

Global sensitivity analysis for stochastic differential equation models

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We are interested in models driven by **parametrized stochastic differential equations** (parametrized SDE) defined as :

$$dX_t = b(X_t, \xi)dt + \sigma(X_t, \xi)dW_t, \quad X_0 = x, \quad (1)$$

with $\xi = (\xi_1, \dots, \xi_m)$ a random vector valued in $\Xi \subseteq \mathbb{R}^m$ modeling the uncertain parameter, $(W_t)_{t \geq 0}$ a standard d -Brownian motion, independent from ξ .

We assume in the following that the drift term $b : \mathbb{R}^d \times \Xi \rightarrow \mathbb{R}^d$ and the diffusion term $\sigma : \mathbb{R}^d \times \Xi \rightarrow \mathbb{R}^{d \times d}$ satisfy :

$$\begin{aligned} |b(x, z) - b(y, z)| + |\sigma(x, z) - \sigma(y, z)| &\leq M|x - y| \\ |b(x, z)|^2 + |\sigma(x, z)|^2 &\leq M^2(1 + |x|^2) \end{aligned} \quad (2)$$

for all $x, y \in \mathbb{R}^d$ and $z \in \Xi$ (for a given $0 \leq M < \infty$).

The set of assumptions (2) ensures the existence and unicity of the solution of (1), as far as the following moment property :

$$\mathbb{E}_{W,\xi} |X_t|^q < +\infty, \text{ for any } q \in \mathbb{N}^* .$$

Let us consider $\mathfrak{U}(x, \xi)$ or $\mathfrak{V}(t, x, \xi)$ integrated (with respect to the intrinsic noise W) quantities of interest (Qols) defined from the solution of (1).

We are interested in measuring the influence of any component (or set of components) of the vector of uncertain parameters $\xi = (\xi_1, \dots, \xi_m)$ on these Qols.

- 1 Sobol' indices for global sensitivity analysis
 - General framework
 - Definition of Sobol' indices
 - Pick-freeze estimation procedure
- 2 Two integrated Qols for our stochastic model
- 3 State of the art for Sobol' index estimation in our framework
 - Pick-freeze combined with Monte Carlo
 - Hybrid Galerkin / MC
- 4 New estimation procedure based on Feynman-Kac representation of the Qol
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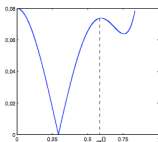
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Let $\mathcal{M} : \begin{cases} \mathbb{R}^m & \rightarrow \mathbb{R} \\ \mathbf{x} & \mapsto y = \mathcal{M}(x_1, \dots, x_m) \end{cases}$ with \mathcal{M} a deterministic model.

We aim at determining the way the **output** of the **model** reacts to variations of the **input parameters**.

A natural way to measure that is, under regularity assumptions on the model \mathcal{M} , to compute the partial derivatives $\frac{\partial \mathcal{M}}{\partial x_j}(\mathbf{x}_0)$, for $j = 1, \dots, m$, and for a nominal value $\mathbf{x}_0 \in \mathbb{R}^m$.



With partial derivatives, we measure local sensitivities around $\mathbf{x}_0 \in \mathbb{R}^m$.

In our study, we are interested in a more global approach. How does the QoI y reacts to variations of the input x_j on its whole set of variations ?

For our study, among numerous alternatives, we focus on variance based sensitivity analysis.

The uncertain parameters are modeled by **independent** random variables $X_j \in \Xi_j \subseteq \mathbb{R}$. Then the probability distribution modeling the uncertain vector $\mathbf{X} \in \Xi \subseteq \mathbb{R}^m$ is a product probability distribution :

$$\mathbb{P}_{\mathbf{X}}(d\mathbf{x}) = \prod_{j=1}^m \mathbb{P}_{X_j}(dx_j).$$

E.g., $\mathbf{X} = (X_1, \dots, X_m) \sim \mathcal{U}([0, 1]^m)$.

Thus, as the uncertainty is propagated through the model, the output $Y \in \mathbb{R}$ is itself a random variable.

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Towards Sobol' sensitivity indices [Sobol', 1993] :

Does the output Y vary more or less when fixing one of its **inputs**?

$\text{Var}(Y|X_j = x_j)$, how to choose x_j ?

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$\text{Var}(Y|X_j = x_j)$, how to choose x_j ? $\Rightarrow \mathbb{E}[\text{Var}(Y|X_j)]$.

