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Sobol' sensitivity analysis for a parametrized diffusion process

MSc Thesis

Master of Science in Industrial and Applied Mathematics (MSIAM)
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Grenoble, June 2017

Acknowledgement

My deepest gratitude goes first and foremost to my supervisors, Professor Clémentine PRIEUR and Assistant Professor HDR Pierre ÉTORÉ, for their constant encouragements and guidances. Without their consistent and illuminating instruction, this thesis could not have reached its present form. I am really thankful to them.

Special thanks should go to my friends, Arthur MACHEREY, Mohamed Reda EL AMRI and Qian SUN, who offer me many useful informations during the intership, and also have put considerable time and effort into their comments on the draft.

Finally, I am indebted to my parents and my girlfriend for their continuous supports and encouragements.

Contents

Abstract

The objective of sensitivity analysis for a mathematical model is to identify the influence of its inputs on its output. Sobol' sensitivity analysis allows us to know the part of the variance of the output explained by each of the model input. Most of the intrusive methodologies in sensitivity analysis are for deterministic models driven by the partial differential equations (PDEs). The Monte Carlo method and the model reduction techniques are often used in this framework (see A. Janon et al., 2014).

Several recent works also present the sensitivity analysis for the stochastic models with both uncertain parameters and intrinsic stochasticity. When performing a Sobol' sensitivity analysis on such a model, one may be interested in the full probability density function of the outputs. For instance, O.P. Le Maître and O.M. Knio (2015) propose a method, based on polynomial chaos (PC) expansion and a stochastic Galerkin projection, for the analysis of variance of stochastic differential equations (SDEs) driven by Wiener noise.

In this work, we discuss the computation of Sobol' indices for a diffusion process with uncertain parameters (a time-homogeneous continuous Markov process satisfying an autonomous SDE in the presence of uncertainties). We first consider the mean value relative to the intrinsic randomness as the quantity of interest for sensitivity analysis. Apart from the Monte Carlo estimator and the PC analysis mentioned above, we propose an alternative appoach, in which we firstly transform the problem from a parametrized SDE to a parametrized PDE, using the famous Feynman-Kac formulae, then we can either use MC samplings for the PDE, or apply PC expansion for the solution of the PDE, combined with stochastic Galerkin technique. Then, we consider the mean exit time of the diffusion process from a compact subset of $\mathbb{R}$ as the quantity of interest.

Symbols

$\mathbb{P}$	probability measure
$\mathbb{E}$	expectation
$\mathbb{E}(\ \vert \bullet)$	conditional expectation given $\bullet$
Var	variance
$\langle , \rangle$	inner product
δ	Kronecker symbol
$\mathbf{0}^p$	zero vector of size p
$\boldsymbol{e}_k$	standard basis vector with 1 in k-th position and 0 in others
$diag(\dots)$	diagonal matrix with non-zero elements $\dots$
$\otimes$	tensor product
∂_x	first order partial derivate w.r.t. x
∂^2_{xx}	second order partial derivate w.r.t. x

Chapter 1

Introduction

In global sensitivity analysis, one considers the uncertain input parameters as random variables, then the model output, as function of inputs, is also a random variable, whose probability distribution is uniquely determined by the model and the distribution of the inputs. The Sobol' indices show us the partial variance of the model output explained by each of the model input.

In this work, we focus on the Sobol' sensitivity analysis of a parameterized diffusion process, which is necessary for the realistic description of many applications. In this case, two different sources of uncertainty occurs - the uncertain parameters and the intrinsic randomness. In our context, when performing a Sobol' sensitivity analysis, we are only interested by the uncertainty due to input parameters on mean quantities of interest.

In this chapter, by introducing properly the parameterized diffusion process, we present the explicit model with some particular assumptions, and define the associated Sobol' indices.

1.1 Parameterized diffusion process

Let us consider a diffusion process $X : [0,T] \times \Theta \to \mathbb{R}$ ($T \in \mathbb{R}_+$) satisfying an autonomous SDE,

$$dX_t = b\left(X_t\right) dt + \sigma\left(X_t\right) dW_t \text{ with } X_0 = Z, \tag{1.1}$$

where $b : \mathbb{R} \to \mathbb{R}$ is the drift coefficient, $\sigma : \mathbb{R} \to \mathbb{R}_+$ is the diffusion coefficient, W_t is a Wiener process defined on the probability space $(\Theta, \mathcal{F}_\Theta, \mathbb{P}_\theta)$.

We give a first assumption to ensure the existence and uniqueness of X_t.

Assumption 1.1.1. *There exists a constant $K \in \mathbb{R}_+$ such that (s.t.) for all (x,y),*

$$|b(x) - b(y)| + |\sigma(x) - \sigma(y)| \leq K|y - x|.$$

Indeed, for an autonomous SDE, this global lipshitz property 1.1.1 implies the linear growth property,

$$|b(x)| + |\sigma(x)| \leq K(1 + |x|), \ \forall x.$$

Let us introduce an associated second-order functional space,

$$L^2(\Theta, \mathbb{P}_\theta) = \{v : \Theta \to \mathbb{R} \text{ s.t. } \mathbb{E}(v^2) := \int_\Theta v^2(x) d\mathbb{P}_\theta(x) < +\infty\}.$$

An additional assumption is given to ensure that $X_t \in L^2(\Theta, \mathbb{P}_\theta)$.

Assumption 1.1.2. *The initial condition Z (see (1.1)) is a random variable independent of W_t s.t. $\mathbb{E}\left(|Z|^2\right) < +\infty$.*

In other words, a SDE (1.1) satisfying the conditions 1.1.1 and 1.1.2, has a unique time-continuous (strong) solution X_t, adapted to the filtration generated by W_t and Z, s.t. $\mathbb{E}\left(\sup_{t\in[0,T]} |X_t|^2\right) < \infty$.

Remark 1.1.3. Such a process X_t is necessarily a time-homogeneous continuous Markov process, i.e. the transition density function of X_t satisfies,

$$p(x,t \mid y,s) = p(x,t-s \mid y,0), \ \ \forall 0 < s < t.$$

See, for instance, Theorem 7.1.2 and Theorem 7.2.4 in (B. Øksendal, 2003) for the proof.

We introduce then the generalized situation, where the drift coefficient and the diffusion coefficient depends also on an uncertain vector $\xi = (\xi_1, \dots, \xi_d)^T$ defined on the finite dimensional probability space $(\Xi, \mathcal{B}_\Xi, \mathbb{P}_\xi)$ with ξ_i are all independently distribued by some probability laws. In this context, the parametrized SDE defined on a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is given by

$$dX_t = \boldsymbol{b}\left(X_t, \xi\right) dt + \boldsymbol{\sigma}\left(X_t, \xi\right) dW_t, \tag{1.2}$$

hence the uncertainty of process X_t come from two sources, the randomness of Wiener process W_t and the randomness of parameters via ξ. For each choice of ξ, we assume that the conditions 1.1.1 and 1.1.2 hold on for the SDE (1.2). In order to perform the sensitivity analysis, another fundamental assumption is given below.

Assumption 1.1.4. *The uncertain parameters ξ and the Wiener process W are independent.*

With this independent condition 1.1.4, the full sample space Ω, the joint probability measure function $\mathbb{P}$ and the second-order functional space associated with (θ, ξ) have the following product structures,

$$\Omega = \Theta \times \Xi, \ \ \mathbb{P} = \mathbb{P}_\theta \otimes \mathbb{P}_\xi \text{ and } L^2(\Omega, \mathbb{P}) = L^2(\Theta, \mathbb{P}_\theta) \otimes L^2(\Xi, \mathbb{P}_\xi).$$

In the paper (O.P. Le Maître and O.M. Knio, 2015), the authors perform a sensitivity analysis of the solution X_t respectively to parameters ξ, stochasticity θ, and coupled terms. In orther words, they consider X_t as the output of a dynamical system with inputs (ξ, θ), described by the coefficients $\boldsymbol{b}$ and $\boldsymbol{\sigma}$, and they are interested in the joint probability measure function $\mathbb{P}$ of X_t.

1.2 Model issues and Sobol' indices

In this work, we consider an alternative approach, where we are interested in a mean quantity of interest with respect to the the randomness of Wiener process, for which one wants to evaluate the Sobol' indices explained by different sources of ξ. In this context, we define a model with inputs (t, x, ξ) and output y_1 by

$$y_1 = \mathcal{M}_1(t, x, \xi) = \mathbb{E}^x(X_t \mid \xi), \tag{1.3}$$

where $\mathbb{E}^x(\bullet) = \mathbb{E}(\bullet \mid X_0 = x)$. Then the associated Sobol' indices are defined by

$$S_I\left(\mathcal{M}_1(t,x,\xi)\right) = \frac{Var(\mathbb{E}(y_1 \mid \xi_I))}{Var(y_1)}, \ \forall I \subseteq \{1,\dots,d\}, \ \xi_I = (\xi_i, i \in I). \tag{1.4}$$

In chapter 3, we are also interested in the sensitivity analysis for the mean exit time from a bounded domain D of such a diffusion process X_t. To this purpose, denoting the first time that X_t exits from D by $\tau_D := \inf\{t \geq 0 : X_t \notin D\}$, we define a model with inputs (x,ξ) and output y_2 by

$$y_2 = \mathcal{M}_2(x,\xi) = \mathbb{E}^x(\tau_D \mid \xi), \tag{1.5}$$

and the associated Sobol' indices by

$$S_I\left(\mathcal{M}_2(x,\xi)\right) = \frac{Var(\mathbb{E}(y_2 \mid \xi_I))}{Var(y_2)}, \ \forall I \subseteq \{1,\dots,d\}, \ \xi_I = (\xi_i, i \in I). \tag{1.6}$$

The objective is then to propose some efficient estimators of $S_I\left(\mathcal{M}_1(t,x,\xi)\right)$ and $S_I\left(\mathcal{M}_2(x,\xi)\right)$, based on various approaches. Basically, we use in the following two tools - Monte Carlo (MC) estimator and Polynomial Chaos (PC) expansion. In chapter 2, we introduce the orthonormal polynomials, which is the core of PC. In chapter 3, we present how to apply these two tools in the parameterized SDE, in order to get the estimator of $S_I\left(\mathcal{M}_1(t,x,\xi)\right)$. An alternative approach is given in chapter 4, where we transfer the problem from the parameterized SDEs to parameterized PDEs, based on various Feymann-Kac formulas. Then we present how to apply the MC and PC in the PDEs, in order to get respectively the estimators of $S_I\left(\mathcal{M}_1(t,x,\xi)\right)$ and $S_I\left(\mathcal{M}_2(x,\xi)\right)$. To these purposes, we give some additional assumptions for the drift coefficient $\boldsymbol{b}$ and the diffusion coefficient $\boldsymbol{\sigma}$,

Assumption 1.2.1. *$\forall x,\xi,\ \boldsymbol{b}(x,\xi)$ and $\boldsymbol{\sigma}(x,\xi)$ are bounded.*

Assumption 1.2.2. *Affine decomposition hypothesis*
We suppose that $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ admit the following decomposition :

$$\forall x,\xi,\ \boldsymbol{b}(x,\xi) = \sum_{q=1}^{Q} \tilde{b}_q(x)\tilde{U}_q(\xi),\ \boldsymbol{\sigma}(x,\xi) = \sum_{q'=1}^{Q'} \tilde{\sigma}_{q'}(x)\bar{U}_{q'}(\xi),$$

where $Q, Q' \in \mathbb{N}^*$, $\tilde{b}_q, \tilde{U}_q, \tilde{\sigma}_{q'}, \bar{U}_{q'}, q = 1,\dots,Q, q' = 1,\dots,Q'$ are given functions.

