PhD Topic / Bayesian Inverse Problems for Wave Propagation towards Exascale

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Contexte et atouts du Poste

Context In the framework of the ExaMA project within the NumPEx program (`https://numpex.irisa.fr/`), we propose a PhD thesis on the topic of *Ensemble and Machine Learning Methods for Bayesian Inverse Problems.* The objective of NumPEx is to develop an exascale software stack, and the ExaMA project is dedicated to the mathematical algorithms to achieve this. The Inria MAKUTU project specilalizes in inverse problems for wave propagation problems and the theoretical and numerical methods needed for their solution.

Mission Confiée

Project Goals In an inverse problem, we seek the (unknown) model parameters from (known) measurements of the system's solution. The direct system—in our case a partial differential equation with its boundary and initial conditions—can be considered as an operator from parameter space into data/observation space. The inverse problem, from data space into parameter space, is ill-posed [1, 2]. The deterministic approach for solving the inverse problem consists of minimizing a cost function that expresses the error, or mismatch, between the model predictions and the measured observations, or data. We usually add a regularization term (Tikhonov approach) to penalize solutions that are too oscillatory. This nonlinear minimization is usually performed by a method from the quasi-Newton family [3].

Bayes' Theorem provides a framework for the solution of a more general inverse problem, where we seek the posterior probability distribution of a function, given prior knowledge of its distribution and measurements of an observed quantity that depends on the unknown, or hidden function. Mathematically, the theorem quantifies a posterior probability distribution (ppd) as a function of an *a priori* distribution that captures any previous knowledge about the parameters, and a likelihood function that is obtained by solving the direct model for given parameter values. The resulting *a posteriori* law is both the solution of the inverse problem and provides a complete quantification of the uncertainty in this solution. The posterior distribution is usually simulated using Markov Chain Monte Carlo (MCMC) methods [2, 4], though in this project we will employ

- ensemble Kalman filters,
- machine learning.

Principales Activités

Research Tasks In this thesis, we want to study, both theoretically and numerically, the solution of inverse problems for wave propagation. A simple case is described by the acoustic wave equation, in a bounded domain, with varying sound speed function over the domain. This case can by easily generalized to more realistic wave propagation problems, including elastic and anisotropic effects.

1. Based on [5], formulate the Bayesian inverse problem (BIP) for the wave equation.
2. Give all details of the existence, and convergence properites of the BIP solution.
3. Propose a MCMC method [2, 4] for solving the BIP.

An alternative approach for solving the BIP, is to use an ensemble Kalman filter (EnKF) [1, 2]. This method is known as ensemble Kalman inversion, and was first formulated in [6].

4. Based on [6], formulate the EKI approach for the wave equation.
5. Give all details of the existence, and convergence properites of the EKI solution.
6. Propose a EnKF method [2] for solving the EKI problem.

In a second phase, we will consider machine learning based surrogates that can be used to replace the very costly evaluation of the direct propagation model, especially in 3D space. The machine learning model will be based on a PINN approach [7].

Both MCMC and EKI are methods that can be readily parallelized. This is the ultimate goal of the ExaMA project: to develop a highly parallelized library for the soution of inverse problems in wave propagation. In a final phase, we will then consider scaling up to very large inverse problems on Exascale-ready computing platforms. For this we will generalize the MELISSA-DA framework [8] to the solution of a wide class of inverse problems for wave propagation. This part of the thesis will be done in close collaboration with the DataMove INRIA team `https://www.inria.fr/en/datamove`.

References

[1] M. Asch, M. Bocquet, M. Nodet. *Data Assimilation: Methods, Algorithms and Applications.* SIAM. 2016.

[2] M. Asch. *A Toolbox for Digital Twins: from Model-Based to Data-Driven.* SIAM. 2022.

[3] J. Nocedal, S. Wright. *Numerical Optimization.* Springer. 2006.

[4] A. Gelman, J. Carlin, H. Stern, D. Dunson, A. Vehtari, D. Rubin. *Bayesian Data Analysis*, 3rd edition. CRC Press, 2014.

[5] A. Stuart. (2010). Inverse problems: A Bayesian perspective. *Acta Numerica*, **19**, 451-559. `doi:10.1017/S0962492910000061`.

[6] M. A. Iglesias, K. J. H. Law and A. M. Stuart. Ensemble Kalman methods for inverse problems. *Inverse Problems* 29 (2013).

[7] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. *Journal of Computational Physics*, Volume 378, 1 February 2019, Pages 686-707. `https://doi.org/10.1016/j.jcp.2018.10.045`

[8] Friedemann S, Raffin B. An elastic framework for ensemble-based large-scale data assimilation. *The International Journal of High Performance Computing Applications.* 2022;36(4):543-563. doi:10.1177/10943420221110507

Compétences

Skills The candidate should have strong skills in applied mathematics for partial differential equations as well as knowledge of probability and stochastic differential equations. The thesis also requires numerical skills and coding experience to solve the underlying partial differential equations and to implement the stochastic simulation methods. Basic knowledge of machine learning will be appreciated. The candidate should be at ease in English, including reading, understanding and communication.

The thesis will be co-supervised by Prof. Mark Asch, who has a long experience in data assimilation and inverse problems.

Avantages

- Restauration subventionnée / Subsidized meals
- Transports publics remboursés partiellement / Partial refund of public transport

- Équipements professionnels à disposition (visioconférence, prêts de matériels informatiques, etc.) / Professional equipment available (videoconference, computers, etc.)

Informations Générales

- Thème/Domaine : Schémas et simulations numériques Calcul Scientifique (BAP E)
- Ville : Pau
- Centre Inria : Centre Inria de l'université de Bordeaux
- Date de prise de fonction souhaitée :2024-10-01
- Durée de contrat : 3 ans
- Date limite pour postuler : 2024-06-31

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