Postdoctoral position in applied mathematics:

Numerical schemes for Sensitivity Analysis of Hypocoercive Systems.

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Job environnements The postdoctoral position will start in September 2024 at Université Grenoble Alpes within Inria project-team AIRSEA[1] located in Grenoble (France). This work is part of the activities of the french thematic network on uncertainty quantification[2]. The candidate will benefit from the scientific environment of Jean Kuntzmann Laboratory[3]. She/he will also benefit from GRICAD[4] supercomputing infrastructure.

Project description Many mathematical models involve input parameters, which are not precisely known. Global sensitivity analysis aims at identifying the parameters whose uncertainty has the largest impact on the variability of a Quantity of Interest (QoI).

In this project we consider models described by hypoelliptic systems of Stochastic Differential Equations (SDE), whose coefficients depend on some uncertainty parameter $\xi = (\xi_1, \ldots, \xi_p) \in \Xi$. More precisely we investigate parametrized SDEs of the form

$$\begin{cases} dX_t &= Y_t dt \\ dY_t &= \sigma(\xi) dW_t - (c(\xi, X_t, Y_t)Y_t + \nabla V(\xi, X_t))dt. \end{cases} \tag{1}$$

We assume the Brownian motion W driving (1) is independent from ξ. In a preliminary work [4], we were interested in QoIs which are averaged quantities with respect to the Brownian motion W. E.g., we considered the averaged exit time starting from $x \in D$ a bounded open subset of $\mathbb{R}^d$, defined as $\mathcal{U}(x, \xi) = \mathbb{E}^x[\tau_D \,|\, \xi]$ with $\tau_D = \inf\{t \geq 0 : \ X_t \notin D\}$. Also, we limited our analysis to a framework of uniform ellipticity. One major drawback of modeling based on elliptic systems is that corresponding trajectories are non-differentiable at any point, which is meaningless for some applications (see, e.g., [1]). Therefore in the present research project, we rather focus on systems for which diffusion only acts on Y-component (see Eq. (1)). Under mild assumptions on damping coefficient c and potential V the system (1) is *hypoelliptic* (see, e.g., [8] for a definition). It enters the scope of *damping Hamiltonian (stochastic) systems* whose properties are well studied, e;g., in [12]. In particular (X, Y) has an invariant probability measure $\mu(dxdy, \xi) = p(x, y, \xi)dxdy$. In that case we will say (loosely speaking) that the system is *hypocoercive* (see [11] for more on *hypocoercivity*). The parametrized QoI we will focus on in this project is the stationary density function $(x, y) \mapsto p(x, y, \xi)$ whose first-order and total sensitivity with respect to each component ξ_i of ξ is to be analysed.

It is well known that $(x, y) \mapsto p(x, y, \xi)$ solves the steady state (parametrized) Fokker-Planck equation:

$$\begin{cases} \dfrac{\tilde{\sigma}^2}{2\varepsilon^2}\partial_{yy}p(x,y,\xi) - y\partial_x p(x,y,\xi) + \partial_y[\{c(\xi,x,y)y + \nabla V(\xi,x)\}p(x,y,\xi)] &= 0 \ \ \forall x, y \in \mathbb{R} \\ \lim\limits_{||(x,y)|| \to \infty} p(x,y,\xi) &= 0 \\ \displaystyle\int p(x,y,\xi)dxdy &= 1. \end{cases} \tag{2}$$

So one of the first and most important tasks for this project will be to develop a numerical scheme for partial differential equation (PDE) described by (2), in a non parametrized context. And then,

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in order to handle uncertain parameter ξ, a second task will be to perform a stochastic Galerkin projection of this scheme (see [10, 9]). Numerical schemes for steady state Fokker-Planck equation are not very well understood. One algorithm has been proposed in [7] without any proof of convergence. Since the years 2000 *hypocoercive* systems have raised a lot of interest (see in particular [11]), but it seems they have been investigated from a numerical perspective only from the years 2020 (e.g., in [3],[6]...). Moreover, in most of these works, evolution (and not steady state) *hypocoercive* PDE is considered, and damping force coefficient c in (1) or (2) is kept constant. The guideline towards the first task of this project will be to follow these works, adding a perturbation to handle non-constant damping force coefficient and considering long-term behavior of the solution.

As far as sensitivity analysis is concerned, the main challenge here is that QoI is a parametrized density function. Recent works in [5] or [2] can handle this framework. Estimation procedures involve the development and use of machine learning and AI tools (random forests, kernel embedding for the computation of Maximum Mean Discrepancy...). The idea here is to leverage Galerkin scheme developed for numerically solving (2) in order to estimate sensitivity measures based on MMD discrepancy (see [2] for a definition) with a suitable kernel.

Among interesting *hypoelliptic systems* is the celebrated FitzHugh-Nagumo model used in neurosciences (see [8] and the references therein for an introduction). In this neuroscience context one QoI is the spike-rate of a neuron, which can be related to the invariant density function of FitzHugh-Nagumo system.

Candidate profile This postdoctoral project is at the crossroad between numerical analysis, probability, statistics and machine learning. Candidates must have good knowledge for at least one of these domains and the motivation to quickly acquire the missing complementary skills. This research work will involve both theoretical developments and practical implementations. Candidates should have demonstrable experience and skill in some of the following topics : scientific creativity, autonomy, writing abilities, oral communication skills (English and/or French), and taste for teamwork.

How to apply The candidates should send a CV, statement of interest and letters of recommendation to Clémentine Prieur (`clementine.prieur@univ-grenoble-alpes.fr`) and Pierre Etoré (`pierre.etore@univ-grenoble-alpes.fr`).

References

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