Indeed, assumption 1.2.1 have been relaxed in (D.K. Pham, 2016), for instance, $\boldsymbol{b}$ satisfies the linear growth condition with an uniform constant K. In chapiter 3, we illustate the different estimators of the Sobol' indices for a parameterized Ornstein-Uhlenbeck (OU) process, which satisfies all the assumptions above (but with the weak condition of $\boldsymbol{b}$) and is widely used in many fields of applications.

Chapter 2

Preliminaries : Orthogonal polynomials

Orthogonal polynomials play an important role in representing the random quantities in the stochastic models. In this chapter, we will see how to construct a stochastic polynomial basis via the orthogonal polynomials.

2.1 General principles

Let $P_n(x)$ be a polynomial of degree n. A set of polynomials $\{P_n(x), n \in \mathbb{N}\}$ is called **orthogonal** if it satisfies the orthogonality condition,

$$\langle P_n, P_m \rangle_W := \int_{\mathcal{D}} P_n(x) P_m(x) W(x) dx = h_n \delta_{nm}, \; n, m \in \mathbb{N},$$

where $\mathcal{D}$ is the support of $\{P_n\}$ (possibly infinite), $W(x)$ is a specified weight function, h_n are non-constants and δ_{nm} is the Kronecker symbol. If $h_n = 1, \forall n$, then the set is called **orthonormal**.

An important property of orthogonal polynomials is that they satisfy a three-terms recurrence relation, which for a set of $\{P_n(x)\}$ can be written

$$-xP_n(x) = A_n P_{n+1}(x) - (A_n + C_n) P_n(x) + C_n P_{n-1}(x), \; n \geq 1,$$

where $A_n, C_n \neq 0$ and $\frac{C_n}{A_{n-1}} > 0$. Thus by specifying P_0 and P_1, it leads to generate all P_n. For instance, see the construction of some classical orthogonal polynomials (Legendre, Hermite, Laguerre, Jacobi) in apprendix A.

2.2 One-dimensional stochastic orthogonal polynomials

Let $L^2(\mathcal{X}, \mathbb{P}_X)$ be a second-order functionals space of a random variable X, endowed with an inner product

$$\langle f, g \rangle_{L^2(\mathcal{X}, \mathbb{P}_X)} = \mathbb{E}(fg) = \int_{\mathcal{X}} f(x) g(x) d\mathbb{P}_X(x).$$

If the weight function $W(x)$ of an orthogonal polynomials basis $\{\Psi_n(x), n \in \mathbb{N}\}$ is equal to the probability density function $p_X(x)$ for the random variable X, then the set $\{\Psi_n(X), n \in$

$\mathbb{N}\}$ is an 1D stochastic orthogonal polynomials basis, i.e.

$$\langle \Psi_n, \Psi_m \rangle_{L^2(\mathcal{X},\mathbb{P}_X)} = \langle \Psi_n(X), \Psi_m(X) \rangle_W = h_n \delta_{nm}, \ \ n, m \in \mathbb{N}.$$

The relationship between classical orthogonal polynomials basis and probability distributions for X is provided in table 2.1 below.

Law	$\mathcal{X}$	$p_X(x)$	Polynomials
Uniform	$[-1,1]$	$\frac{1}{2}$	Legendre
Gaussian	$\mathbb{R}$	$\frac{1}{\sqrt{2\pi}} e^{-x^2/2}$	Hermite
Gamma	$\mathbb{R}_+$	$\frac{x^{\gamma-1}e^{-x}}{\Gamma(\gamma)}$	Laguerre
Beta	$[-1,1]$	$\frac{(1+y)^{\alpha-1}(1-y)^{\beta-1}}{2^{\alpha+\beta-1}B(\alpha,\beta)}$	Jacobi

Table 2.1: Some standard distributions and classical orthogonal polynomials, where Γ is the Gamma function with parameters $\gamma > 0$ and B is the Beta function with parameter $\alpha > 0, \beta > 0$. (cf. apprendix A.3 & A.4)

Once we have the orthogonal polynomials functions $\Psi_n, n \in \mathbb{N}$ for the random variable X, after rescaling each Ψ_n by the associated orthogonal coefficient h_n, we obtain an 1D stochastic orthonormal basis.

2.3 Multidimensional stochastic orthogonal polynomials

In our framework, $\xi = (\xi_1, \ldots, \xi_d)^T$ is a random vector, in which all random variables ξ_i are mutually independent. Thus the construction of the d-dimensional orthonormal basis can be reduced to a one-dimensional construction. Denoting $(\Xi_i, \mathcal{B}_{\Xi_i}, \mathbb{P}_{\xi_i})$ the probability space associated with random variable ξ_i, the sample space Ξ, the joint probability measure $\mathbb{P}_\xi$ and the second-order functional space associated with ξ have the following product structures, due to the independence of the ξ_i :

$$\Xi = \prod_{i=1}^{d} \Xi_i, \ \ \mathbb{P}_\xi(z) = \otimes_{i=1}^{d} \mathbb{P}_{\xi_i}(z_i) \text{ and } L^2(\Xi, \mathbb{P}_\xi) = \otimes_{i=1}^{d} L^2(\Xi_i, \mathbb{P}_{\xi_i}).$$

On each dimension, we select a 1D orthonormal basis $\{\Psi^{(i)}_{\alpha_i}(z_i), \alpha_i \in \mathbb{N}^d\}$ of $L^2(\Xi_i, \mathbb{P}_{\xi_i})$, according to the marginal probability measure associated with ξ_i (use e.g. the polynomials in table 2.1 with normalization). Then

$$\Psi_\alpha(z) = \prod_{i=1}^{d} \Psi^{(i)}_{\alpha_i}(z_i) \text{ with } \alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$$

is an orthonormal basis of $L^2(\Xi, \mathbb{P}_\xi)$. Indeed,

$$\langle \Psi_\alpha, \Psi_\beta \rangle_{L^2(\Xi,\mathbb{P}_\xi)} = \prod_{i=1}^{d} \langle \Psi^{(i)}_{\alpha_i}, \Psi^{(i)}_{\beta_i} \rangle_{L^2(\Xi_i,\mathbb{P}_{\xi_i})} = \prod_{i=1}^{d} \delta_{\alpha_i\beta_i} = \delta_{\alpha\beta}.$$

In the following, we denote $\langle \bullet, \bullet \rangle_{L^2(\Xi,\mathbb{P}_\xi)}$ simply by $\langle \bullet, \bullet \rangle$.

2.4 Multidimensional polynomials approximation

In practice, we work always with a truncated finite numbers of polynomials. Every d-dimensional finite polynomials space can be represented by an associated set of indices $\mathcal{I}$. For instance, the space of d-dimensional polynomials with **partial** degree p is denoted by

$$\mathcal{I}_{d,p} = \{\alpha \in \mathbb{N}^d \mid |\alpha|_\infty := \max_{i\in\{1,\dots,d\}} \alpha_i \leq p\}, \ \mathcal{P}_{d,p} = span\{z^\alpha = \prod_{i=1}^{d} z_i^{\alpha_i} \mid \alpha \in \mathcal{I}_{d,p}\},$$

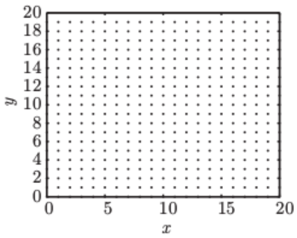
and the space of d-dimensional polynomials with **total** degree p is denoted by

$$\mathcal{J}_{d,p} = \{\alpha \in \mathbb{N}^d \mid |\alpha| := \sum_{j=1}^{d} \alpha_j \leq p\}, \ \mathcal{Q}_{d,p} = span\{z^\alpha = \prod_{j=1}^{d} z_j^{\alpha_j} \mid \alpha \in \mathcal{J}_{d,p}\}.$$

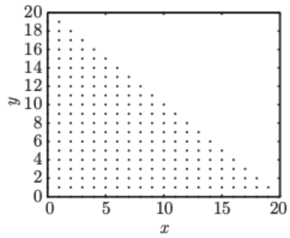
We deduce then respectively the degree of freedom of $\mathcal{P}_{d,p}$ and $\mathcal{Q}_{d,p}$,

$$\deg_{d,p}^{\mathcal{P}} := \dim(\mathcal{P}_{d,p}) = (p+1)^d, \ \deg_{d,p}^{\mathcal{Q}} := \dim(\mathcal{Q}_{d,p}) = \binom{d+p}{p},$$

hence $\mathcal{Q}_p \subseteq \mathcal{P}_p, \forall d$. The figure 2.1 shows more intuitively in the two-dimensional case.



(a) Space $\mathcal{P}_{2,p}$



(b) Space $\mathcal{Q}_{2,p}$

Figure 2.1: Comparison of degree of freedom for the two-dimensional polynomials spaces

In this work, we work within the space $\mathcal{Q}_{d,p}$, which is also called the **tensor product space**. One can see more approximate spaces in (J. Beck et al., 2012).

Remark 2.4.1. Let $K = \{0, 1, \dots, P\}$, then by using an appropriate indexing function (e.g. lexicographical order),

$$\kappa : \begin{cases} \mathcal{J}_{d,p} \to K \\ \quad \alpha \mapsto k = \kappa(\alpha), \end{cases}$$

the multidimensional orthonormal basis function can also be represented by $\{\Psi_k(z), k \in K\}$ with $P = \deg_{d,p}^{\mathcal{Q}} - 1$.

Chapter 3

Existing approaches for sensitivity analysis of parametrized SDEs

In this chapter, we present two kinds of appoaches applied in SDEs to estimate the Sobol' indices $S_I\left(\mathcal{M}_1(t,x,\xi)\right), \ \forall I \subseteq \{1,\dots,d\}$. Naturally, MC samplings for the trajectories of the SDEs with various choices of uncertainties lead to a first class of estimators. Another approach is based on the PC expansion for the parametrized diffusion process, combined with the Galerkin stochastic method for the parametrized SDE.

3.1 Monte Carlo based approach

In this section, we recall firstly how to simulate the trajectories of the diffusion process, given by

$$dX_t = b\left(X_t\right)dt + \sigma\left(X_t\right)dW_t \text{ with } X_0 = Z. \tag{3.1}$$

Then we propose the Monte Carlo estimators of the Sobol' indices in our context.

3.1.1 Simulation of a diffusion process

Consider a time discretization $0 = t_0 < t_1 < \cdots < t_N = T$ with a fixed stepsize $\Delta t = \frac{T}{N}$.
If the solution of the diffusion process X_t is explicit, then we're able to compute some conditional moments of X. Thus, from the Markovian property (remark 1.1.3), the diffusion process X can be simulated by the transition density function in the time interval $[0,T]$.

When no explicit solution is available we can use a numerical scheme to approximate a solution to Eq.(3.1) in $[0,T]$. For $i = 0,\dots,N$, we denote the approximate solution at time t_i by X_i and the increments of the Wiener process by $\Delta W_i = W(t_{i+1}) - W(t_i)$. Then we have $\Delta W_i \sim \mathcal{N}(0,\Delta t)$ i.i.d.. We give two schemes in this paper, the Euler and the Milstein scheme.

The Euler scheme of the SDE (3.1) is written by

$$X_{i+1} = X_i + b(X_i)\Delta t + \sigma(X_i)\Delta W_i, \tag{3.2}$$

which has order of strong convergence 0.5 (i.e. $\exists K > 0$ s.t. $\mathbb{E}(|X(T) - X_N|) \leq K\sqrt{\Delta t}$), and has order of weak convergence 1 (i.e. $\exists K > 0$ s.t. $|\mathbb{E}\left(f(X(T))\right) - \mathbb{E}\left(f(X_N)\right)| \leq K\Delta t$, for any polynomial f).

