the DNN model predictions are represented with solid dots for different number of observations $n = 5, 10, 20, 30, 38$.

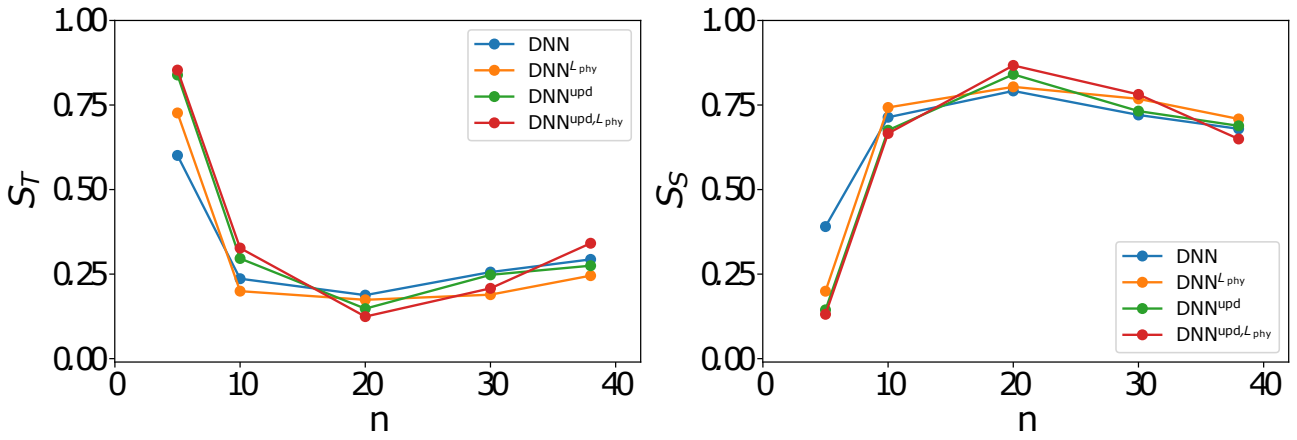

Fig. 5. First-order sensitivity index estimators for: (a) printer extrusion temperature, and (b) speed using DNN models.

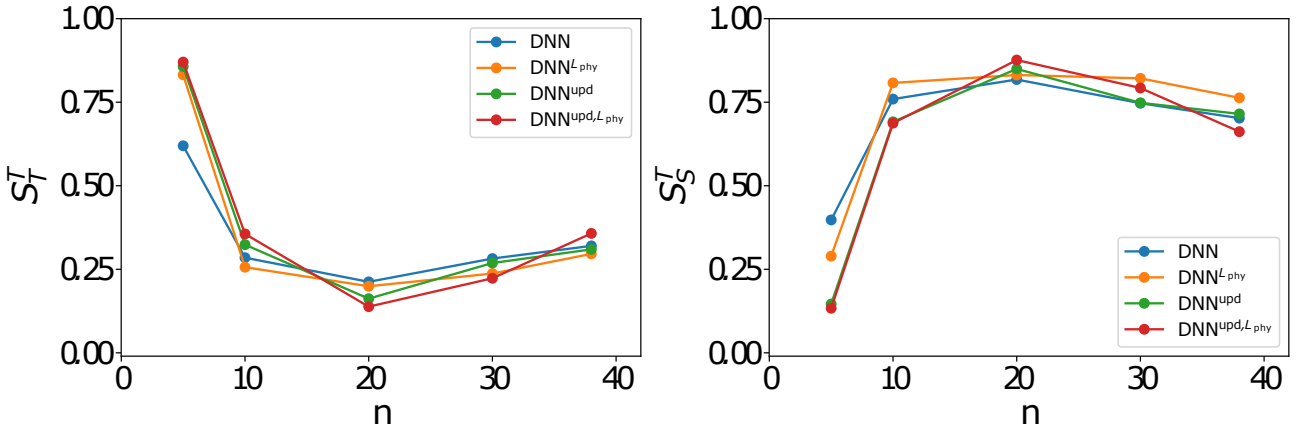

Fig. 6. Total-effect sensitivity index estimates for: (a) printer extrusion temperature, and (b) speed using DNN models.

All DNN models converge to similar first-order and total-effect sensitivity estimates for both input parameter and these values are consistent with the results obtained using GP models. The main difference between the results obtained using GP and DNN models is that the sensitivity estimates evaluated based on the DNN model predictions do not show a strong convergence, which may be because of the noisy data or the quality of the data.

4.2.2. GSA using DNN models with MC dropout

DNN models with MC dropout results in bounds for the sensitivity estimates as opposed to DNN models without MC dropout. The mean values of $S_{m,n}^{X_{d_1}}$ MC dropout predictions are represented with solid dots based on 100 stochastic forward passes through the networks for

different number of observations. The 95% prediction intervals are represented with bars above and below the solid dots for the corresponding model.

