M2 Internship: Physics-Informed Generative Neural Networks for stochastic PDEs

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To apply send a CV and a motivation letter with subject "Application for PINNS internship".

1 Context

Spatio-temporal data arise in many applications of modern ecology or climate sciences (Porcu et al. 2021). Statistical modeling of such data is an important challenge, with an historical focus on Gaussian random fields (GRFs) and kriging for prediction (Chilès et al. 1999). In a seminal article, Lindgren et al. (2011) proposed an inference methodology using the fact that certain GRFs can be expressed as solutions of stochastic partial differential equations (SPDEs). The most famous example being spatial Matèrn GRFs being solution of the diffusion-like equation

$$(\kappa - \Delta)^{\alpha/2} u = \mathcal{W}, \tag{1}$$

where $\mathcal{W}$ is a stochastic forcing term (*e.g.* a white noise), and $\theta = (\kappa, \alpha)$ are the model parameters, linked to the Matèrn covariance function. This approach bridges the link between physical and statistical modeling. This led to a large body of work refining Equation (1) to model a broader class of random fields, and to the development of statistical inference procedures for estimating the model parameters (Lindgren et al. 2022). Most of these methods rely on a mesh-based approach, using finite element or volume methods to discretise the equation on a finite set of basis functions. A recent generalisation of this method to spatio-temporal data is proposed in Clarotto et al. (2024).

On the other hand, in the deterministic setting, physics-informed neural networks (PINNs, Raissi et al. 2019) have recently been introduced to solve partial differential equations $\mathcal{N}_\theta[u] = 0$, where $\mathcal{N}_\theta$ is an arbitrary differential operator. One seeks to find the best neural network u_ν (ν being the set of weights and biases) representing the solution by minimizing its PDE residuals computed at randomly sampled collocation points. This mesh-less approach has proven useful in a variety of contexts, and can be extended to inverse problems where one seeks to learn the differential operator's parameters θ given some observations of the solution.

2 Goal of this internship: generative model with PINNs for SPDEs

This internship aims at generalizing the PINN approach for solving SPDEs. To do so, several modification of the deterministic framework are necessary and ought to be explored.

First, one needs the neural network to represent a stochastic process, which can be done by *generative modeling* where the network $u_\nu(Z)$ has an additional latent variable $Z \sim \mathbb{Q}$ as input. Then, the quantity of interest becomes the distribution $\mathbb{P}_\nu$ of the PDE operator of the network $\mathcal{N}_\theta[u_\nu](Z)$, which has to be compared to the stochastic forcing term $\mathcal{W}$. This can be interpreted as a generative model (VAEs, GANs, etc.), as defined in *e.g.* Salmona et al. (2022), where we study $\mathbb{P}_\nu := \mathcal{N}_\theta[u_\nu](\cdot)\#\mathbb{Q}$ is the push-forward of the base distribution of Z through the PINN.

Second, one needs to define a proper loss function accounting for the stochastic nature of the objects at hand. As SPDEs prescribe equality in distribution, a natural choice is to consider a similarity measure between the probability distributions $D(\mathbb{P}_\nu, \mathcal{W})$. Several choices are possible, such as the Kullback-Leibler divergence, the Wasserstein-p distance as in Arjovsky et al. (2017), or the maximum-mean discrepancy associated to some reproducing kernel (Gretton et al. 2012), each leading to different learning strategies for the network's parameters ν.

The new PINN's architecture would then be able to simulate different types of spatial random field according to the parameters of the SPDE. Finally, addition of real data would enable conditional simulations of the spatial field using classical Gaussian conditioning, or methods similar to the one proposed in Bhavsar et al. (2024). The method could be applied to geoscience or environmental data based on the intern's preferences. Possible application scenarios include meteorological simulations (solar radiation, temperature, rain...), air pollution mapping, prediction of soil properties, estimation of sea surface temperature and salinity, etc.

Related work A body of related works on PINNs for SPDEs (Ma et al. 2023) employ a truncated Karhunen-Loeve expansion of the solution of time-dependent SPDEs, representing them with a finite-dimensional series of random variables. The loss function is defined through the weak form of the equation, with so-called "bi-orthogonal" conditions to constrain the basis functions. However, the Karhunen-Loeve decomposition can be computationally expensive and challenging for large-scale problems, and truncating the series to a finite number of terms for practical computation can also introduce errors. On the other hand, by using a generative model able to directly sample the SPDE solution, the proposed approach would bypass the challenges described above.

Organization Starting from Equation (1), this internship will investigate and carefully implement the different methodologies discussed above. The implementation will use the Python package `jinns`, developed at MIA Paris-Saclay and based on the JAX ecosystem[1].

During the internship the student is expected to perform the following tasks :

- Bibliography on the recent literature on generative models and PINNs;
- Conception of a generative PINN model with losses based on KL divergence or Wasserstein-p distance;
- Implementation of a new Python module for stochastic and generative PINNs in `jinns`;
- Application of generative PINNs to real-world data, flexible depending on intern's preferences.

3 Profile & environment

The candidate should be a 2nd year master or last year engineer student, in Statistics/Machine Learning, with courses on latent variable modeling, deep learning or spatial statistics. Scientific programming skills in Python are required, while familiarity with the JAX ecosystem is a bonus.

- Location : UMR MIA Paris-Saclay, Palaiseau Campus, 22 place de l'agronomie, 91120 Palaiseau, France
- Supervision : Lucia Clarotto is an expert in spatial statistics with SPDEs, Hugo Gangloff & Nicolas Jouvin do their research on PINNs and are the developers of the `jinns` Python package.
- Starting date: flexible, starting in February or after.

[1] https://jax.readthedocs.io/en/latest/

- Duration: 5-6 months
- Salary: as an intern, you'll receive a "gratification" which is unfortunately capped around 700 euros/month.

The candidate will have an office, and benefit from the work environment of the MIA Paris-Saclay laboratory, with many PhD students & postdocs working on statistical modeling and machine learning for the life sciences.

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