On the other hand, the Milstein scheme is given by

$$X_{i+1} = X_i + b(X_i)\Delta t + \sigma(X_i)\Delta W_i + \frac{1}{2}\sigma(X_i)\partial_x\sigma(X_i)((\Delta W_i)^2 - \Delta t), \tag{3.3}$$

which has order of strong convergence 1.

3.1.2 Monte Carlo estimators

Return to the parametrized diffusion process, given by

$$dX_t = \boldsymbol{b}\,(X_t,\xi)\,dt + \boldsymbol{\sigma}\,(X_t,\xi)\,dW_t. \tag{3.4}$$

Let us draw randomly by Monte Carlo (quasi Monte Carlo, hypercubes latins, etc.) two i.i.d. samples, (with respect to the probability law of $(\xi_1,\ldots,\xi_d)$), $\xi^A = \{\xi^A_{i,j}\}_{i=1,\ldots,d,j=1\ldots,n}$ and $\xi^B = \{\xi^B_{i,j}\}_{i=1,\ldots,d,j=1\ldots,n}$. Consider a new sample $\xi^I = \{\xi_{i,j}\}_{i=1,\ldots,d,j=1\ldots,n}$, $I\subseteq\{1,\ldots,d\}$, where if $i\in I$, then $\xi_{i,\bullet} = \xi^B_{i,\bullet}$, else $\xi_{i,\bullet} = \xi^A_{i,\bullet}$.

Draw next $m\in\mathbb{N}^*$ independent gaussian vectors $\zeta^{(k)} = \left(\zeta^k_1,\ldots,\zeta^k_N\right)^T$, $k = 1,\ldots,m$, where $\zeta^k_l \sim \mathcal{N}(0,1)$ i.i.d. for $l = 1\ldots,N$.

With each batch $(\xi^I,\zeta^{(k)})$ and $(\xi^B,\zeta^{(k)})$, we simulate the trajectories $X^{I,(k)}_t$ and $X^{B,(k)}_t$, based on the transition density function or an approximate scheme (3.2), (3.3). We compute then the scenarios

$$y^I = \frac{1}{m}\sum_{k=1}^m X^{I,(k)}_t \text{ and } y^B = \frac{1}{m}\sum_{k=1}^m X^{B,(k)}_t.$$

Finally, we can approximate the Sobol' indices $S_I\left(\mathcal{M}_1(t,x,\xi)\right)$, $\forall I\subseteq\{1,\ldots,d\}$ by a MC estimator,

$$S_I\left(\mathcal{M}_1(t,x,\xi)\right) \approx \frac{\frac{1}{n}\sum_{j=1}^n y^B_j y^I_j - \left(\frac{1}{n}\sum_{j=1}^n \frac{y^B_j+y^I_j}{2}\right)^2}{\frac{1}{n}\sum_{j=1}^n \frac{(y^B_j)^2+(y^I_j)^2}{2} - \left(\frac{1}{n}\sum_{j=1}^n \frac{y^B_j+y^I_j}{2}\right)^2}.$$

3.2 Polynomial Chaos based appoach

This method is well developped in the paper (O.P. Le Maître and O.M. Knio, 2015), in which one can see the computation of Sobol' indices from PC coefficients is immediate. We explain in the following how to apply this approach in our case.

3.2.1 PC expansion for a parametrized diffusion process

For almost any trajectory of W_t, we are lead to consider a PC expansion of the diffusion process X_t in the approximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi,\mathbb{P}_\xi)$,

$$X_t \approx \sum_{k=0}^P [X_k]_t \Psi_k(\xi),$$

where $[X_k]$ are the coefficient process to determine, which are independent of ξ but only depend on W_t, $\Psi_k(\xi)$ are d-dimensional orthonormal polynomial functions and $P+1 = \binom{d+p}{p}$ (see in remark 2.4.1).

One advantage of the PC expansion for the parametrized diffusion process is that it enables us to compute their approximate statistics from the coefficient process $[X]_t$, based on the independence of $[X_k]$ and ξ, also on the orthogonality of the stochastic basis Ψ_k.

$$\begin{aligned}\mathbb{E}^x(X_t \mid \xi = \xi') &\approx \mathbb{E}^x\left(\sum_{k=0}^{P}[X_k]_t\Psi_k(\xi) \mid \xi = \xi'\right)\\ &= \sum_{k=0}^{P}\Psi_k(\xi')\mathbb{E}^x([X_k]_t \mid \xi = \xi') = \sum_{k=0}^{P}\mathbb{E}^x([X_k]_t)\Psi_k(\xi'),\end{aligned}$$

$$\begin{aligned}\mathbb{E}\left(\mathbb{E}^x(X_t \mid \xi = \xi')\right) &\approx \mathbb{E}\left(\sum_{k=0}^{P}\mathbb{E}^x([X_k]_t)\Psi_k(\xi')\right)\\ &= \sum_{k=0}^{P}\mathbb{E}^x([X_k]_t)\mathbb{E}(\Psi_k(\xi')) = \mathbb{E}^x([X_0]_t),\end{aligned}$$

$$\begin{aligned}Var\left(\mathbb{E}^x(X_t \mid \xi = \xi')\right) &\approx \mathbb{E}\left(\left(\mathbb{E}^x(X_t \mid \xi = \xi')\right)^2\right) - \left(\mathbb{E}^x([X_0]_t)\right)^2\\ &= \sum_{k=0}^{P}\left(\mathbb{E}^x([X_k]_t)\right)^2 - \left(\mathbb{E}^x([X_0]_t)\right)^2 = \sum_{k=1}^{P}\left(\mathbb{E}^x([X_k]_t)\right)^2,\end{aligned}$$

$$\mathbb{E}\left(\mathbb{E}^x(\mathcal{M}_1(t,x,\xi) \mid \xi = \xi_I\right) \approx \mathbb{E}\left(\sum_{k=0}^{P}\mathbb{E}^x([X_k]_t)\Psi_k(\xi) \mid \xi = \xi_I\right) = \sum_{k'\in K_I}\mathbb{E}^x([X_{k'}]_t)\Psi_{k'}(\xi_I),$$

where $I \subseteq \{1,\dots,d\}$ and $K_I := \{k \in \{1,\dots,P\} \mid \Psi_k(z) = \Psi_k(z = \xi_I)\}$.

$$Var\left((\mathbb{E}^x(\mathcal{M}_1(t,x,\xi) \mid \xi = \xi_I)\right) \approx \sum_{k'\in K_I}\left(\mathbb{E}([X_{k'}]_t)\right)^2.$$

Thus, one can estimate the Sobol' indices by

$$S_I\left(\mathcal{M}_1(t,x,\xi)\right) \approx \frac{\sum_{k'\in K_I}\left(\mathbb{E}^x([X_{k'}]_t)\right)^2}{\sum_{k=1}^{P}\left(\mathbb{E}^x([X_k]_t)\right)^2}.$$

The next problem is how to determine the mean trajectory of each coefficient process $[X_k]_t$, $k = 0,\dots,P$. To this purpose, the stochastic Galerkin method combined with samplings will be applied.

3.2.2 Stochastic Galerkin method for a parametrized SDE

It is called stochastic Galerkin method, since we follow a Galerkin projection on a stochastic basis. More precisely, we replace the diffusion process X in the parametrized SDE (3.4) by the PC expansion, then within the assumption 1.2.1 (or the weak assumptions in (D.K. Pham, 2016)) we project the obtained equation in the approximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi,\mathbb{P}_\xi)$,

$$d[X_k] = \langle \boldsymbol{b}\left(\sum_{l=0}^{P}[X_l]\Psi_l,\xi\right),\Psi_k\rangle dt + \langle \boldsymbol{\sigma}\left(\sum_{l=0}^{P}[X_l]\Psi_l,\xi\right),\Psi_k\rangle dW_t, \forall k = 0,\dots,P.$$

Let us denote

$$[\boldsymbol{b}_k] := \langle \boldsymbol{b}\left(\sum_{l=0}^{P}[X_l]\Psi_l, \xi\right), \Psi_k\rangle \text{ and } [\boldsymbol{\sigma}_k] := \langle \boldsymbol{\sigma}\left(\sum_{l=0}^{P}[X_l]\Psi_l, \xi\right), \Psi_k\rangle.$$

We get then a system of $P+1$ coupled SDEs,

$$d[X_k] = [\boldsymbol{b}_k]([X_0], \dots, [X_P])dt + [\boldsymbol{\sigma}_k]([X_0], \dots, [X_P])dW_t, \ k = 0, \dots, P.$$

Denoting $[\boldsymbol{X}] = ([X_0], \dots, [X_P])^T \in \mathbb{R}^{P+1}$, the previous system can be expressed by the following form, due to the affine decomposition hypothesis 1.2.2 of $\boldsymbol{b}, \boldsymbol{\sigma}$ in the space $\mathcal{Q}_{d,p}$.

$$\begin{cases} d[\boldsymbol{X}]_t = \boldsymbol{B}[\boldsymbol{X}]_t dt + \boldsymbol{\Sigma}[\boldsymbol{X}]_t dW_t, \ t > 0 \\ [\boldsymbol{X}]_0 = (\langle X_0, \Psi_0\rangle, \dots, \langle X_0, \Psi_P\rangle)^T = (X_0, 0 \dots, 0)^T \in \mathbb{R}^{P+1}, \end{cases} \tag{3.5}$$

where $\boldsymbol{B}, \boldsymbol{\Sigma} \in \mathcal{M}_{P+1}(\mathbb{R})$.

One can apply an approximate scheme (e.g. Euler, Milstein) to simulate the trajectories of the coupled processes $[\boldsymbol{X}]$. However, we should emphasize that the coefficient processes $[X_k], k = 0, \dots, P$ are all driven by a **unique** Wiener process. For the j-th sample of the discretized Wiener process increments, $\Delta W_i^j = W_{i+1}^j - W_i^j, \ i = 0, \dots, N, \ j = 1, \dots, m$, we denote $[X_k]^j$ the simulated trajectory, then the mean trajectory of the coefficient process $[X_k]$ can be approximated by

$$\mathbb{E}^x([X_k]) \approx \frac{1}{m}\sum_{j=1}^{m}[X_k]^j.$$

Chapter 4

New methods based on Feynman-Kac formulas

In this chapter, we firstly introduce the Feynman-Kac formula, which allows us to transform our problem from the parametrized SDE to a parametrized parabolic PDE, then we apply PC expansion to the solution of the parametrized PDE. Once we know the coefficients of PC expansion, one can see that the estimation of the Sobol' indices $S_I(\mathcal{M}_1(t,x,\xi))$ is immediate, thanks to the orthogonality of the stochastic basis and the linearity of the PC expansion. In order to solve the parametrized PDE, we still apply the stochastic Galerkin technique. In a similar way, one can apply another Feynman-Kac formula (we call it localized Feynman-Kac formula in this work) to transform the parametrized SDE to a parametrized elliptic PDE with Dirichlet conditions. Using the same approaches as in the parabolic case, we can immediately approximate the Sobol' indices $S_I(\mathcal{M}_2(x,\xi))$.

4.1 Parabolic case

The famous Feynman-Kac formula reveales profoundly the relation between the solutions of SDEs and the solutions of parabolic PDEs.

4.1.1 Feynman-Kac formula

Theorem 4.1.1. *Let us consider an autonomous SDE,*

$$dX_t = b(X_t)\,dt + \sigma(X_t)\,dW_t, \tag{4.1}$$

where the coeffcient functions b and σ are bounded and satisfy the lipschiz condition 1.1.1. We assume also that $0 < m \le \sigma^2(x),\ \forall x \in \mathbb{R}$.

