

Postdoctoral position:
Interacting particle systems for optimization and sampling

September 2023

Scientific context and motivations

The project lies at the interface between numerical optimization, computational statistics and partial differential equations (PDEs). The central goal is to improve, mathematically analyse and implement efficient high-dimensional sampling and optimization methods based on interacting particle systems.

Methods for sampling and optimisation are often two sides of the same coin. A prominent example of this is statistical inference: sampling approaches typically aim at generating samples from the probability measure describing the unknown parameter given the data and prior knowledge, known as the Bayesian posterior distribution, while optimization approaches aim at calculating the maximum likelihood or maximum a posteriori estimator, i.e. the pointwise maximizer of the Bayesian posterior. Sampling and optimisation methods also coexist in the field of machine learning, where use of the former is driven by the need for explainable and transparent algorithms, which requires to analyse the parameter uncertainties present in trained neural networks.

Many key recent developments in the fields of sampling and optimisation are based on the use of interacting particle systems and their analysis at the level of the nonlocal Fokker–Planck equation describing the systems in the limit of infinitely many particles, known as the mean field limit. This approach to numerical algorithms based on interacting particle systems emerged initially from the optimization community and has since then has brought considerable insight. It has enabled, notably, significant progress towards proving rigorously the longtime convergence of widely-used interacting particle methods, including the ensemble Kalman filter and particle swarm optimization.

Description of the project

Improving, implementing and mathematically analysing sampling and optimization methods based on interacting particle systems are the primary aims of this postdoctoral project. Two particular classes of methods will be considered: consensus-based methods inspired by particle swarm optimisation [4, 1], and ensemble Kalman-based methods [3, 2], which were recently revealed to have a close connection to interacting Langevin diffusions.

The first research track of this postdoctoral project concerns the analysis and improvement of consensus-based optimization and sampling methods. The main goals are to improve and generalize existing theoretical results related to the mean field limit and long-time behaviour of these methods. We will also study whether the methodologies can be improved in terms of computational efficiency and, in the context of sampling, accuracy of the invariant measure as an approximation of the target probability distribution. In order to complete the latter objective, simple approaches based on metropolization and preconditioning will be tested.

The second research track is devoted to numerical aspects for consensus-based methods, including implementation, testing, and discretization. Consensus-based optimization will be studied at the discrete-time level, and the postdoctoral research will participate in an effort to produce robust and efficient implementations of consensus-based methods intended for dissemination.

Expected profile

The expected profile is that of an independent researchers with strong analytical skills. Applicants should hold a PhD in applied mathematics and have experience in scientific computation, stochastic analysis and partial differential equations. Prior experience in computational statistics and the analysis of mean field equations is desirable.

Keywords. Interacting particle systems, Bayesian inverse problems, sampling and optimization.

Selection process. The full application should contain:

- A complete curriculum vitae, including a list of publications.
- A short cover letter explaining why the candidate is a good fit for this project.

Location. The successful candidate will take up the position as soon as possible and be based at École des Ponts, 77420 Champs-sur-Marne (RER A, station Noisy-Champs) and Inria Paris, rue Simone Iff, 75012 Paris (RER A, station Gare de Lyon, and Métro 6, station Dugommier). See <https://team.inria.fr/matherials/> for more details on the location and activities of our research team.

Contact. Candidates are encouraged to discuss their application with Urbain Vaes (urbain.vaes@inria.fr).

References

- [1] J. A. Carrillo, F. Hoffmann, A. M. Stuart, and U. Vaes. Consensus-based sampling. *Stud. Appl. Math.*, 2022.
- [2] A. Garbuno-Inigo, F. Hoffmann, W. Li, and A. M. Stuart. Interacting Langevin diffusions: gradient structure and ensemble Kalman sampler. *SIAM J. Appl. Dyn. Syst.*, **19**(1), 2020.
- [3] M. A. Iglesias, K. J. H. Law, and A. M. Stuart. Ensemble Kalman methods for inverse problems. *Inverse Probl.*, **29**(4), 2013.
- [4] R. Pinnau, C. Totzeck, O. Tse, and S. Martin. A consensus-based model for global optimization and its mean-field limit. *Math. Models Methods Appl. Sci.*, **27**(01):183–204, 2017.