Then, noting $\text{Var}[\mathbb{E}(Y|X_j)] = \text{Var}(Y) - \mathbb{E}[\text{Var}(Y|X_j)]$, we define the first-order Sobol' index wrt X_j as :

$$S_j = \text{Var}[\mathbb{E}(Y|X_j)] / \text{Var}[Y].$$

The larger $0 \leq S_j \leq 1$, the more influential the j^{th} input, X_j .

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Remark : if $Y = \sum_{j=1}^m \beta_j X_j$, one gets

$S_j = \beta_j^2 \text{Var}[X_j] / \text{Var}[Y] = \rho_j^2$, with ρ_j the linear correlation coefficient.

More generally, we can define Sobol' indices of any order :

$$S_j = \frac{\text{Var} [\mathbb{E} (Y|X_j)]}{\text{Var}[Y]}, \quad 1 \leq j \leq m$$

$$S_{j,k} = \frac{\text{Var} [\mathbb{E} (Y|X_j, X_k)] - \text{Var} [\mathbb{E} (Y|X_j)] - \text{Var} [\mathbb{E} (Y|X_k)]}{\text{Var}[Y]},$$

$$1 \leq j \neq k \leq m$$

...

$$\text{We have } 1 = \sum_{j=1}^m S_j + \sum_{1 \leq j \neq k \leq m} S_{j,k} + \dots + S_{1,\dots,m}.$$

It is also possible to define, for any $1 \leq j \leq m$, the total Sobol' index

$$S_j^{\text{tot}} = \sum_{\mathbf{u} \subseteq \{1, \dots, m\}, j \in \mathbf{u}} S_{\mathbf{u}}.$$

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We still assume that the input parameters are independent.

Let \mathbf{X}^1 and \mathbf{X}^2 be two independent copies of \mathbf{X} .

For $j = 1, \dots, m$, we define :

$$\mathbf{z}^j = (X_1^2, \dots, X_{j-1}^2, X_j^1, X_{j+1}^2, \dots, X_m^2)$$

Let $Y = \mathcal{M}(\mathbf{X}^1)$ and, for $j = 1, \dots, m$, $Y^j = \mathcal{M}(\mathbf{z}^j)$.

We can prove :

$$S_j = \frac{\text{Cov}(Y, Y^j)}{\text{Var}[Y]}.$$

For any $j \in \{1, \dots, m\}$, let $X_j^{1,i}$ and $X_j^{2,i}$, $i = 1, \dots, N$ be two independent samples of size N of the parameter X_j .

We define :

$$\mathbf{X}^{1,i} = (X_1^{1,i}, \dots, X_{j-1}^{1,i}, X_j^{1,i}, X_{j+1}^{1,i}, \dots, X_m^{1,i}) \quad i = 1, \dots, N$$

$$\mathbf{Z}^{j,i} = (X_1^{2,i}, \dots, X_{j-1}^{2,i}, X_j^{1,i}, X_{j+1}^{2,i}, \dots, X_m^{2,i}) \quad i = 1, \dots, N, j = 1, \dots, m$$

We evaluate the model $(1 + m)N$ times :

$$Y^i = \mathcal{M}(\mathbf{X}^{1,i}) \quad i = 1, \dots, N$$

$$Y^{j,i} = \mathcal{M}(\mathbf{Z}^{j,i}) \quad i = 1, \dots, N, j = 1, \dots, m.$$

Pick-freeze estimator : [Monod et al., 2006, Janon et al., 2014]

$$\hat{S}_{j,N} = \frac{\frac{1}{N} \sum_{i=1}^N Y^i Y^{j,i} - \left(\frac{1}{N} \sum_{i=1}^N \frac{Y^i + Y^{j,i}}{2} \right)^2}{\frac{1}{N} \sum_{i=1}^N \frac{(Y^i)^2 + (Y^{j,i})^2}{2} - \left(\frac{1}{N} \sum_{i=1}^N \frac{Y^i + Y^{j,i}}{2} \right)^2}$$

Total and higher order interaction indices can also be estimated.

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Let $(X_t)_{t \geq 0}$ be the unique solution of (1). Recall that existence and unicity are ensured by (2). The process $(X_t)_{t \geq 0}$ is subject to two uncertainty sources : the intrinsic noise modeled by the process $(W_t)_{t \geq 0}$ and the uncertainty due to a lack of knowledge on ξ .

We want to define two Qols which are integrated with respect to the intrinsic randomness of the system.