Let us consider a parabolic PDE,

$$\begin{cases} \partial_t u(t,x) + k(x)u(t,x) = \mathcal{A}u(t,x) + g(x), \ \forall (t,x) \in (0,T] \times \mathbb{R} \\ u(0,x) = f(x), \ \forall x \in \mathbb{R} \\ \lim_{|x|\to\infty} |u(t,x)| = 0, \ \forall t \in [0,T], \end{cases}$$

where $f : \mathbb{R} \to \mathbb{R}$ is a continuous bounded function s.t. $f \in L^2(\mathbb{R})$ and $\lim_{|x|\to\infty} |f(x)| = 0$, $g, k : \mathbb{R} \to \mathbb{R}$ are also continuous bounded functions, and the operator $\mathcal{A}$ acting on functions *in* φ *of* $\mathcal{C}^2(\mathbb{R})$ *by*

$$(\mathcal{A}\varphi)(t,x) = \frac{1}{2}\sigma^2(x)\partial_{xx}\varphi(t,x) + b(x)\partial_x\varphi(t,x),\ \ \forall(t,x) \in (0,T] \times \mathbb{R}.$$

Then the function $u(t,x)$ *of class* $\mathcal{C}^{1,2}([0,T]\times\mathbb{R};\mathbb{R})$ *has the stochastic representation*

$$u(t,x) = \mathbb{E}^x\left[f(X_t)\exp\left(-\int_0^t k(X_s)ds\right) + \int_0^t g(X_s)\exp\left(-\int_0^s k(X_r)dr\right)ds\right]. \tag{4.2}$$

See the proof in chapter 3 of (E. Pardoux and A. Răşcanu, 2014).

In particular, setting $k = g \equiv 0$ and $f(x) = x,\ \forall x \in \mathbb{R}$, Eq.(4.2) becomes $u(t,x) = \mathbb{E}^x(X_t)$, where $u(t,x)$ is solution to the Cauchy problem,

$$\begin{cases} \partial_t u(t,x) = \mathcal{A}u(t,x),\ \forall(t,x) \in (0,T]\times\mathbb{R} \\ \quad u(0,x) = x,\ \ \forall x \in \mathbb{R}. \end{cases}$$

Indeed, this approach can be extended to the case of parametrized SDE (1.2), since from the begining we have assumed that $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ satisfy the conditions in Feynman-Kac formula. Thus, the random variable

$$u(t,x,\xi) = \mathbb{E}^x(X_t \mid \xi) = \mathcal{M}_1(t,x,\xi) = y_1$$

is the solution of the parametrized parabolic PDE,

$$\begin{cases} \partial_t u(t,x,\xi) = \dfrac{1}{2}\boldsymbol{\sigma}^2(x,\xi)\partial^2_{xx}u(t,x,\xi) + \boldsymbol{b}(x,\xi)\partial_x u(t,x,\xi),\ \ \forall(t,x) \in (0,T]\times\mathbb{R} \\ \quad u(0,x,\xi) = x,\ \ \forall x \in \mathbb{R}. \end{cases}$$

In practice, we are interested in the solution of the parametrized PDE defined in a bounded open domain $D = (l,r) \subset \mathbb{R}$,

$$\begin{cases} \partial_t u(t,x,\xi) = \dfrac{1}{2}\boldsymbol{\sigma}^2(x,\xi)\partial^2_{xx}u(t,x,\xi) + \boldsymbol{b}(x,\xi)\partial_x u(t,x,\xi),\ \ \forall(t,x) \in (0,T]\times D \\ \quad u(0,x,\xi) = x,\ \ \forall x \in \mathbb{R}. \\ \quad u(t,l,\xi) = \mathbb{E}^{x=l}(X_t \mid \xi),\ \ \forall t \in (0,T] \\ \quad u(t,r,\xi) = \mathbb{E}^{x=r}(X_t \mid \xi),\ \ \forall t \in (0,T] \end{cases} \tag{4.3}$$

4.1.2 PC expansion for Sobol' indices

We decompose the solution $u(t,x,\xi)$ of the parametrized PDE (4.3) by PC expansion in the appoximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi,\mathbb{P}_\xi)$,

$$u(t,x,\xi) \approx \sum_{k=0}^{P} u_k(t,x)\Psi_k(\xi),$$

where $u_k(t,x)$ are deterministic coefficients and $\Psi_k(\xi)$ are d-dimensional orthonormal polynomial functions. Once we have the coefficients of the expansion, we can compute some approximate statistics with the formulas,

$$\mathbb{E}(u(t,x,\xi)) \approx \mathbb{E}\left(\sum_{k=0}^{P} u_k(t,x)\Psi_k(\xi)\right) = \sum_{k=0}^{P} u_k(t,x)\mathbb{E}_\xi(\Psi_k(\xi)) = \sum_{k=0}^{P} u_k(t,x)\delta_{0k} = u_0(t,x),$$

$$Var(u(t,x,\xi)) = \mathbb{E}\left(u^2(t,x,\xi)\right) - \left[\mathbb{E}\left(u(t,x,\xi)\right)\right]^2 \approx \sum_{k=0}^{P} u_k^2(t,x) - u_0(t,x) = \sum_{k=1}^{P} u_k^2(t,x),$$

$$\mathbb{E}\left[u(t,x,\xi) \mid \xi = \xi_I\right] \approx \sum_{k' \in K_I} \Psi_{k'}(\xi_I)\mathbb{E}(u_{k'}(t,x)) = \sum_{k' \in K_I} u_{k'}(t,x)\Psi_{k'}(\xi_I),$$

where $I \subseteq \{1,\ldots,d\}$ and $K_I := \{k \in \{1,\ldots,P\} \mid \Psi_k(z) = \Psi_k(z = \xi_I)\}$,

$$Var\left[\mathbb{E}\left(u(t,x,\xi) \mid \xi = \xi_I\right)\right] \approx \sum_{k' \in K_I} u_{k'}^2(t,x).$$

These lead to estimate the Sobol' indices by

$$S_I\left(\mathcal{M}_1(t,x,\xi)\right) = \frac{Var[\mathbb{E}(y_1 \mid \xi_I)]}{Var(y_1)} \approx \frac{\sum_{k' \in K_I} u_{k'}^2(t,x)}{\sum_{k=1}^{P} u_k^2(t,x)}.$$

4.2 Elliptic case

As we know, there exists also a probabilistic representation for the solution of elliptic PDEs.

4.2.1 Localized Feynman-Kac formula

Theorem 4.2.1. *Let us consider an elliptic PDE with Dirichlet conditions,*

$$\begin{cases} \mathcal{A}(x)u(x) - k(x)u(x) = -g(x), & \forall x \in D \\ u(x) = f(x), & \forall x \in \partial D, \end{cases}$$

where $\mathcal{A}$ is an elliptic operator of type

$$\mathcal{A}(x)\varphi(x) = \frac{1}{2}\sigma^2(x)\varphi''(x) + b(x)\varphi'(x), \quad \forall \varphi \in \mathcal{C}^2(D;\mathbb{R}), \quad \forall x \in D,$$

and the coefficient b and σ are the bounded functions of the SDE (4.1) satisfying else

$$0 < m \le \sigma^2(x) \le M < \infty, \quad |(\sigma^2)'(x)| \le M, \quad |b'(x)| \le M, \quad \forall x \in D.$$

Assuming that the functions $k \ge 0$ and g are of class $\mathcal{C}^2(\bar{D};\mathbb{R})$, hence g is bounded in $\bar{D} = [l,r]$.

Then the solution u of class $\mathcal{C}^2(\bar{D};\mathbb{R})$ has the probabilistic representation

$$u(x) = \mathbb{E}^x\left[f(X_{\tau_D})\exp\left(-\int_0^{\tau_D} k(X_r)dr\right) + \int_0^{\tau_D} g(X_s)\exp\left(-\int_0^{s} k(X_r)dr\right)ds\right]. \quad (4.4)$$

See the proof in chapter 3 of (E. Pardoux and A. Răşcanu, 2014).

In particular, setting $f = k \equiv 0$ and $g \equiv 1$, the mean exit time $u(x) = \mathbb{E}^x[\tau_D]$ will be the solution of the elliptic PDE with a homogenous Dirichlet condition,

$$\begin{cases} -\mathcal{A}(x)u(x) = 1, & \forall x \in D \\ u(x) = 0, & \forall x \in \partial D. \end{cases}$$

We extend then this approch to the parametrized SDE (1.2), hence the random variable

$$u(x,\xi) = \mathbb{E}^x[\tau_D \mid \xi] = \mathcal{M}_2(x,\xi) = y_2$$

will be the solution of the parametrized elliptic PDE with homogenous Dirichlet condition,

$$\begin{cases} -\frac{1}{2}\boldsymbol{\sigma}^2(x,\xi)u''(x,\xi) - \boldsymbol{b}(x,\xi)u'(x,\xi) = 1, \ \forall x \in D \\ \hfill u(x,\xi) = 0, \ \forall x \in \partial D. \end{cases} \tag{4.5}$$

4.2.2 PC expansion for Sobol' indices

In a similar way to the parabolic case, decomposing the solution $u(x,\xi)$ of the parametrized PDE (4.5) by PC expansion in the appoximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi, \mathbb{P}_\xi)$,

$$u(x,\xi) \approx \sum_{k=0}^{P} u_k(x)\Psi_k(\xi),$$

we get the following approximate statistics,

$$Var(u(x,\xi)) \approx \sum_{k=1}^{P} u_k^2(x) \text{ and } Var\left[\mathbb{E}\left(u(x,\xi) \mid \xi = \xi_I\right)\right] \approx \sum_{k' \in K_I} u_{k'}^2(x),$$

which leads to

$$S_I\left(\mathcal{M}_2(x,\xi)\right) = \frac{Var[\mathbb{E}(y_2 \mid \xi_I)]}{Var(y_2)} \approx \frac{\sum_{k' \in K_I} u_{k'}^2(x)}{\sum_{k=1}^{P} u_k^2(x)}.$$

4.3 General principles of stochastic Galerkin method

We see in both two previous sections that the problem returns to determine the coefficients of expansion. We present in this section the stochastic Galerkin technique for general PDEs with uncertain parameters. Let us consider a parametrized differential equation

$$\mathcal{A}(t,x,\xi;u) = f(t,x,\xi),$$

where u is the solution, f is the source term and $\mathcal{A}$ is a general differential operator that may contain spatial derivatives, time derivatives, and linear terms. Appropriate initial and boundary conditions are assumed.

We substitude the PC expansion of $u = \sum_{k=0}^{P} u_k \Psi_k$ into the differential equation, and we project the resulting equation in the same space $\mathcal{Q}_{d,p}$,

$$\langle \mathcal{A}\left(t,x,\xi;\sum_{l=0}^{P} u_l \Psi_l\right), \Psi_k \rangle = \langle f(t,x,\xi), \xi \rangle, \ k = 0,\dots,P.$$

By the orthogonality of the stochastic basis, the parametrized differential equation reduces to a system of $(P+1)$ coupled deterministic differential equations for the coefficients of expansion u_k, $k = 0,\dots,P$. Due to the ideal affine decomposition hypothesis 1.2.2 of $\boldsymbol{b}, \boldsymbol{\sigma}$ in the space $\mathcal{Q}_{d,p}$, and using an appropriate spatial and temporal discretization of the coefficients, the problem reduces to solve a linear system (or evolution of linear systems in parabolic case).

An alternative approach is to firstly discretise the parametrized PDE, and then project the discretized scheme in the stochastic basis. We will detail all these points for the parametrized OU process in next chapter.

Remark 4.3.1. The convergence of stochastic Galerkin method have been studied in serveral works, for instance see section 6 in (A. Nouy, 2017). According to the author's discussions, we should add an unformly bounded condition for the diffusion coeffcient $\boldsymbol{\sigma}$ in this work, in order to ensure the unformly coercive and unformly continuous of the bilinear form of the Eq.(4.3) and Eq.(4.5), which leads to the convergence.

