PhD offer

Efficient methods for spatio-temporal models estimation

Research units :

— Geostatistics team, Centre for Geosciences, Mines Paris, PSL

— MIA Paris Saclay, AgroParisTech/INRAE, Université Paris-Saclay

Supervisors : Lucia Clarotto (AgroParisTech), Nicolas Desassis and Thomas Romary (Mines Paris)
Duration : 3 years (starting autumn 2025)
Profile : The candidate should have a Master's degree in engineering, applied mathematics, computer science, statistics or data science, with courses in deep learning and/or spatial statistics. Proficient scientific programming skills in Python are required, especially with Deep Learning frameworks (Pytorch, Tensorflow or JAX).
Salary : $\sim$ 2200€/month (gross). The PhD is funded by the Geolearning chair.
Location : Centre for Geosciences, Mines Paris PSL (Fontainebleau) and/or MIA Paris Saclay, Campus Agro Paris-Saclay (Palaiseau)

The candidate will have an office in both locations, and benefit from the work environment of both laboratories, with many PhD students & postdocs working on statistical modeling and machine learning for geosciences and life sciences. Being part of the Geolearning chair will offer great opportunities to discuss similar topics with the other students and researchers of the chair.

Context

Geostatistics aims at modeling natural phenomena that evolve in space and time and predicting their behavior at unobserved locations, while quantifying the associated uncertainties. Most geostatistical models rely on Gaussian processes, as they allow for an easy prediction of the variable of interest at unobserved times/locations together with the computation of the prediction variance. In this context, the observations are assumed to be derived from a particular realization of a Gaussian process whose parameters have to be estimated. The second order moment, that shapes the regularity of the process, is classically chosen among parametric families of covariance functions. Their parameters are then estimated by maximizing the likelihood of the data. In the past few years, sophisticated spatio-temporal models based on stochastic partial differential equations (SPDEs) have been proposed [3]. Built upon a stochastic representation of physical processes such as advection and diffusion, they allow for a more natural way to model spatio-temporal phenomena than standard spatio-temporal covariance models. Their flexibility can also be enhanced when considering nonstationary extensions [7], that is when diffusion and advection vary across space and time.

In practice, however, maximum likelihood estimation often becomes a computational bottleneck as the amount of data increases — an issue that frequently arises in a spatio-temporal context. It is therefore of major importance to develop scalable estimation techniques.

The finite element discretization of the SPDEs yields a sparse precision matrix (inverse covariance) for the spatio-temporal random field [9, 11]. This speeds up the computation of the likelihood but the optimization problem remains hard, especially when considering non stationary models.

While SPDEs based models are hard to infer, they are fast to simulate from. Therefore, another way of addressing the parameter estimation problem consists in working in a simulation based inference framework [4]. This terms to simulate a large number of realizations of spatio-temporal random fields, with known parameters, and to learn to solve the parameter estimation problem. This approach is also called amortized inference [15] : while training the model is computationally intensive, this cost is amortized by the efficiency of subsequent parameter inference. Two approaches have been proposed within this framework : the first aims to train a neural network capable of estimating the parameters of a random field, given a realization [6, 8, 12], while the second rather aims to obtain an approximation of the likelihood, thus providing an easy-to-calculate proxy [13], that is subsequently maximized.

Goals

The PhD aims to tackle the computational challenges of the inference of complex spatio-temporal models, exploring different approaches. Several possibilities exist to address this problem, among which two are detailed below, but we are open to propositions formulated by the candidate.

Automatic Differentiation (AD) [1] has already been applied in the context of Gaussian Processes in gradient-based optimization method for the estimation of parametric spatial covariance functions, notably in the library `GPyTorch` [5]. A first objective could be to enable AD for optimizing the likelihood of complex spatio-temporal models based on SPDEs, while exploring flexible parameterizations for non-stationarity within this framework.

Another approach will be based on amortized inference. An initial internship in 2024 focused on implementing an architecture similar to the one proposed in [12] based on graph neural networks (GNNs) to infer parameters of stationary spatial fields. One goal of the PhD will be to generalize the approach to a setting adapted to spatio-temporal data. The main challenges of this generalization include designing a GNN architecture that accounts for spatio-temporal neighborhood structures and handling the estimation of a significantly larger number of parameters.

Alternative approaches may also be considered, including hybrid models that integrate neural networks within Gaussian processes [14], such as Deep Gaussian Markov Fields [10], as well as variational inference methods [2]. In addition, Bayesian inference will be investigated within this framework.

This work will benefit the spatial statistics community by enabling fast parameter estimation in complex spatio-temporal models. A comprehensive comparison between the proposed methods and state-of-the-art approaches will be conducted, focusing on computational complexity, estimation accuracy, and scalability. Applications to real datasets in environmental sciences (e.g. solar radiation for short term photovoltaic power prediction, wind speed for wind power generation, air pollutants monitoring, ...) will also be carried out.

How to apply ?

To apply or for any questions, please contact Lucia Clarotto (lucia.clarotto@agroparistech.fr), Thomas Romary (thomas.romary@minesparis.psl.eu) and Nicolas Desassis (nicolas.desassis@minesparis.psl.eu). Please send us your CV, cover letter and 2nd-year Master academic transcript.

Références

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