Let us assume uniform ellipticity of the system (Ellip) :

$$\exists \lambda > 0 \text{ such that } \forall x, y \in \mathbb{R}^d, \forall z \in \Xi, \quad y^T [\sigma \sigma^T](x, z) y \geq \lambda |y|^2.$$

Let D a bounded open subset of \mathbb{R}^d (with regularity on ∂D) and $f \in \mathcal{C}^2(\bar{D})$ (satisfying the compatibility assumption, regularity and boundedness conditions). We define $\tau_D = \inf\{t \geq 0 : X_t \notin D\}$ and the following Qols

$$\mathfrak{U}(x, \xi) = \mathbb{E}^x[\tau_D | \xi] \quad \text{and} \quad \mathfrak{V}(t, x, \xi) = \mathbb{E}^x[f(X_t) \mathbf{1}_{t \leq \tau_D} | \xi].$$

We aim at studying the sensitivity of \mathfrak{U} (and \mathfrak{W}) to variations of the components of ξ by computing Sobol' indices :

$$S_I(\mathfrak{U}) = \frac{\mathbb{V}[\mathbb{E}(\mathfrak{U}(\xi)|\xi_I)]}{\mathbb{V}(\mathfrak{U}(\xi))}, \quad \forall I \subseteq \{1, \dots, m\}, \quad \xi_I = \{\xi_\ell, \ell \in I\}$$

Remark : the variances in the numerator and denominator are finite under our assumptions.

We define $\mathcal{F}_{\mathfrak{U}}$ and $\mathcal{F}_{\mathfrak{W}}$ as :

$$\mathcal{F}_{\mathfrak{U}}(W, \xi) = \tau_D \quad \text{and} \quad \mathcal{F}_{\mathfrak{W}}(W, \xi) = f(X_t) \mathbf{1}_{t \leq \tau_D}.$$

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Approach 1 : pick-freeze (PF) combined with Monte Carlo (MC).

In a first time, we compute a MC approximation of

$$\mathfrak{U}(\xi) = \mathbb{E}[\tau_D | \xi]$$

$$\bar{E}^M[\hat{\mathcal{F}}_{\mathfrak{U}}](\xi) := \frac{1}{M} \sum_{k=1}^M \hat{\mathcal{F}}_{\mathfrak{U}}(W^{(k)}, \xi), \quad W^k \text{ i.i.d., distributed as } W.$$

Then we estimate $S_I(\mathfrak{U})$ with a *pick-freeze* scheme on the proxy

$$\xi \mapsto \bar{E}^M[\hat{\mathcal{F}}_{\mathfrak{U}}](\xi).$$

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Approach 2 : hybrid Galerkin / MC.

Let $\{\Psi_q\}_{q \in \mathbb{N}}$ be an orthonormal basis of $L^2(\Xi, \mathbb{P}_\xi)$, $\langle \cdot, \cdot \rangle$.

In [Le Maître and Knio, 2015], the authors consider the representation ($d = 1$)

$$X_t = \sum_{q \in \mathbb{N}} [X_t]_q(W) \Psi_q(\xi)$$

and approximate the $[X_t]_q(W)$'s by solving the system of stochastic differential equations

$$d[X_t]_q(W) = \langle b(\sum_r [X_t]_r(W) \Psi_r), \Psi_q \rangle dt + \langle \sigma(\sum_r [X_t]_r(W) \Psi_r), \Psi_q \rangle dW_t$$

for $0 \leq q \leq P$ (the basis is truncated to its $P + 1$ first terms).

From the orthonormality of the basis, we get :

$$\mathbb{V}(\mathbb{E}[X_t | \xi]) \approx \sum_{q=1}^P \{\mathbb{E}([X_t]_q)\}^2.$$

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New approach based on Feynman-Kac representation of the QoI [Etoré et al., 2020]

Let us first consider the non-parametrized framework ($b(x, z) = b(x)$ and $\sigma(x, z) = \sigma(x)$).

Let X be the solution of $dX_t = b(X_t)dt + \sigma(X_t)dW_t$ and

$$\tau_D = \inf\{t \geq 0 : X_t \notin D\}$$

(with the same assumptions as previously).

Let $a = \sigma\sigma^T$. Then $\mathbb{E}^x(\tau_D) = u(x)$, $x \in \bar{D}$, with u solution of the partial differential equation (PDE)

$$\begin{cases} \frac{1}{2} \sum_{k,j=1}^d a_{kj}(x) \partial_{x_k x_j}^2 u(x) + \sum_{k=1}^d b_k(x) \partial_{x_k} u(x) = -1 & \forall x \in D \\ u(x) = 0 & \forall x \in \partial D. \end{cases}$$

([Karatzas and Shreve, 1991]).

We now come back to the parametrized SDE.

