Uncertainty Quantification for data-limited Inverse Problems via efficient probabilistic ML methods

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In many applications, quantities of interest cannot be observed directly because they lie, for example, in the past, are too far away from the observer, or their observation would require disproportionate effort. Instead, these quantities are usually determined by measuring other quantities that are easier to observe and whose functional relationship with the actual quantity of interest is known. Mathematically speaking, we aim for the inversion of the function which maps the quantity of interest onto the observable quantity leading to the term *inverse problem* [1, 2]. Such problems are often found in medical imaging, where one is interested in the internal structure of a patients' body, but the patient should not simply be cut open. Alternatively, one observes the interaction of radiation with the tissue. The knowledge on how different types of tissue interact with radiation can be utilized to reconstruct the patient's inner structure [3, 4].

Reconstructing a quantity of interest from an observable is often challenging since even if a functional relationship between both quantities is available, perturbations might lead to the inverse problem being ill-posed. With the increase of computational power, various techniques have been developed to solve inverse problems, most of which rely on regularization theory [5]. Using regularization, one can overcome the ill-posedness of the inverse problem and obtain a reconstruction of the quantity of interest. Nevertheless, this approach somewhat neglects the ill-posed nature of the inverse problem. Aiming for a single solution of the inverse problem is often misleading since there might not even exist a (unique) solution. As an alternative, Bayesian inversion theory has been developed which reformulates the inverse problem as follows. Instead of asking what value the quantity has taken, Bayesian inversion theory asks what is the probability that the quantity has taken on a particular value. This approach extends the solution concept of an inverse problem with the goal of finding a probability distribution instead of a single reconstruction.

The main advantage of Bayesian inversion is the possibility to calculate different point estimates and perform uncertainty quantification for them. Given the ill-posed nature of an inverse problem, being able to quantify the credibility of the estimate is essential [6]. Thus, we are not only interested in calculating point estimates but always consider the combination of both the point estimate and the corresponding confidence.

In our work, we deal with inverse problems related to the diffusion equation, i.e. an elliptic partial differential equation (PDE) which models a diffusion process in a heterogeneous medium. In particular, we are interested in the reconstruction of the underlying diffusivity field encoding the structural information of the medium by observing only the solution of the PDE. We consider piece-wise constant diffusivity fields which model inclusions in the medium in which the diffusion process takes place, which has numerous applications e.g. in medical imaging or geology [7, 8, 9].

One of the main challenges in PDE-driven Bayesian inversion is to overcome the high computational effort associated with the inversion process which involves solving the PDE possibly hundreds of thousands of times. We employ a deep learning approach which allows us to solve the elliptic PDE significantly faster than by using traditional solvers. In particular, we make use of a *Deep Operator Network* recently proposed in [10] which has already been used to learn the solution operator to various PDEs [11, 12]. We show that our deep neural network approximates the solution operator of the elliptic PDE in some operator norm and present numerical results illustrating the computational benefit that can be achieved by our method.

References

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