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FIRST ORDER SOBOLE INDICES FOR PHYSICAL MODELS VIA INVERSE REGRESSION

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Résumé. Dans un contexte d’inversion Bayésienne de modèles physiques, on souhaite effectuer une analyse de sensibilité pour comprendre et ajuster le modèle. Pour ce faire, on introduit des indicateurs inspirés des indices de Sobol, mais visant le modèle inverse. Comme le modèle inverse n’a en général pas d’expression analytique, on propose d’utiliser un modèle paramétrique pour l’approximer. Les paramètres de ce modèle peuvent être estimés par un algorithme EM. On peut ensuite exploiter l’expression analytique de la postérieur par une intégration numérique de type Monte-Carlo, ce qui permet une estimation efficace de ces pseudo indices de Sobol.

Mots-clés. Analyse de sensibilité, indices de Sobol, problème inverse, régression, apprentissage statistique

Abstract. In a bayesian inverse problem context, we aim at performing sensitivity analysis to help understand and adjust the physical model. To do so, we introduce indicators inspired by Sobol indices but focused on the inverse model. Since this inverse model is not generally available in closed form, we propose to use a parametric surrogate model to approximate it. The parameters of this model may be estimated via standard EM inference. Then we can exploit its tractable form and perform Monte-Carlo integration to efficiently estimate these pseudo Sobol indices.

Keywords. Sensitivity analysis, Sobol indices, inverse problem, regression, statistical learning

1 Introduction

A wide class of problems from medical imaging [Mesejo et al., 2016, Lemasson et al., 2016, Nataraj et al., 2018] to astrophysics [Deleforge et al., 2015, Schmidt and Fernando, 2015] can be formulated as inverse problems [Tarantola, 2005, Giovannelli and Idier, 2015]. An inverse problem refers to a situation where one aims at determining the causes of a phenomenon from experimental observations of its effects. Such a resolution generally starts by the so-called *direct or forward* modelling of the phenomenon. It theoretically

describes how input parameters \mathbf{x} are translated into effects \mathbf{y} . Then from experimental observations of these effects, the goal is to estimate the parameters values that best explain the observed measures.

Typical features or constraints that can occur in practice are that 1) both direct and inverse relationships are (highly) non-linear, *e.g.* the direct model is available but is a (complex) series of ordinary differential equations as in [Mesejo et al., 2016, Hovorka et al., 2004]; 2) the observations \mathbf{y} are high-dimensional because they represent signals in time or spectra, as in [Schmidt and Fernando, 2015, Bernard-Michel et al., 2009, Ma et al., 2013]; 3) many such high-dimensional observations are available and the application requires a very large number of inversions, *e.g.* [Deleforge et al., 2015, Lemasson et al., 2016]; 4) the vector of parameters \mathbf{x} to be predicted is itself multi-dimensional with correlated dimensions so that predicting its components independently is sub-optimal, *e.g.* when there are known constraints such as their sum is one like for concentrations or probabilities, [Deleforge et al., 2015, Bernard-Michel et al., 2009].

A common issue when dealing with inverse problems is to be sure that the problem is well defined. In this regard some natural questions arise. Is the direct model one-to-one? And if it's the case, are the output sensitive enough to the parameters? If not, small noise in the observations may lead to high errors in predictions (high variance in probabilistic settings), making the model barely usable in practice. To answer these questions, one may use Sensitivity Analysis, which aims at providing qualitative or quantitative indicators on the variation of the output \mathbf{y} with respect to the input \mathbf{x} . Sensitivity analysis may be useful on its own, to gain inner knowledge on the forward model. Besides, sensitivity analysis of the inverse model (variation of the output \mathbf{x} with respect to \mathbf{y}) can help choosing the measurements to perform for an optimal determination of the model parameters.

Among various methods, we focus in this paper on Sobol sensitivity analysis, applied to an inverse problem setup. We aim at computing what we call pseudo Sobol indices for the inverse model. We propose to use a surrogate model, estimated via a regression approach and exploited via numerical integration.

2 Sobol indices for an inverse problem

We start by specifying the notations for our inverse problem, before introducing the so-called Gaussian Locally-Linear Mapping model (GLLiM) ([Deleforge et al., 2015]) as a surrogate model, and proposing an efficient way to estimate inverse Sobol indices.