For any realization ξ of the uncertain parameter, let $X(\xi)$ solution de

$$dX_t(\xi) = b(X_t, \xi)dt + \sigma(X_t, \xi)dW_t.$$

By using the Feynman-Kac representation with the drift and diffusion terms $b(\cdot, \xi)$ and $\sigma(\cdot, \xi)$, we get

$\mathfrak{U}(x, \xi) = \mathbb{E}^x[\tau_D | \xi] = u(x, \xi)$ with $u(\cdot, \xi)$ solution of

$$\begin{cases} \frac{1}{2} \sum_{k,j=1}^d a_{kj}(x, \xi) \partial_{x_k x_j}^2 u(x, \xi) + \sum_{k=1}^d b_k(x, \xi) \partial_{x_k} u(x, \xi) = -1 & \forall x \in D \\ u(x, \xi) = 0 & \forall x \in \partial D \end{cases}$$

(with $a = \sigma \sigma^T$).

Thus ...

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Now the aim is to compute numerically $\mathfrak{U}(x, \xi)$ in a way which eases the computation of Sobol' indices...

Good news : such numerical tools do exist !
(see, e.g., [Nouy, 2009])

Notation : let $\mathcal{V} = H_0^1(D) \otimes L^2(\Xi, \mathbb{P}_\xi)$ endowed with

$$u \mapsto \mathbb{E}_\xi \|u(\cdot, \xi)\|_{H^1(D)}^2 =: \|u\|_{\mathcal{V}}^2,$$

and for $u, v \in \mathcal{V}$

$$\mathcal{A}(u, v) = \mathbb{E}_\xi \left(\int_D (\nabla u(\cdot, \xi))^T \tilde{a}(\cdot, \xi) \nabla v(\cdot, \xi) + \int_D (\nabla u(\cdot, \xi))^T \tilde{b}(\cdot, \xi) v(\cdot, \xi) \right).$$

Lemma

$\mathfrak{U}(x, \xi) \in \mathcal{V}$ and it coincides with the unique weak solution of (\mathcal{P}_{ell}) in the sense that

$$\forall v \in \mathcal{V}, \quad \mathcal{A}(\mathfrak{U}, v) = F(v)$$

with $\forall v \in \mathcal{V}, \quad F(v) = \mathbb{E}_\xi \left(\int_D v(\cdot, \xi) \right).$

Galerkin approximation of \mathfrak{U} :

Let $\mathcal{V}^{N,P} = V^N \otimes \mathcal{S}^P \subseteq \mathcal{V}$ with

$V^N = \text{Span}(\{\phi_i^N\}_{i=1}^{N-1}) \subseteq H_0^1(D)$ (finite elements)

and $\mathcal{S}^P = \text{Span}(\{\Psi_q\}_{q=0}^P)$ (with $\{\Psi_q\}_{q \in \mathbb{Q}}$ orthonormal basis of $L^2(\Xi, \mathbb{P}_\xi)$),

chosen such that $\mathcal{V}^{N,P} \subseteq \mathcal{V}^{N+1,P+1}$ and $\bigcup_{N,P} \mathcal{V}^{N,P}$ is dense in \mathcal{V} .

Theorem

Let $\mathfrak{U}^{N,P}$ be the unique solution in $\mathcal{V}^{N,P}$ of

$$\forall v \in \mathcal{V}^{N,P}, \quad \mathcal{A}(\mathfrak{U}^{N,P}, v) = F(v).$$

Then

$$\|\mathfrak{U}^{N,P} - \mathfrak{U}\|_{\mathcal{V}} \xrightarrow{N \rightarrow \infty, P \rightarrow \infty} 0.$$

For the computation of $\mathfrak{U}^{N,P} = \sum_{j=1}^{N-1} \sum_{q=0}^P U_j^q \Psi_q \phi_j$ we seek for

$U = (U^0, \dots, U^P)^T$, with $U^q = (U_1^q, \dots, U_{N-1}^q) \in \mathbb{R}^{1 \times (N-1)}$, $0 \leq q \leq P$

solution of $\mathbf{A}U = \mathbf{F}$ where $\mathbf{A} = (\mathbf{A}_{pq})_{0 \leq p, q \leq P}$ and $\mathbf{F} = (\mathbf{F}_0, \dots, \mathbf{F}_P)^T$ are defined as :

$$\begin{cases} \mathbf{A}_{pq} = (\mathcal{A}(\Psi_q \phi_j, \Psi_p \phi_i))_{1 \leq i, j \leq N-1} & \forall 0 \leq p, q \leq P, \\ \mathbf{F}_p = (F(\Psi_p \phi_1), \dots, F(\Psi_p \phi_{N-1})) & \forall 0 \leq p \leq P. \end{cases}$$