Assumption 4.3.2. *We assume that $\boldsymbol{\sigma}$ in Eq.(4.3) and Eq.(4.5) satisfies*

$$0 < m \leq \boldsymbol{\sigma}(x, \xi) \leq M < \infty, \text{ for almost all } x \text{ and } \xi,$$

where m, M independent of ξ.

Indeed, this condition is stronger than the ones in Feynman-Kac formulas 4.1.1 and 4.2.1 where the lower bounds and upper bounds of $\boldsymbol{\sigma}$ depend on each choice of ξ.

Chapter 5

Numerical example : Parametrized Ornstein-Uhlenbeck process

In this chapter, we firstly define two models $\mathcal{M}_1$ and $\mathcal{M}_2$ with the associated Sobol' indices $S_I(\mathcal{M}_1)$ and $S_I(\mathcal{M}_2)$, for a particular parametrized OU process. Moreover, the explicit solutions of $S_I(\mathcal{M}_1)$ have been computed, based on their known conditional moments. In order to perform the PC expansion for our exemple, we precise then how to construct the two-dimensional orthonormal Legendre polynomials. For the approximation of $S_I(\mathcal{M}_1)$, we present the detail numerical schemes to solve the stochastic Galerkin formalisms respectively for the parametrized SDE and for the parametrized PDE, as mentioned in the two previous chapters. For the approximation of $S_I(\mathcal{M}_2)$, we present a numerical scheme to solve the stochastic Galerkin formalisms for the associated PDE, and also a MC estimator at PDE level as a benchmark. Finally, some numerical results have been given based on the concerned methods.

5.1 Model and Sobol' indices

In this section, we recall some useful properties of the OU process at first. Then we define properly a parametrized OU process, the two concerned models with the associated Sobol' indices. In particular, we're interested in the explicit solutions of $S_I(\mathcal{M}_1)$.

5.1.1 Properties of the OU process

Let us consider a simplified OU process given by the SDE

$$dX_t = -\alpha X_t dt + \beta dW_t,\ t > 0 \text{ with } X_0 = x,$$

where $\alpha, x \in \mathbb{R}$, and $\beta \in \mathbb{R}_+$.

Define $Y_t = e^{\alpha t} X_t$ and applying the Itô's formula with $f(t,x) = e^{\alpha t} x$ yields

$$dY_t = \left(\partial_t f(t,X_t) + \alpha \partial_x f(t,X_t) + \frac{1}{2}\beta^2 \partial_{xx}^2 f(t,X_t)\right) dt + \beta \partial_x f(t,X_t) dW_t = \beta e^{\alpha t} dW_t,$$

hence $Y_t = Y_0 + \beta \int_0^t e^{\alpha s} dW_s$. Finally, $X_t = X_0 e^{\alpha t} + \beta \int_0^t e^{-\alpha(t-s)} dW_s$.

The conditional moments of X_t can then be directly computed,

$$\mathbb{E}(X_t \mid X_0 = x) = xe^{-\alpha t} \text{ and } Var(X_t \mid X_0 = x) = \frac{\beta^2}{2\alpha}(1 - e^{-2\alpha t}). \tag{5.1}$$

We deduce that the transition density function of X_t is Gaussian,

$$p(y, t \mid x, 0) = \frac{1}{\beta\sqrt{\frac{\pi}{\alpha}(1 - e^{-2\alpha t})}} \exp\left(-\frac{\alpha(y - xe^{-\alpha t})^2}{\beta^2(1 - e^{-2\alpha t})}\right).$$

For the time discretization $0 = t_0 < t_1 < \cdots < t_N = T$ with fixed stepsize $\Delta t = \frac{T}{N}$, we deduce an exacte scheme by the Markovian property of X_t,

$$X_{i+1} = X_i e^{-\alpha \Delta t} + \beta\sqrt{\frac{1 - e^{-2\alpha\Delta t}}{2b}}\zeta_i, \ \zeta \sim \mathcal{N}(0,1) \text{ i.i.d.}, \ i = 0, \ldots, N-1. \tag{5.2}$$

5.1.2 OU process with uncertain parameters

Let us now consider the OU process X_t with uncertain parameters $\xi = (\xi_1, \xi_2)^T$, driven by the follwing parametrized SDE,

$$dX_t = -\alpha(\xi_1)X_t dt + \beta(\xi_2)dW_t, \ t > 0 \text{ with } X_0 = x \in \mathbb{R}, \tag{5.3}$$

where $\xi_i \sim \mathcal{U}([0,1])$ i.i.d., $i = 1, 2$ independent of the Wiener process W_t, the drift coefficient α and the diffusion coefficient β are characterized respectively by their mean $\mu_i \in \mathbb{R}$ and standard deviation $\sigma_i \in \mathbb{R}$, $i = 1, 2$.

In this case, one can show more precisely that

$$\begin{cases} \alpha(\xi_1) = \mu_1 + \sqrt{3}\sigma_1(2\xi_1 - 1) \sim \mathcal{U}\left([\mu_1 - \sqrt{3}\sigma_1, \mu_1 + \sqrt{3}\sigma_1]\right) \\ \beta(\xi_2) = \mu_2 + \sqrt{3}\sigma_2(2\xi_2 - 1) \sim \mathcal{U}\left([\mu_2 - \sqrt{3}\sigma_2, \mu_2 + \sqrt{3}\sigma_2]\right) \end{cases} \tag{5.4}$$

Remark 5.1.1. We assume that the characterized parameters of β should satisfy $\mu_2 > \sqrt{3}\sigma_2$, which directly leads to the uniformly bounded condition 4.3.2.

In this context, according to the definitions in section 1.2, the first model for sensitivity analysis becomes,

$$y_1 = \mathcal{M}_1(t, x, \xi) = \mathbb{E}^x(X_t(\omega, \xi) \mid \xi).$$

Then the associated (first order) Sobol' indices are defined by

$$S_i\left(\mathcal{M}_1(t, x, \xi)\right) = \frac{Var(\mathbb{E}(y_1 \mid \xi_i))}{Var(y_1)}, \ i = 1, 2.$$

One can immediately deduce the Sobol' indices for the interaction of ξ_1 and ξ_2,

$$S_{\text{inter}}\left(\mathcal{M}_1(t, x, \xi)\right) = 1 - S_1\left(\mathcal{M}_1(t, x, \xi)\right) - S_2\left(\mathcal{M}_1(t, x, \xi)\right).$$

Similarly, we have the second model defined by

$$y_2 = \mathcal{M}_2(x, \xi) = \mathbb{E}^x(\tau_D \mid \xi),$$

with the associated Sobol' indices,

$$\begin{cases} S_i\left(\mathcal{M}_2(x,\xi)\right) = \dfrac{Var(\mathbb{E}(y_2 \mid \xi_i))}{Var(y_2)}, \ i = 1,2, \\ S_{\text{inter}}\left(\mathcal{M}_2(x,\xi)\right) = 1 - S_1\left(\mathcal{M}_2(x,\xi)\right) - S_2\left(\mathcal{M}_2(x,\xi)\right). \end{cases}$$

Remark 5.1.2. We wont precise the MC approach applied in the parametrized SDE in the following. Indeed, one can directly apply the algorithm mentioned in section 3.1.2 for $\xi = (\xi_1, \xi_2)$, using the exact scheme (5.2). We will only show the numerical results in the last part.

5.1.3 Explicit solutions of Sobol' indices

We deduce by the conditional moment (5.1), $\mathbb{E}^x(X_t \mid \xi) = xe^{-\alpha(\xi_1)t}$. Based on the known probability law (5.3) of $\alpha(\xi_1)$, we compute then the explicit expressions of the follwing statistics,

$$\begin{aligned} E_1 &:= \mathbb{E}\left(\mathbb{E}^x(X_t \mid \xi)\right) = x\mathbb{E}\left(e^{-\alpha(\xi_1)t}\right) = x\int_{\mu_1-\sqrt{3}\sigma_1}^{\mu_1+\sqrt{3}\sigma_1} e^{-ut}\frac{1}{2\sqrt{3}\sigma_1}du \\ &= \frac{x}{2\sqrt{3}\sigma_1 t}e^{-\mu_1 t}\left(e^{\sqrt{3}\sigma_1 t} - e^{-\sqrt{3}\sigma_1 t}\right) = xe^{-\mu_1 t}\frac{\sinh(\sqrt{3}\sigma_1 t)}{\sqrt{3}\sigma_1 t}, \\ E_2 &:= \mathbb{E}\left[\left(\mathbb{E}^x(X_t \mid \xi)\right)^2\right] = x^2\mathbb{E}\left(e^{-2\alpha(\xi_1)t}\right) = x^2 e^{-2\mu_1 t}\frac{\sinh(2\sqrt{3}\sigma_1 t)}{2\sqrt{3}\sigma_1 t}, \end{aligned}$$

which lead to the total variance

$$Var(y_1) = Var\left(\mathbb{E}^x(X_t \mid \xi)\right) = E_2 - E_1^2.$$

On the other hand, we can also compute the explicit partial variances caused by each ξ_i, $i = 1,2$,

$$\begin{cases} Var(\mathbb{E}(y_1 \mid \xi_1)) = Var(\mathbb{E}(xe^{-\alpha t} \mid \xi_1)) = Var(xe^{-\alpha(\xi_1)t}) = Var(y_1), \\ Var(\mathbb{E}(y_1 \mid \xi_2)) = Var(\mathbb{E}(xe^{-\alpha t} \mid \xi_2)) = Var(\mathbb{E}_\xi(xe^{-\alpha t})) = 0, \end{cases}$$

which lead to the explicit Sobol' indices,

$$S_1\left(\mathcal{M}_1(t,x,\xi)\right) = 1,\ S_2\left(\mathcal{M}_1(t,x,\xi)\right) = 0 \text{ and } S_{\text{inter}}\left(\mathcal{M}_1(t,x,\xi)\right) = 0.$$

5.2 2D orthonormal Legendre polynomials

In order to perform the PC expansion for our exemple, we need the 2D orthonormal Legendre polynomials defined on $[0,1]$. A set of 1D Legendre polynomials $\{P_n(x),\ n \in \mathbb{N}\}$ defined on $[-1,1]$ can be etabished by the recurrence in appendix A.1. By an affine transformation $x \mapsto 2x-1$, we obatin a set of 1D Legendre polynomials $\{\tilde{P}_n(x),\ n \in \mathbb{N}\}$ defined on $[0,1]$, which is determined by the recurrence

$$\begin{cases} \tilde{P}_0(x) = 1 \\ \tilde{P}_1(x) = 2x - 1 \\ (n+1)\tilde{P}_{n+1}(x) = (2n+1)(2x-1)\tilde{P}_n(x) - n\tilde{P}_{n-1}(x),\ n \ge 1, \end{cases}$$

with the associated orthogonality $\langle \tilde{P}_n, \tilde{P}_m \rangle_{\tilde{W}} = \frac{1}{2n+1}\delta_{nm}$.

Then a set of 1D orthonormal Legendre polynomials $\{\bar{P}_n(x),\ n \in \mathbb{N}\}$ is obtained by $\bar{P}_n(x) = \sqrt{2n+1}\tilde{P}_n(x)$. A few of such polynomials have been shown in figure 5.1.