2.1 Context

The parameters and observations are assumed to be random variables $\mathbf{X} \in \mathbb{R}^L$ and $\mathbf{Y} \in \mathbb{R}^D$ of dimension L and D respectively where D is usually much greater than L . The forward model is then described by a likelihood function linking parameters values \mathbf{x} to

the probability of observing some \mathbf{y} and denoted by $\mathcal{L}_{\mathbf{x}}(\mathbf{y}) = p(\mathbf{y} | \mathbf{X} = \mathbf{x})$. We will further assume that the relationship between \mathbf{x} and \mathbf{y} is described by a known function F and that the uncertainties on the theoretical model are independent on the input parameter \mathbf{x} . In other words,

$$\mathbf{Y} = F(\mathbf{X}) + \epsilon \quad (1)$$

where ϵ is a random variable. For instance ϵ can be assumed to be a centered Gaussian variable with covariance matrix Σ , so that $\mathcal{L}_{\mathbf{x}}(\mathbf{y}) = \mathcal{N}(\mathbf{y}; F(\mathbf{x}), \Sigma)$, where $\mathcal{N}(\cdot; F(\mathbf{x}), \Sigma)$ denotes the Gaussian pdf with mean $F(\mathbf{x})$ and covariance Σ . We denote the prior density on \mathbf{X} by $p(\mathbf{x})$.

Sensitivity analysis often deals with the forward model. Thus, first order Sobol indices are defined as

$$S_{l,d} = \frac{\text{Var}[\mathbb{E}[Y_d|X_l]]}{\text{Var}[Y_d]} \quad (2)$$

As we will show later on, our approach also yields estimation of Sobol indices for F . However, we mainly propose in this paper to study the sensitivity of the inverse model. It's challenging because it requires the expression of F^{-1} which is not available. Reversing the role of X and Y , we propose to define the inverse Sobol indices as

$$S_{d,l}^* = \frac{\text{Var}[\mathbb{E}[X_l|Y_d]]}{\text{Var}[X_l]} \quad (3)$$

We propose in the next section a model which enables the computation of S^* by exploiting an explicit density.

2.2 Surrogate model

We propose to use a learning approach. We approximate (\mathbf{X}, \mathbf{Y}) by a Gaussian Locally-Linear Mapping model (GLLiM) which builds upon Gaussian Mixture Models to approximate non linear functions ([Deleforge et al., 2015]). This is modeled by introducing a latent variable $Z \in \{1, \dots, K\}$ such that

$$\mathbf{Y} = \sum_{k=1}^K \mathbb{I}_{Z=k} (\mathbf{A}_k \mathbf{X} + \mathbf{b}_k + \epsilon_k) \quad (4)$$

where \mathbb{I} is the indicator function, \mathbf{A}_k a $D \times L$ matrix and \mathbf{b}_k a vector of \mathbb{R}^D that define an affine transformation. Variable ϵ_k corresponds to an error term which is assumed to be zero-mean and not correlated with \mathbf{X} capturing both the observation noise and the reconstruction error due to the affine approximation.

In order to keep the posterior tractable, we assume that $\epsilon_k \sim \mathcal{N}(\mathbf{0}, \Sigma_k)$ and \mathbf{X} is a mixture of K Gaussians : $p(\mathbf{x}|Z = k) = \mathcal{N}(\mathbf{x}; \mathbf{c}_k, \Gamma_k)$ and $p(Z = k) = \pi_k$. The GLLiM model is thus characterized by the parameters $\theta = \{\pi_k, \mathbf{c}_k, \Gamma_k, \mathbf{A}_k, \mathbf{b}_k, \Sigma_k\}_{k=1:K}$

This model can be learned against a training set, sampled along the prior on \mathbf{X} and the likelihood defined in (1), via an EM algorithm. More specifically, we sample a dictionary $(\mathbf{x}_n, \mathbf{y}_n)_{n=1..N}$ where \mathbf{x}_n are realizations of the prior $p(\mathbf{x})$ and $\mathbf{y}_n = F(\mathbf{x}_n) + \epsilon_n$. We then run the EM algorithm on $(\mathbf{x}_n, \mathbf{y}_n)_{n=1..N}$ to estimate $\boldsymbol{\theta}$ and use the resulting GLLiM distribution denoted by p_G (and depending on $\boldsymbol{\theta}$) as a surrogate model for the pdf of (\mathbf{X}, \mathbf{Y})