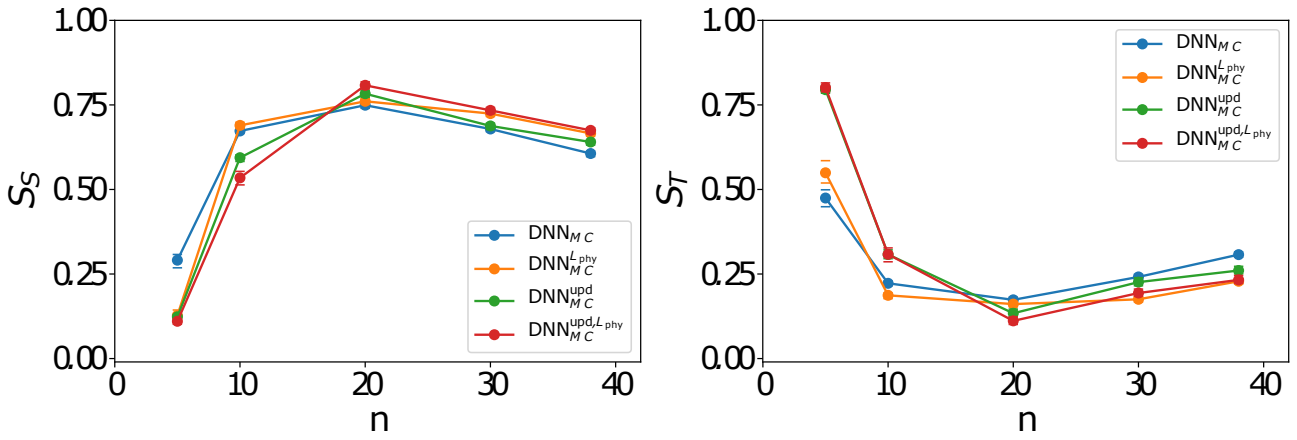

Fig. 7. First-order sensitivity index estimators for: (a) printer extrusion temperature, and (b) speed using DNN models with MC dropout.

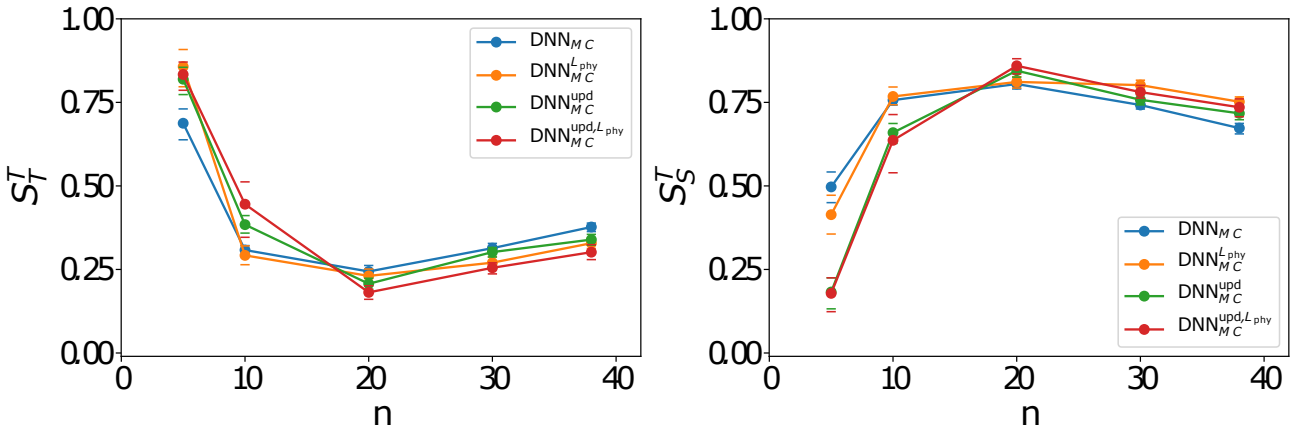

Fig. 8. Total-effect sensitivity index estimates for: (a) printer extrusion temperature, and (b) speed using DNN models with MC dropout.

The optimized dropout rate p_d used for the MC dropout simulations is 0.05. All four models converge to similar first-order and total-effect sensitivity estimates for both printer extrusion temperature and speed. The relative contribution of printer extrusion speed to the variability of the porosity (≈ 0.65) is greater than printer extrusion temperature (≈ 0.25). The MC dropout results converge to similar values obtained using the DNN models without MC dropout. Further, the prediction intervals decrease as more number of experimental data used to train the models and they are significantly smaller than the ones obtained using GP models.

The effect of dropout rate p_d for a fixed number of observations (n=38) in the first-order Sobol index estimates of DNN models using MC dropout is shown in Fig. 9. The total-effect Sobol index estimates of DNN models using MC dropout with different dropout rates for $n = 38$ is given in Fig. 10. The values of first-order and total-effect sensitivity index obtained using DNN models with MC dropout for printer extrusion temperature, and speed increase with increasing dropout rates except the range (0.0-0.025). These results show that the dropout rate is also needed to be optimized together with the other hyperparameters to be able to achieve accurate sensitivity estimates.