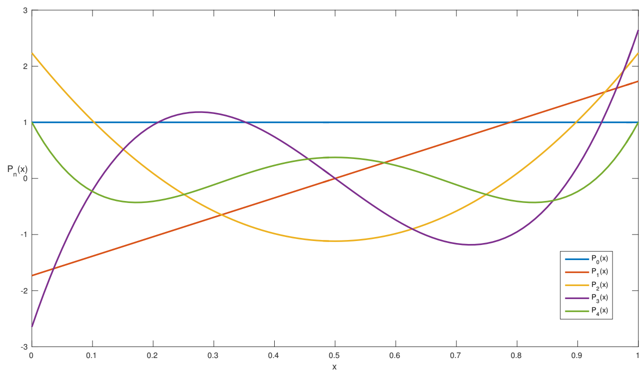


Figure 5.1: The first few 1D orthonormal Legendre polynomials defined on $[0,1]$

Let us consider $\Psi^{(1)}_{r_1}(\xi_1) = \bar{P}_{r_1}(\xi_1)$ and $\Psi^{(2)}_{r_2}(\xi_2) = \bar{P}_{r_2}(\xi_2)$, then according to the section 2.3, a set of 2D orthonormal Legendre polynomials $\{\Psi_r(\xi),\ r \in \mathbb{N}^2\}$ can be constructed by

$$\Psi_r(\xi) = \Psi^{(1)}_{r_1}(\xi_1)\Psi^{(2)}_{r_2}(\xi_2).$$

Finally using the following indexing function

$$\kappa : \begin{cases} \mathbb{N} \times \mathbb{N} \to \mathbb{N} \\ (r_1, r_2) \mapsto k = \dfrac{(r_1 + r_2 + 1)(r_1 + r_2 + 2)}{2} - r_1 - 1, \end{cases}$$

we can also represent such polynomials by $\Psi_k,\ k \in \mathbb{N}$. Some their explicit expressions are given in Table 5.1.

k	(r_1, r_2)	$\Psi_k(\xi_1, \xi_2)$
0	$(0,0)$	1
1	$(1,0)$	$\sqrt{3}(2\xi_1 - 1)$
2	$(0,1)$	$\sqrt{3}(2\xi_2 - 1)$
3	$(2,0)$	$\sqrt{5}(6\xi_1^2 - 6\xi_1 + 1)$
4	$(1,1)$	$3(2\xi_1 - 1)(2\xi_2 - 1)$
5	$(0,2)$	$\sqrt{5}(6\xi_2^2 - 6\xi_2 + 1)$
6	$(3,0)$	$\sqrt{7}(20\xi_1^3 - 30\xi_1^2 + 12\xi_1 - 1)$
7	$(2,1)$	$\sqrt{15}(6\xi_1^2 - 6\xi_1 + 1)(2\xi_2 - 1)$
8	$(1,2)$	$\sqrt{15}(2\xi_1 - 1)(6\xi_2^2 - 6\xi_2 + 1)$
9	$(0,3)$	$\sqrt{7}(20\xi_2^3 - 30\xi_2^2 + 12\xi_2 - 1)$

Table 5.1: The first ten 2D orthonormal Legendre polynomials

From the distributions (5.4) and the table 5.1, one can immediately find a PC expansion for the drift coefficient and the diffusion coefficient,

$$\alpha(\xi_1) = \mu_1\Psi_0(\xi) + \sigma_1\Psi_1(\xi) \text{ and } \beta(\xi_2) = \mu_2\Psi_0(\xi) + \sigma_2\Psi_2(\xi).$$

Remark 5.2.1. One can see the construction of indexing function more precisely by the following table.

(r_1, r_2)	0	1	2	3	$\cdots$
0	0	2	5	9	$\iddots$
1	1	4	8	13	$\iddots$
2	3	7	12	18	$\iddots$
3	6	11	17	24	$\iddots$
$\vdots$	$\iddots$	$\iddots$	$\iddots$	$\iddots$	$\iddots$

Table 5.2: Construction of the indexing function κ

5.3 Stochastic Galerkin solver for the parametrized SDE

As mentioned in section 3.2, we decompose the parametrized OU process X_t by PC expansion in the approximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi, \mathbb{P}_\xi)$,

$$X_t \approx \sum_{k=0}^{P} [X_k]_t \Psi_k(\xi),$$

and we project the parametrized SDE (5.3) in the space $\mathcal{Q}_{d,p}$: for $k = 0, \dots, P$,

$$\begin{aligned} d[X_k]_t &= -\langle (\mu_1 \Psi_0 + \sigma_1 \Psi_1) \left(\sum_{l=0}^{P} [X_l]_t \Psi_l \right), \Psi_k \rangle dt + \langle \mu_2 \Psi_0 + \sigma_2 \Psi_2, \Psi_k \rangle dW_t \\ &= -\left(\mu_1 \delta_{0k} + \sigma_1 \sum_{l=0}^{P} [X_l]_t \langle \Psi_1 \Psi_l, \Psi_k \rangle \right) dt + (\mu_2 \delta_{0k} + \sigma_2 \delta_{2k})\, dW_t. \end{aligned}$$

Let us define respectively $[\boldsymbol{X}] = ([X_0], \dots, [X_P])^T$, $\boldsymbol{A} = (a_{ij})_{i,j=0,\dots,P} \in \mathcal{M}_{P+1}(\mathbb{R})$, where $a_{ij} = \mu_1 \delta_{ij} + \sigma_1 \langle \Psi_1 \Psi_i, \Psi_j \rangle$ and $\boldsymbol{b} = (b_0, \dots, b_P)^T \in \mathbb{R}^{P+1}$, where $b_k = \mu_2 \delta_{0k} + \sigma_2 \delta_{2k}$. We get then a system of $(P+1)$ coupled SDEs of the following form :

$$\begin{cases} d[\boldsymbol{X}]_t = -\boldsymbol{A}[\boldsymbol{X}]_t dt + \boldsymbol{b} dW_t, \ t > 0 \\ [\boldsymbol{X}]_0 = (\langle X_0, \Psi_0 \rangle, \dots, \langle X_0, \Psi_P \rangle)^T = (x, 0, \dots, 0)^T \in \mathbb{R}^{P+1} \end{cases}$$

We simulate then m trajectoires of $[\boldsymbol{X}]$ in $[0, T]$ by an Euler scheme : for the j-th sample trajectory, it becomes

$$\begin{cases} [\boldsymbol{X}]_{i+1}^{(j)} = [\boldsymbol{X}]_i^{(j)} - \boldsymbol{A}[\boldsymbol{X}]_i^{(j)} \Delta t + \boldsymbol{b} \sqrt{\Delta t} \zeta_i^{(j)}, \ i = 0, \dots, N-1 \\ [\boldsymbol{X}]_0^{(j)} = [\boldsymbol{X}]_0, \end{cases}$$

where $\zeta_i^{(j)} \sim \mathcal{N}(0,1)$ i.i.d. and $[\boldsymbol{X}]_i^{(j)} = \left([X_0]_i^{(j)}, \dots, [X_P]_i^{(j)} \right)^T \in \mathbb{R}^{P+1}$.

Finally, we can approximate the first order Sobol' indices by

$$S_i\left(\mathcal{M}_1(t,x,\xi)\right) \approx \frac{\sum_{l \in K_i} \left(\frac{1}{m} \sum_{j=1}^{m} [X_l]^{(j)} \right)^2}{\sum_{k=1}^{P} \left(\frac{1}{m} \sum_{j=1}^{m} [X_k]^{(j)} \right)^2}, \ i = 1, 2,$$

where $K_i = \{k \in \{1, \dots, P\} \mid \Psi_k(z) = \Psi_k(z = \xi_i)\}$, $i = 1, 2$, which also leads to compute $S_{\text{inter}}\left(\mathcal{M}_1(t,x,\xi)\right)$ by $1 - \sum_{i=1}^{2} S_i\left(\mathcal{M}_1(t,x,\xi)\right)$.

5.4 Stochastic Galerkin solver for the parametrized PDE

The link between a parametrized SDE and a parametrized PDE has been given in section 4.1. In particular, we apply it to the OU process for x in the domain $\bar{D} = [0,1]$. The output of the model $\mathcal{M}_1(t,x,\xi) = u(t,x,\xi) = \mathbb{E}^x[X_t(\omega,\xi) \mid \xi]$ is the solution to the parametrized PDE,

$$(\mathcal{P}_u)\begin{cases} \partial_t u(t,x,\xi) = -\alpha(\xi_1)x\partial_x u(t,x,\xi) + \dfrac{1}{2}\beta(\xi_2)^2\partial^2_{x,x}u(t,x,\xi), \ \forall (t,x) \in (0,T] \times (0,1) \\ u(0,x,\xi) = x, \ \forall x \in (0,1) \\ u(t,0,\xi) = \mathbb{E}^{x=0}_\omega[X_t \mid \xi] = 0, \ \forall t \in (0,T] \\ u(t,1,\xi) = \mathbb{E}^{x=1}_\omega[X_t \mid \xi] = e^{-\alpha(\xi_1)t}, \ \forall t \in (0,T]. \end{cases}$$

Then we decompose the solution $u(t,x,\xi)$ by PC expansion in the approximate space $\mathcal{Q}_{d,p}$ of $L^2(\Xi,\mathbb{P}_\xi)$,

$$u(t,x,\xi) \approx \sum_{k=0}^{P} u_k(t,x)\Psi_k(\xi),$$

and we follow a Galerkin projection for the parametrized PDE $(\mathcal{P}_{OU})$ in the space $\mathcal{Q}_{d,p}$: for $k = 0,\dots,P$,

$$\begin{aligned} \partial_t u_k &= \langle -(\mu_1\Psi_0 + \sigma_1\Psi_1)x\sum_{l=0}^{P}\partial_x u_l\Psi_l, \Psi_k\rangle + \langle \frac{1}{2}(\mu_2\Psi_0 + \sigma_2\Psi_2)^2\sum_{l=0}^{P}\partial^2_{xx}u_l\Psi_l, \Psi_k\rangle \\ &= -\left(\mu_1\delta_{lk}x\partial_x u_k + \sigma_1\sum_{l=0}^{P}\langle\Psi_1\Psi_l,\Psi_k\rangle x\partial_x u_l\right) \dots \\ &\quad + \left(\frac{\mu_2^2}{2}\delta_{lk}\partial^2_{xx}u_k + \mu_2\sigma_2\sum_{l=0}^{P}\langle\Psi_2\Psi_l,\Psi_k\rangle\partial^2_{xx}u_l + \frac{\sigma_2^2}{2}\sum_{l=0}^{P}\langle\Psi_2^2\Psi_l,\Psi_k\rangle\partial^2_{xx}u_l\right) \end{aligned}$$

It becomes in fact a system of $P+1$ deterministic coupled equations,

$$\partial_t\begin{pmatrix} u_0 \\ \vdots \\ u_P \end{pmatrix} = -\boldsymbol{A}x\partial_x\begin{pmatrix} u_0 \\ \vdots \\ u_P \end{pmatrix} + \boldsymbol{B}\partial^2_{xx}\begin{pmatrix} u_0 \\ \vdots \\ u_P \end{pmatrix},$$

where $\boldsymbol{A} \in \mathcal{M}_{P+1}(\mathbb{R})$ defined in previous section, $\boldsymbol{B} = (b_{ij})_{i,j=0,\dots,P} \in \mathcal{M}_{P+1}(\mathbb{R})$ with $b_{ij} = \left(\frac{1}{2}\mu_2^2\delta_{ij} + \mu_2\sigma_2\langle\Psi_2\Psi_i,\Psi_j\rangle + \frac{1}{2}\sigma_2^2\langle\Psi_2^2\Psi_i,\Psi_j\rangle\right)$.

