PhD thesis project *Uncertainty quantification in Stochastic Differential Equations and applications to Neurosciences*

Advisors:

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Project context and objectives:

Many mathematical models involve input parameters, which are not precisely known. Global sensitivity analysis aims to identify the parameters whose uncertainty has the largest impact on the variability of a quantity of interest - for instance by computing Sobol' sensitivity indices. In this project we consider stochastic models described by Stochastic Differential Equations (SDE), whose coefficients depend on some uncertainty parameter $\xi \in \mathbb{R}^d$. More specifically, we are interested in harmonic oscillators perturbed with a gaussian white noise. We consider a vector of uncertain parameters $\xi = (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d$ and the process $\big(Z_t := (X_t, Y_t) \in \mathbb{R}^2\,,\ t \geq 0\big)$ governed by the following Itô stochastic differential equation:

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

Under some conditions on the damping coefficient c and the potential V the process is hypoelliptic and is ergodic with a unique invariant probability measure $\mu(dxdy, \xi) = p(x, y, \xi)dxdy$, and the rate of convergence in the ergodic theorem is exponential. We aim at studying the influence of the uncertain parameters $\xi_1, \ldots, \xi_d$ on quantities of interest defined from the density $p(x, y, \xi)$ of $\mu(dxdy, \xi)$. This density is known to solve the stationary Fokker-Planck Partial Differential Equation (PDE)

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

with the constraint $p \geq 0$. Note that the second order operator appearing in the first line of (1) is the formal adjoint of the infinitesimal generator associated to $\{(X_t, Y_t)\,,\ t \geq 0\}$. Note also that the PDE (1) is hypoelliptic, it suffers of "loss of ellipticity".

Sensitivity analysis for models driven by systems of stochastic differential equations were presented, e.g., in [LMK15, EPPL20]. The main challenges of the present project are the hypoellipticity of the diffusion under study and the specific nature of the quantities of interest for sensitivity analysis. The main steps to tackle these challenges will consist in:

- deriving a numerical scheme for the Fokker-Planck equation and studying its convergence
- proposing a metamodel for $\xi \mapsto p_n(\cdot, \cdot, \xi)$ numerical solution of the Fokker-Planck equation (based, e.g., on Stochastic Galerkin or stochastic collocation, presented in [N09])
- computing from evaluations of this metamodel sensitivity indices for different quantities of interest.

To start with we can consider as a toy model the Kramer oscillator with $\xi = (\sigma, \kappa, \alpha, \beta) \in \big(\mathbb{R}_+^*\big)^4$, $\sigma(\xi) = \sigma$, $c(\xi, X_t, Y_t) = \kappa$ and with the Duffing's potential $V(\xi, x) = \alpha x^4/4 - \beta x^2/2$. Explicit formulae for $p(x, y, \xi)$ are available in this case. They can provide benchmarks for testing numerical procedures under investigation.

An important application we have in mind for this project is to handle the hypoelliptic Fitzhugh-Nagumo model arising from neurosciences (see for instance [LS18]). In that case one has $c(\xi, x, y) = \frac{1}{\varepsilon}(3x^2 - 1 + \varepsilon)$, $V(\xi, x) = \frac{1}{\varepsilon}\left(\frac{x^4}{4} + \frac{\gamma - 1}{2}x^2 + (s + \beta)x\right)$ and $\sigma = \frac{\tilde{\sigma}}{\varepsilon}$, and one can see $\xi = (\varepsilon, \tilde{\sigma}, \gamma, s, \beta)$ as the uncertain parameter. The quantity X_t is the electric potential at time t at the surface of a neuron. Then the component Y_t is interpreted as its velocity.

In [LS18] it is proved that the quantity $\int_0^{+\infty} yp(u,y,\xi)dy$ approximates the neuronal spike rate (subject to uncertainty ξ) above a given threshold u.

It might also be interesting to consider directly as quantity of interest the density function

$$y \mapsto p(u,y,\xi)/\int p(u,v,\xi)dv.$$

Sensitivity analysis for QoIs that are probability distribution functions is a topic in full expansion (see, e.g., [FKL20] or [Dav21]). Estimation procedures involve the development and use of machine learning and AI tools (random forests, kernel embedding for the computation of Maximum Mean Discrepancy...)

Project will be advised by Pierre Etoré, researcher at LJK (topics: stochastic processes and their simulation, link with PDEs, numerical and statistical aspects...). It could lead to collaborations with Clémentine Prieur (LJK, topic: sensitivity analysis, statistics) and Adeline Leclercq-Samson (LJK, topic: probability and statistics for neurosciences).

Keywords

Hypoelliptic diffusions - Stochastic Differential Equations - Partial Differential Equations - Uncertainty quantification - Stochastic Galerkin methods - Wasserstein distances - Machine learning -stochastic collocation - kernel embedding

Required competences

We seek for a student in probability and statistics with some knowledge and/or interest in PDE issues. Some knowledge of scientific computing is required (Python or Matlab, R, C/C++).

References

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