2.3 Sobol indices for the GLLiM model

We have shifted the computation of Sobol indices from the real model to an approximated one, and in this section (\mathbf{X}, \mathbf{Y}) will thus denote random variables following the GLLiM distribution. The purpose is to exploit the tractable density p_G given by the GLLiM model. Indeed, from p_G , the conditional distribution is available in closed form :

$$p_G(\mathbf{x}|\mathbf{Y} = \mathbf{y}, \boldsymbol{\theta}) = \sum_{k=1}^K w_k^*(\mathbf{y}) \mathcal{N}(\mathbf{x}; \mathbf{A}_k^* \mathbf{y} + \mathbf{b}_k^*, \boldsymbol{\Sigma}_k^*) \quad (5)$$

$$\text{with } w_k^*(\mathbf{y}) = \frac{\pi_k \mathcal{N}(\mathbf{y}; \mathbf{c}_k^*, \boldsymbol{\Gamma}_k^*)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{y}; \mathbf{c}_j^*, \boldsymbol{\Gamma}_j^*)}$$

A new parametrization $\boldsymbol{\theta}^* = \{\mathbf{c}_k^*, \boldsymbol{\Gamma}_k^*, \mathbf{A}_k^*, \mathbf{b}_k^*, \boldsymbol{\Sigma}_k^*\}_{k=1:K}$ is used to illustrate the similarity between the two conditional distributions. The parameters $\boldsymbol{\theta}^*$ are easily deduced from $\boldsymbol{\theta}$ as follows:

$$\begin{aligned} \mathbf{c}_k^* &= \mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k \\ \boldsymbol{\Gamma}_k^* &= \boldsymbol{\Sigma}_k + \mathbf{A}_k \boldsymbol{\Gamma}_k \mathbf{A}_k^\top \\ \boldsymbol{\Sigma}_k^* &= (\boldsymbol{\Gamma}_k^{-1} + \mathbf{A}_k^\top \boldsymbol{\Sigma}_k^{-1} \mathbf{A}_k)^{-1} \\ \mathbf{A}_k^* &= \boldsymbol{\Sigma}_k^* \mathbf{A}_k^\top \boldsymbol{\Sigma}_k^{-1} \\ \mathbf{b}_k^* &= \boldsymbol{\Sigma}_k^* (\boldsymbol{\Gamma}_k^{-1} \mathbf{c}_k - \mathbf{A}_k^\top \boldsymbol{\Sigma}_k^{-1} \mathbf{b}_k) \end{aligned} \quad (6)$$

To compute $\mathbb{E}[X_l|Y_d]$ as required in (3), we observe that (\mathbf{X}, Y_d) still follows a GLLiM distribution, with $D = 1$ and

$$\begin{aligned} \mathbf{A}_k^{(d)} &:= \mathbf{A}_k[d, :] && \text{(row } d) \\ \mathbf{b}_k^{(d)} &:= \mathbf{b}_k[d] && \text{(coefficient } d) \\ \boldsymbol{\Sigma}_k^{(d)} &:= \boldsymbol{\Sigma}_k[d, d] && \text{(coefficient in row and column } d) \end{aligned} \quad (7)$$

Since (5) is a Gaussian mixture, $\mathbb{E}[X_l|Y_d = y_d]$ is easy to compute from (5), with $\boldsymbol{\theta}$ adjusted as in (7) :

$$f_d(y_d) := \mathbb{E}[X_l|Y_d = y_d] = \sum_{k=1}^K w_k^*(y_d) (\mathbf{A}_k^* y_d + \mathbf{b}_k^*) \quad (8)$$

Unfortunately, the variance of $f_d(Y_d)$ is not straightforward. Thus, we propose to compute it via Monte-Carlo integration. It can be shown that \mathbf{Y} follows a Gaussian mixture model, with parameters $(\pi_k, \mathbf{c}_k^*, \mathbf{\Gamma}_k^*)_{k=1..K} : p_G(\mathbf{y}|\boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{y}; \mathbf{c}_k^*, \mathbf{\Gamma}_k^*)$, from which we can efficiently produce samples.