Denoting $U = (u_0,\dots,u_P)^T$, we rewrite the system of PDEs with the initial condition and boundary condition obtained also by Galerkin projection in the space $\mathcal{Q}_{d,p}$,

$$(\mathcal{P}_U)\begin{cases} \partial_t U(t,x) = -\boldsymbol{A}x\partial_x U(t,x) + \boldsymbol{B}\partial^2_{x,x}U(t,x), \ \forall (t,x) \in (0,T] \times (0,1) \\ U(0,x) = (\langle x,\Psi_0\rangle,\dots,\langle x,\Psi_P\rangle)^T = (x,0,\dots,0)^T \in \mathbb{R}^{P+1}, \ \forall x \in (0,1) \\ U(t,0) = \mathbf{0}^{P+1}, \ \forall t \in (0,T] \\ U(t,1) = \left(\langle e^{-\alpha t},\Psi_0\rangle,\dots,\langle e^{-\alpha t},\Psi_P\rangle\right)^T \in \mathbb{R}^{P+1}, \ \forall t \in (0,T] \end{cases}$$

We use the finite difference method to solve the system of PDEs $(\mathcal{P}_U)$. Let us consider a grid of discretizations $0 = t_0 < t_1 < \dots < t_N = T$ with stepsize $\Delta t = \frac{T}{N}$ and

$0 = x_0 < x_1 < \cdots < x_M = 1$ with stepsize $\Delta x = \frac{1}{M}$. For $k = 0, \ldots, P$, we denote the exact solution by $u_k(t_i, x_j)$ and its approximation at (t_i, x_j) by $u_k^{i,j}$. In vector form, we can approximate $U(t_i, x_j) \in \mathbb{R}^{P+1}$ by $U^{i,j} := \left(u_0^{i,j}, \ldots, u_P^{i,j}\right)^T$ at each point (t_i, x_j).

In particular, we use the Crank-Nicholson scheme which is a evenly weighted combination of the explicit and implicit schemes, as shown in Figure 5.2.

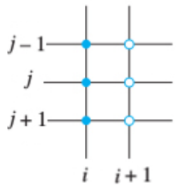


Figure 5.2: Crank-Nicolson scheme - At each time step, the open circles are the unknowns and the filled circles are known from the previous step.

For each point in the grid, we use a forward-difference formula for the time derivative, and center-difference approximations for the remainder of $(\mathcal{P}_U)$: for $i = 0, \ldots, N-1,\ j = 1, \ldots, M-1$,

$$\frac{U^{i+1,j} - U^{i,j}}{\Delta t} = \frac{1}{2}\left(-\boldsymbol{A}x_j \frac{U^{i,j+1} - U^{i,j-1}}{2\Delta x} + \boldsymbol{B}\frac{U^{i,j-1} - 2U^{i,j} + U^{i,j+1}}{(\Delta x)^2}\right) \ldots$$
$$+ \frac{1}{2}\left(-\boldsymbol{A}x_j \frac{U^{i+1,j+1} - U^{i+1,j-1}}{2\Delta x} + \boldsymbol{B}\frac{U^{i+1,j-1} - 2U^{i+1,j} + U^{i+1,j+1}}{(\Delta x)^2}\right),$$

which leads to

$$\frac{1}{\Delta t}U^{i+1,j} + \frac{1}{4\Delta x}\boldsymbol{A}x_j\left(U^{i+1,j+1} - U^{i+1,j-1}\right) - \frac{1}{2(\Delta x)^2}\boldsymbol{B}\left(U^{i+1,j-1} - 2U^{i+1,j} + U^{i+1,j+1}\right)$$
$$= \frac{1}{\Delta t}U^{i,j} - \frac{1}{4\Delta x}\boldsymbol{A}x_j\left(U^{i,j+1} - U^{i,j-1}\right) + \frac{1}{2(\Delta x)^2}\boldsymbol{B}\left(U^{i,j-1} - 2U^{i,j} + U^{i,j+1}\right). \tag{5.5}$$

Let us introduce then the Kronecker product of a $m \times n$ matrix $\mathcal{A}$ and a $p \times q$ matrix $\mathcal{B}$: $\mathcal{A} \otimes \mathcal{B}$ is a $mp \times nq$ block matrix defined as

$$\mathcal{A} \otimes \mathcal{B} = \begin{pmatrix} a_{11}\mathcal{B} & \cdots & a_{1n}\mathcal{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathcal{B} & \cdots & a_{mn}\mathcal{B} \end{pmatrix}.$$

Denoting respectively $D = diag(x_1, \ldots, x_{M-1}) \in \mathcal{M}_{M-1}(\mathbb{R})$,

$$A = \begin{pmatrix} 0 & 1 & & O \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ O & & -1 & 0 \end{pmatrix} \in \mathcal{M}_{M-1}(\mathbb{R}),\ B = \begin{pmatrix} -2 & 1 & & O \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ O & & 1 & -2 \end{pmatrix} \in \mathcal{M}_{M-1}(\mathbb{R})$$

and $U^i = \left(U^{i,1}, \ldots, U^{i,M-1}\right)^T \in \mathbb{R}^{(M-1)(P+1)},\ \forall i = 0, \ldots, N$, the Crank-Nicholson scheme

(5.5) can be represented in form of block matrix product,

$$\left(\frac{1}{\Delta t}I^{(M-1)} \otimes I^{(P+1)} + \frac{1}{4\Delta x}(DA)\otimes \boldsymbol{A} - \frac{1}{2(\Delta x)^2}B\otimes \boldsymbol{B}\right)U^{i+1} - F^{i+1}$$
$$= \left(\frac{1}{\Delta t}I^{(M-1)} \otimes I^{(P+1)} - \frac{1}{4\Delta x}(DA)\otimes \boldsymbol{A} + \frac{1}{2(\Delta x)^2}B\otimes \boldsymbol{B}\right)U^{i} + F^{i},$$

where $F^i = \left(F^{i,1}, \mathbf{0}^{P+1}, \dots, \mathbf{0}^{P+1}, F^{i,M-1}\right)^T \in \mathbb{R}^{(M-1)(P+1)}$ is a block vector composed of vectors $F^{i,1} = \left(f_0^{i,1}, \dots, f_P^{i,1}\right)^T \in \mathbb{R}^{P+1}$ and $F^{i,M-1} = \left(f_0^{i,M-1}, \dots, f_P^{i,M-1}\right)^T \in \mathbb{R}^{P+1}$, defined respectively by

$$F^{i,1} = \frac{x_1}{4\Delta x}\boldsymbol{A}U^{i,0} + \frac{1}{2(\Delta x)^2}\boldsymbol{B}U^{i,0} = \mathbf{0}^{P+1},$$

$$F^{i,M-1} = -\frac{x_{M-1}}{4\Delta x}\boldsymbol{A}U^{i,M} + \frac{1}{2(\Delta x)^2}\boldsymbol{B}U^{i,M} = \left(-\frac{x_{M-1}}{4\Delta x}\boldsymbol{A} + \frac{1}{2(\Delta x)^2}\boldsymbol{B}\right)U(t_i,1)$$
$$= \left(-\frac{x_{M-1}}{4\Delta x}\boldsymbol{A} + \frac{1}{2(\Delta x)^2}\boldsymbol{B}\right)\left(\left\langle e^{-\alpha t_i}, \Psi_0\right\rangle, \dots, \left\langle e^{-\alpha t_i}, \Psi_P\right\rangle\right)^T$$

Thus, for $k = 0, \dots, P$, $f_k^{i,1} = 0$ and

$$f_k^{i,M-1} = \left(-\frac{x_{M-1}}{4\Delta x}a_{k\bullet} + \frac{1}{2(\Delta x)^2}b_{k\bullet}\right)\left(\left\langle e^{-\alpha t_i}, \Psi_0\right\rangle, \dots, \left\langle e^{-\alpha t_i}, \Psi_P\right\rangle\right)^T$$
$$= \sum_{l=0}^{P}\left(-\frac{x_{M-1}}{4\Delta x}a_{kl} + \frac{1}{2(\Delta x)^2}b_{kl}\right)\langle e^{-\alpha t_i}, \Psi_l\rangle,$$

where $a_{k\bullet}$ is the k-row of matrix $\boldsymbol{A}$ and a_{kl} is the element of k-row and l-column.

Defining

$$\begin{cases} \boldsymbol{L} = \dfrac{1}{\Delta t}I^{(M-1)} \otimes I^{(P+1)} + \dfrac{1}{4\Delta x}(DA)\otimes \boldsymbol{A} - \dfrac{1}{2(\Delta x)^2}B\otimes \boldsymbol{B} \\ \boldsymbol{R} = \dfrac{1}{\Delta t}I^{(M-1)} \otimes I^{(P+1)} - \dfrac{1}{4\Delta x}(DA)\otimes \boldsymbol{A} + \dfrac{1}{2(\Delta x)^2}B\otimes \boldsymbol{B}, \end{cases}$$

the final linear system writes,

$$\boldsymbol{L}U^{i+1} = \boldsymbol{R}U^i + (F^{i+1} + F^i), \tag{5.6}$$

with the initial condition defined by

$$U^0 = (\langle x_1, \Psi_0\rangle \ \dots \ \langle x_1, \Psi_P\rangle, \ \dots \ ,\langle x_{M-1}, \Psi_0\rangle \ \dots \ \langle x_{M-1}, \Psi_P\rangle)^T \in \mathbb{R}^{(M-1)(P+1)},$$

where $\langle x_j, \Psi_k\rangle = x_j\delta_{0k}$.

Remark 5.4.1. We have proved completely in appendix B that the Crank-Nicholson scheme (5.5) is unconditionally stable in L^2 norm and is second order both in time and in space, which make this scheme superior to the explicit or implicit scheme for $(\mathcal{P}_U)$, although its expression is rather complicated.

Remark 5.4.2. In the above discussion, we have firstly projected the parametrized PDE $(\mathcal{P}_u)$ in the space $\mathcal{Q}_{d,p}$, then we discretise the obtained system of PDEs $(\mathcal{P}_U)$ by a Crank-Nicholson scheme. In fact, we have studied also an alternative approach in appendix C, where we firstly discretise the parametrized PDE $(\mathcal{P}_u)$ with also a Crank-Nicholson scheme, and then we project the discretized scheme in the space $\mathcal{Q}_{d,p}$. Finally, we find that the two linear systems obtained respectively by the two different approaches are permutation equivalent with approximations of boundary conditions.

As mentioned in section 4.1.2, once we know the projection coefficients $u_k(t,x),\ \forall k = 0,\dots,P$, the first order Sobol' indices can be approximated by

$$S_i\left(\mathcal{M}_1(t,x,\xi)\right) \approx \frac{\sum_{l\in K_i} u_l^2(t,x)}{\sum_{k=1}^{P} u_k^2(t,x)},\ i=1,2,$$

where $K_i = \{k \in \{1,\dots,P\} \mid \Psi_k(z) = \Psi_k(z=\xi_i)\},\ i=1,2$, which also leads to compute $S_{\text{inter}}\left(\mathcal{M}_1(t,x,\xi)\right)$ by $1-\sum_{i=1}^{2} S_i\left(\mathcal{M}_1(t,x,\xi)\right)$.