Then we get : $\mathfrak{U}^{N,P}(x, \xi) = \sum_{q=0}^P \mathfrak{U}_q^N(x) \Psi_q(\xi)$ with

$$\mathfrak{U}_q^N(x) = \sum_{j=1}^{N-1} U_j^q \phi_j(x), \quad \forall 0 \leq q \leq P.$$

Lastly, we compute $S_I(\mathfrak{U})$ using Parseval's identity :

$$\frac{\sum_{q \in K_I} [\mathfrak{U}_q^N(x)]^2}{\sum_{q=1}^P [\mathfrak{U}_q^N(x)]^2} \text{ with } K_I = \{p \in \{1, \dots, P\} : \Psi_p(\xi) = \Psi_p(\xi_I)\}.$$

Remark : with this approach, we compute approximation of Sobol' indices without any MC scheme.

Example : $dX_t = -\alpha(\xi)X_t dt + \sigma(\xi)dW_t$ where

$\xi = (\xi_1, \xi_2)^T$ with ξ_1, ξ_2 i.i.d. distributed as $\mathcal{U}([0, 1])$ and

$$\alpha(\xi) = \mu_1 + \sqrt{3}\sigma_1(2\xi_1 - 1) \quad \text{and} \quad \sigma(\xi) = \mu_2 + \sqrt{3}\sigma_2(2\xi_2 - 1).$$

We take $D = (0, 10)$.

	Galerkin	MC combined with PF
$S_1(\mathfrak{U})$	$(N = 1000, P = 10)$ 0.0253	$(N = M = 10^4, \delta t = 10^{-3})$ 0.024927
$S_2(\mathfrak{U})$	$(N = 1000, P = 10)$ 0.9747	$(N = M = 2 \times 10^4, \delta t = 10^{-4})$ 0.971277

TABLE – Sobol' indices for $\mathfrak{U}(x, \xi)$, $x = 5$, in the Ornstein-Uhlenbeck example with $\mu_1 = 1$, $\mu_2 = 9$ and $\sigma_1 = \sigma_2 = 0.2$.

For the Qol $\mathfrak{Q}(T, x, \xi)$, one has to solve the parametrized parabolic PDE (...)

It also works well.

Let us choose $f \equiv 1$. We get $\mathfrak{Q}(T, x, \xi) = \mathbb{P}^x(\tau_D \leq T)$.

	Galerkin / Crank-Nicholson	MC combined with PF
$S_1(\mathfrak{Q})$	$(M = 300, N = 1000, P = 10)$ 0.0961	$(N = M = 5 \times 10^4, \delta t = 6 \times 10^{-4})$ 0.095812
$S_2(\mathfrak{Q})$	$(M = 300, N = 1000, P = 10)$ 0.9039	$(N = M = 5 \times 10^4, \delta t = 6 \times 10^{-4})$ 0.903182

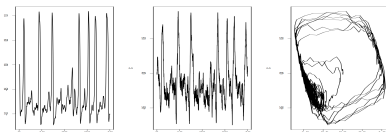
TABLE – Sobol' indices for $\mathfrak{Q}(T, x, \xi, x = 1, T = 0.3)$ in the Ornstein-Uhlenbeck example, with $\mu_1 = 1$, $\mu_2 = 2$ and $\sigma_1 = \sigma_2 = 0.2$.

Remark : in terms of computation time, our new approach takes a few seconds against more than one hour for the MC / PF one.

Conclusions :

- we developed a methodology for performing GSA on QoIs integrated wrt to the intrinsic noise of the system ;
- the implementation does not require any MC scheme.

Perspectives : in collaboration with colleagues in Grenoble, we aim at applying such a methodology to better understand spike emission described by **FitzHugh-Nagumo model** defined as :

$$\begin{cases} dV_t = \frac{1}{\varepsilon}(V_t - V_t^3 - C_t - s)dt \\ dC_t = (\gamma V_t - C_t + \beta)dt + \tilde{\sigma}dW_t \end{cases}$$


- V_t the membrane potential of a single neuron,
- C_t a recovery variable / channel kinetics,
- ε the time scale separation, s the stimulus input,
- β, γ positive constants determining the position of the fixed point and the duration of the excitation,
- W_t a Brownian motion, $\tilde{\sigma} > 0$ the diffusion coefficient.

This model is governed by hypoelliptic SDE [Leon et al., 2018].
Our first perspective is to extend our methodology to the hypoelliptic framework.

Another perspective is to choose adaptively the truncation of the bases involved in the decomposition of our Qol.

We are also interested in non integrated Qol, such as the invariant density of the FitzHugh-Nagumo model (ongoing work).

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Thanks for your attention !