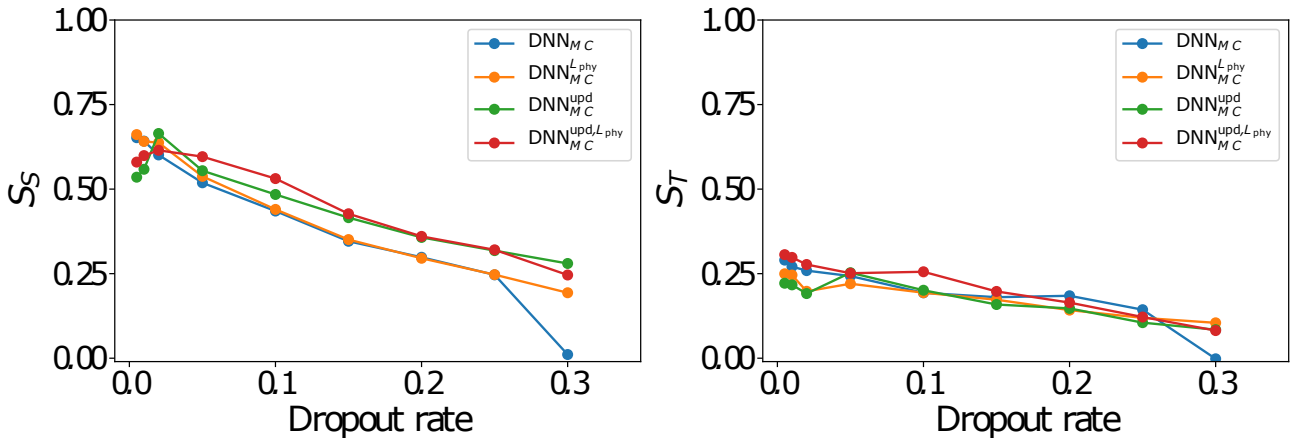

Fig. 9. First-order sensitivity index estimators for: (a) printer extrusion temperature, and (b) speed using DNN models with MC dropout.

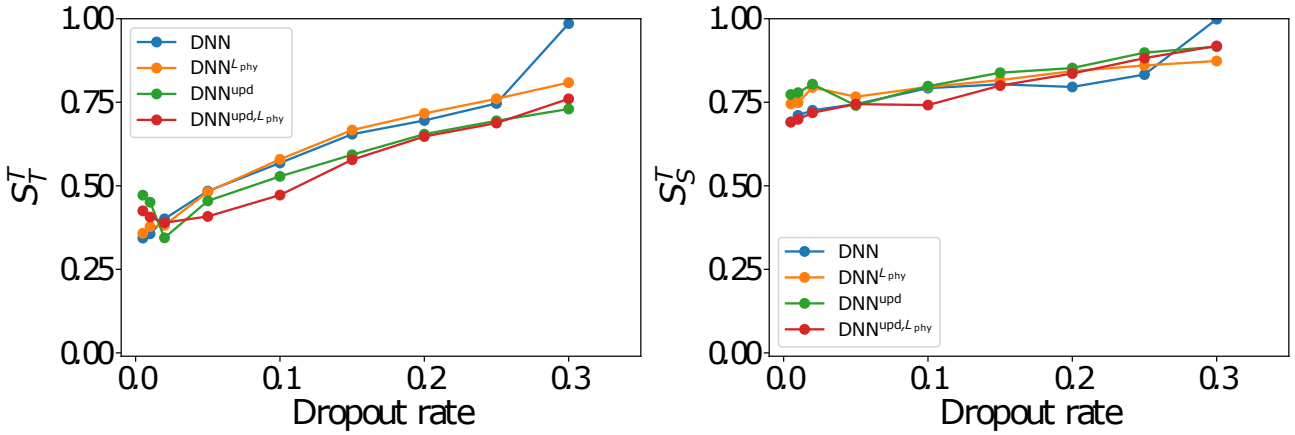

Fig. 10. Total-effect sensitivity index estimates for: (a) printer extrusion temperature, and (b) speed using DNN models with MC dropout.

5. Conclusion

In this paper, methodologies for information fusion and machine learning for sensitivity analysis using physics knowledge and experimental data while accounting for model uncertainty were developed. Variance-based sensitivity analysis is used to quantify the relative contribution of uncertainty source to the variability of the output quantity. Two types of ML models were considered, namely, GP and DNN models. Several PIML models were developed by leveraging two strategies for incorporating physics knowledge into ML models: (1) incorporating loss functions in the ML models to enforce physics constraints, and (2) pre-training an ML model with simulation data and then updating it with experimental data. The effect of ML model uncertainty on the sensitivity index estimate is analyzed, and the accuracy and computational of the various PIML models are compared.

The results show that the application of PIML strategies to both GP and DNN allows accurate Sobol index computations even with smaller amounts of experimental data while producing physically meaningful results. Thus, the proposed approach helps to fill the physics knowledge gap in the ML models while estimating the Sobol indices accurately by correcting for the approximation in the physics-based models. Numerical examples studied show that training the GP models for estimating the Sobol indices require more computational effort than the DNN models.

In future work, the proposed framework needs to be tested for problems with a larger number of dimensions both in the input and output, with multiple combinations to further analyze the convergence of Sobol index estimates for different PIML strategies. Future work can also explore the weighting of the two sources of data since the data produced by physics-based models and experiments have different levels of credibility.

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