Finally, since \mathbf{X} is also a mixture of Gaussian distributions, its variance has a closed form :

$$Cov(\mathbf{X}) = \sum_{k=1}^K \pi_k [\mathbf{\Gamma}_k + \mathbf{c}_k \mathbf{c}_k^\top] - \left(\sum_{k=1}^K \pi_k \mathbf{c}_k \right) \left(\sum_{k=1}^K \pi_k \mathbf{c}_k \right)^\top$$

To sum up, given a GLLiM model characterized by $\boldsymbol{\theta}$, we propose to compute the Sobol indices of the inverse problem $S_{d,l}^*$ by sampling $(y_d^{(n)})_{n=1..N}$ according to its mixture of Gaussian distributions and estimating $v_d := Var(f_d(Y_d))$ with Monte-Carlo integration using samples $(y_d^{(n)})_{n=1..N}$. The index $S_{d,l}^*$ can be then computed by

$$S_{d,l}^* = \frac{v_d}{Cov(\mathbf{X})_{l,l}}$$

3 Illustration on a photometric model

We apply the proposed approach to the Hapke's model, a highly-non linear model used in remote sensing. It is a semi-empirical photometric model that relates physically meaningful parameters to the reflectivity of a granular material for a given geometry of illumination and viewing. A geometry denoted by G is described by three angles (θ_0, θ, ϕ) . Thus, our forward model takes the form $F(\mathbf{x}) = (f_{hapke, G_1}(\mathbf{x}), \dots, f_{hapke, G_D}(\mathbf{x}))$ where D is the number of geometries, and $\mathbf{x} = (\omega, \bar{\theta}, b, c)$ are the physical parameters. The exact expression of f_{hapke} may be found for example in [Schmidt and Fernando, 2015]. The figure 1 plots the inverse Sobol indices for the three parameters $(\omega, \bar{\theta}, c)$, with respect to the geometries.

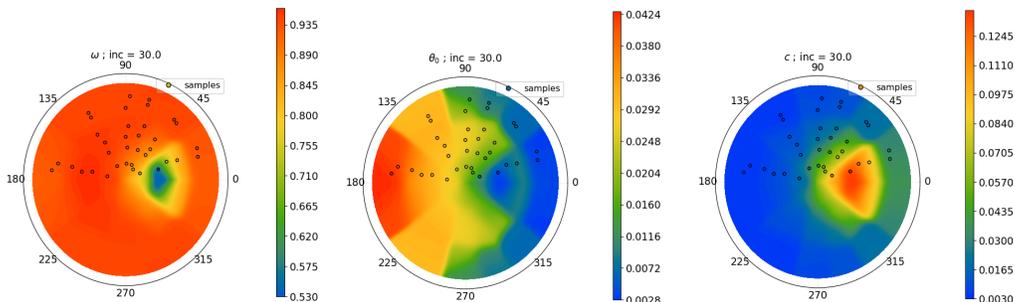


Figure 1: $D = 36$ geometries, with fixed incidence $\theta_0 = 30^\circ$. Radial coordinate is θ , polar angular coordinate is ϕ .

4 Conclusion

We proposed an efficient computation of sensitivity indicators inspired by Sobol indices using a surrogate model. We focused on the Sobol indices for inverse models. Regarding forward models, a surrogate model is not usually needed as the forward model is often available in closed form. Still, our approach also yields direct Sobol indices, by reversing the role of \mathbf{X} and \mathbf{Y} . It could be used in a setup where only a dictionary of samples (\mathbf{x}, \mathbf{y}) is available, and not the functional model F .

So far, we have implicitly assumed that \mathbf{Y} components were independent, which is a common assumption when using Sobol indices. If it is wrong, Sobol indices are still well defined, but the property of variance decomposition does not hold anymore. Studies on sensitivity analysis in the dependent case suggest to use generalized Sobol indices, which take into account the dependency between components. For instance, a future work could be to apply the methodology proposed in [Chastaing et al., 2014].

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