I-optimal sequential design for Bayesian inverse problems with Gaussian process surrogate models

P. Lartaud[†,1,2], P. Humbert[2], J. Garnier[1],

PhD expected duration: Oct. 2021 – Sep. 2024

[1] CMAP, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France
{paul.lartaud,josselin.garnier}@polytechnique.edu

[2] CEA DAM-DIF, Bruyères-le-Châtel 91297 Arpajon, France
philippe.humbert@cea.fr

Abstract

In the context of nuclear safeguards and security, passive neutron correlation measurements can be used to identify an unknown fissile matter [2]. This approach has been widely used and documented but the focus on the uncertainty quantification is more recent. The common approach is to solve an inverse problem with a Bayesian approach, while building a surrogate model to overcome the computational burden of the true direct model [3]. The training data for the surrogate can be obtained using state-of-the-art neutronic Monte-Carlo codes, but the limited computational budget restricts the number of data points that can be obtained. As a consequence, a large portion of the uncertainties in the inverse problem may reside in the lack of knowledge of the surrogate itself. Hence the problem at stake: given some observations of an inverse problem, how can we refine the surrogate model in the region of interest by feeding it with well-chosen design points ? To answer this question, we developed an I-optimal stepwise uncertainty reduction (ISUR) strategy for the sequential design of computer experiments in the context of Bayesian inverse problems with Gaussian process surrogate models. This method is based on the Stepwise Uncertainty Reduction (SUR) paradigm introduced in [1] and [4]. Let $\mathbb{M}$ be the space of Gaussian measures on an appropriate functional space. We consider an inverse problem with noisy observations $\mathbf{y} \in \mathbb{R}^N$ and we are trying to identify the posterior distribution $p(x|\mathbf{y})$ for some parameters $x \in \mathcal{X} \subset \mathbb{R}^p$. The newly proposed method is derived from I-optimal designs with a metric of uncertainty given by the function $\mathcal{H} \colon \mathbb{M} \to [0, +\infty)$ where the functional is defined for $\nu \in \mathbb{M}$ by:

$$\mathcal{H}(\nu) = \mathbb{E}_{p_\nu}\left[k_\nu(\tilde{x}, \tilde{x})\right] = \int_{\mathcal{X}} k_\nu(\tilde{x}, \tilde{x}) p_\nu(\tilde{x}|\mathbf{y}) d\tilde{x} \tag{1}$$

where $k_\nu(\tilde{x}, \tilde{x})$ is the predictive variance on $\tilde{x}$ of the GP associated with the measure ν and $p_\nu(\tilde{x}|\mathbf{y})$ is the posterior distribution obtained from noisy observations $\mathbf{y}$ and using the GP surrogate model as a direct model.
This metric can be understood as the integrated predictive variance of the GP surrogate over the posterior distribution of the inverse problem. We show that the ISUR criteria for this particular metric can be derived analytically and we verify the supermartingale property and the almost-sure convergence of the metric towards 0. The results can also be extended to a multi-dimensional framework in which $\mathbf{y} \in \mathbb{R}^{N \times d}$. Finally we also introduced a simpler D-optimal design strategy and compare the two methods with a naive design on a number of test cases.

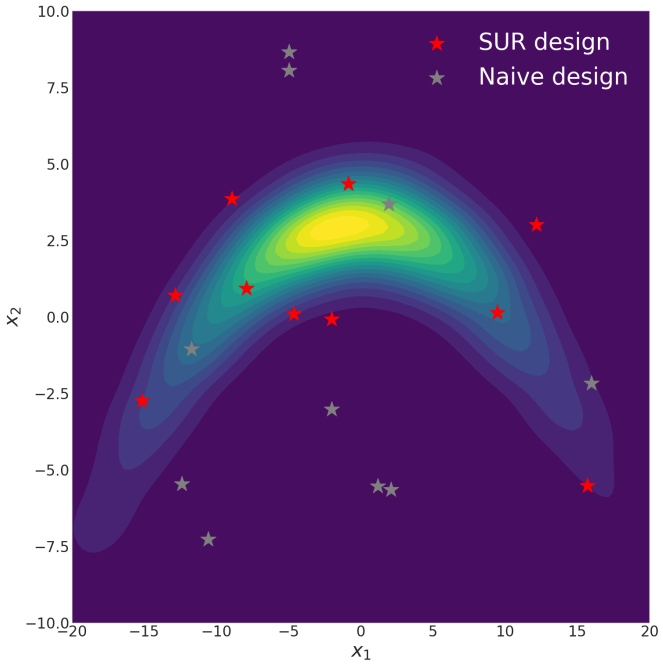

Figure 1: New design points with naive (grey) and ISUR (red) strategies on an analytical inverse problem test case with a banana-shaped posterior distribution

Short biography (PhD student)

I am a third-year PhD student working at CEA DAM Île-de-France and École polytechnique under the supervision of Josselin Garnier. This work is funded by the CEA and aims at providing robust uncertainty quantification methods for the identification of nuclear materials using passive neutron correlation measurements.

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