5.5 The mean exit time of the parametrized OU process from a bounded domain

Always setting $\bar{D}=[0,1]$, according to the discussion in section 4.2.1, the random variable

$$u(x,\xi) = \mathbb{E}^x[\tau_D \mid \xi] = \mathcal{M}_2(x,\xi)$$

is the solution of the parametrized elliptic PDE with homogenous Dirichlet condition,

$$\begin{cases} \alpha(\xi_1)xu'(x,\xi) - \dfrac{\beta(\xi_2)^2}{2}u''(x,\xi) = 1,\ \forall x\in D \\ \qquad\qquad\qquad\qquad u(x,\xi) = 0,\ \forall x \in \partial D. \end{cases} \tag{5.7}$$

5.5.1 Review of the finite element method (FEM)

Let us consider an elliptic PDE,

$$\begin{cases} \alpha x u'(x) - \dfrac{\beta^2}{2}u''(x) = 1,\ \forall x\in D \\ \qquad\qquad\qquad u(x) = 0,\ \forall x\in\partial D. \end{cases} \tag{5.8}$$

The variational formulation of Eq.(5.8) is given by

$$(\mathcal{Q})\text{ find } u\in V = H_0^1([0,1]) \text{ s.t. } a(u,v) = l(v),\ \forall v\in V,$$

where

$$\begin{cases} a(u,v) = \displaystyle\int_0^1 \frac{\beta^2}{2}u'(x)v'(x) + \alpha x u'(x)v(x)dx \\ \quad l(v) = \displaystyle\int_0^1 v(x)dx. \end{cases}$$

An internal approximation of the variational formulation writes,

$$(\mathcal{Q}_h)\text{ find } u_h\in V_h\subset V \text{ s.t. } a(u_h,v_h) = l(v_h),\ \forall v_h\in V_h.$$

Let us discretise the domain $\bar{D}$ into n_e elements $e_k = [z_{k-1}, z_k]$ of uniform width $h = \frac{1}{n_e}$, with $n_e + 1$ vertices $z_k = kh,\ k = 0, \ldots, n_e$. Let us choose the internal approximate space

$$V_h = \{v \in \mathcal{C}([0,1]) : v|_{e_k} \in \mathbb{P}_1(e_k),\ k = 1, \ldots, n_e \text{ and } v(a) = 0 = v(b)\} = \text{span}\{\phi_1, \ldots, \phi_{N_h}\},$$

where $N_h = n_e - 1$. Each global basis funcion ϕ_j is piecewice linear and satisfies $\phi_j(x_i) = \delta_{ij}$, see figure 5.3.

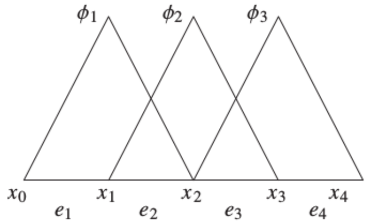


Figure 5.3: A few piecewise linear global basis functions

We can then express the Galerkin solution as $u_h(x) = \sum_{j=1}^{N_h} u_j \phi_j(x),\ u_j \in \mathbb{R}$. Substituting it into $\mathcal{Q}$ and setting $v_h = \phi_i \in V_h$ gives

$$\sum_{j=1}^{N_h} u_j a(\phi_j, \phi_i) = l(\phi_i),\ i = 1, \ldots, N_h.$$

Let us define the matrix $\tilde{A} \in \mathcal{M}_{N_h}(\mathbb{R})$ and the vector $\tilde{b} \in \mathbb{R}^{N_h}$ respectively by

$$\tilde{a}_{ij} = a(\phi_i, \phi_j),\ \tilde{b}_i = l(\phi_i),\ i, j = 1 \ldots, N_h$$

then the coefficients of projection are obtained by solving the linear system

$$\tilde{A}\boldsymbol{u} = \tilde{b}, \tag{5.9}$$

where $\boldsymbol{u} = (u_1, \ldots, u_{N_h})^T$. More precisely, we have

$$\tilde{a}_{ij} = \sum_{k=1}^{n_e} \int_{e_k} \left(\frac{\beta^2}{2} \phi_i'(x)\phi_j'(x) + \alpha x \phi_i'(x)\phi_j(x) \right) dx \text{ and } \tilde{b}_i = \sum_{k=1}^{n_e} \int_{e_k} \phi_i(x) dx.$$

Then we work with local basis functions for $\mathbb{P}_1$ (i.e. within each element e_k, see figure 5.4), defined by

$$\phi_1^k(x) = \phi_{k-1}|_{e_k}(x) = \frac{z_k - x}{h} \text{ and } \phi_2^k(x) = \phi_k|_{e_k}(x) = \frac{x - z_{k-1}}{h}.$$

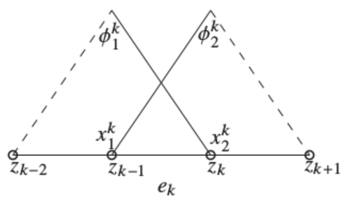


Figure 5.4: Local basis functions for $\mathbb{P}_1$

We define the element matrix $A^k \in \mathcal{M}_2(\mathbb{R})$ by

$$a_{st}^k := \int_{e_k} \left(\frac{\beta^2}{2} \phi_s'(x)\phi_t'(x) + \alpha x \phi_s'(x)\phi_t(x) \right) dx, \quad s,t = 1,2,$$

and the element vector $b^k \in \mathbb{R}^2$ by $b_s^k := \int_{e_k} \phi_s(x)dx$. By affine transformations to the reference support $[0,1]$, one can show that

$$A^k = \frac{\beta^2}{2} \begin{pmatrix} 1/h & -1/h \\ -1/h & 1/h \end{pmatrix} + \alpha z_k \begin{pmatrix} -1/2 & -1 \\ 1/2 & 1 \end{pmatrix}, \text{ and } b^k = \begin{pmatrix} h/2 \\ h/2 \end{pmatrix}.$$

For two element e_i and e_{i+1} meeting at vertex z_i, we perform the assembly of matrices as follows,

$$\tilde{a}_{i,i-1} = a_{21}^i, \ \tilde{a}_{i,i} = a_{22}^i + a_{11}^{i+1}, \ \tilde{a}_{i,i+1} = a_{12}^{i+1}.$$

5.5.2 Monte Carlo FEM

Indeed, we can consider the elliptic PDE (5.8) as the parametrized PDE (5.7) given a $\xi = \xi'$. Thus, according to the linear system (5.9), we can consider $\boldsymbol{u}(\xi) = \tilde{A}^{-1}(\xi)\tilde{b}$ as the output of a deterministic model, hence a MC estimator of the Sobol' indices can be deduced immediately :

1. Draw randomly by Monte-Carlo (quasi Monte-Carlo, LHS, etc.) two independent uniform samplings :

$$\xi_A = \begin{pmatrix} \xi_{1,1}^A & \xi_{2,1}^A \\ \vdots & \vdots \\ \xi_{1,n}^A & \xi_{2,n}^A \end{pmatrix}, \ \xi_B = \begin{pmatrix} \xi_{1,1}^B & \xi_{2,1}^B \\ \vdots & \vdots \\ \xi_{1,n}^B & \xi_{2,n}^B \end{pmatrix}.$$

2. We construct the samplings matrices ξ^{C_1}, ξ^{C_2} from ξ_A and ξ_B :

$$\xi^{C_1} = \begin{pmatrix} \xi_{1,1}^B & \xi_{2,1}^A \\ \vdots & \vdots \\ \xi_{1,n}^B & \xi_{2,n}^A \end{pmatrix}, \xi^{C_2} = \begin{pmatrix} \xi_{1,1}^A & \xi_{2,1}^B \\ \vdots & \vdots \\ \xi_{1,n}^A & \xi_{2,n}^B \end{pmatrix}.$$

3. We evaluate $3n$ the models by $\boldsymbol{u}(\xi) = \tilde{A}^{-1}(\xi)\tilde{b}$:

$$\boldsymbol{u}(\xi_{\bullet j}^B), \ \boldsymbol{u}(\xi_{\bullet j}^{C_1}), \ \boldsymbol{u}(\xi_{\bullet j}^{C_1}), \ j = 1, \dots, n,$$

4. We approximate the Sobol' indices by

$$S_i\left(\mathcal{M}_2(x,\xi)\right) \approx \frac{\frac{1}{n}\sum_{j=1}^n \boldsymbol{u}(\xi_{\bullet j}^B)\boldsymbol{u}(\xi_{\bullet j}^{C_i}) - \left(\frac{1}{2n}\sum_{j=1}^n \boldsymbol{u}^2(\xi_{\bullet j}^B) + \boldsymbol{u}^2(\xi_{\bullet j}^{C_i})\right)^2}{\frac{1}{2n}\sum_{j=1}^n \boldsymbol{u}^2(\xi_{\bullet j}^B)\boldsymbol{u}^2(\xi_{\bullet j}^{C_i}) - \left(\frac{1}{2n}\sum_{j=1}^n \boldsymbol{u}^2(\xi_{\bullet j}^B) + \boldsymbol{u}^2(\xi_{\bullet j}^{C_i})\right)^2}, \ i = 1,2$$

5.5.3 Stochastic FEM

Following the ideas in the article (A. Nouy, 2009), we derive an alternative variational formulation at the stochastic level. We search a weak solution u in the space $L^2(\Xi, \mathbb{P}_\xi, V) = \{v : \Xi \to V \text{ s.t. } \mathbb{E}\left(\|v\|_V^2\right) < \infty\}$. Note that this space can also be assimilated to a tensor product space,

$$L^2(\Xi, \mathbb{P}_\xi, V) \simeq V \otimes L^2\left(\Xi, \mathbb{P}_\xi\right) := V \otimes \mathcal{S}.$$

The variational formulation of Eq.(5.7) on $D \times \Xi$ at the stochastic level writes then,

$$(\mathcal{P}) \text{ find } u \in V \otimes \mathcal{S} \text{ s.t. } \boldsymbol{a}(u,v) = \boldsymbol{l}(v), \ \forall v \in V \otimes \mathcal{S},$$

where

$$\begin{aligned}\boldsymbol{a}(u,v) &:= \mathbb{E}\left[\int_D \left(\frac{1}{2}\beta^2(\bullet)u'(x,\bullet)v'(x,\bullet) + \alpha x(\bullet)u'(x,\bullet)v(x,\bullet)\right)dx\right] \\ &= \int_\Xi \int_D \left(\frac{1}{2}\beta^2(\theta_2)u'(x,\theta)v'(x,\theta) + \alpha(\theta_1)xu'(x,\theta)v(x,\theta)\right)dxd\mathbb{P}_\xi(\theta)\end{aligned}$$

and

$$\boldsymbol{l}(v) := \mathbb{E}\left[\int_D v(x,\bullet)dx\right] = \int_\Xi \int_D v(x,\theta)dxd\mathbb{P}_\xi(\theta).$$

Let $\mathcal{S}_p := \mathcal{Q}_{d,p}$ a stochastic basis, an internal approximation of $(\mathcal{P})$ is given by

$$(\mathcal{P}_{hp}) \text{ find } u_{hp} \in V_h \otimes \mathcal{S}_p \subset V \otimes \mathcal{S} \text{ s.t. } \boldsymbol{a}(u_{hp}, v_{hp}) = \boldsymbol{l}(v_{hp}), \ \forall v_{hp} \in V_h \otimes \mathcal{S}_p$$

Let us define a tensor product space of the finite elements basis V_h and the stochastic basis $\mathcal{S}_p$ by

$$V_h \otimes \mathcal{S}_p := \text{span}\{\phi_i \Psi_k, \ \forall i = 1,\dots,N_h, \ \forall k = 0,\dots,P\}.$$

We apply the Galerkin projection of $u_{hp}(x,\xi)$ on this basis,

$$u_{hp}(x,\xi) = \sum_{i=1}^{N_h}\sum_{k=0}^{P} u_{ik}\phi_i(x)\Psi_k(\xi), \ u_{ik} \in \mathbb{R}$$

Substituting it in $(\mathcal{P}_{hp})$ and setting $v_{hp} = \phi_j(x)\Psi_l(\xi)$, we can show that

$$\begin{aligned}&\int_\Xi \int_D \frac{1}{2}\beta^2(\theta_2)\left(\sum_{i=1}^{N_h}\sum_{k=0}^{P} u_{ik}\phi_i'(x)\Psi_k(\theta)\right)\phi_j'(x)\Psi_l(\theta)dxd\mathbb{P}_\xi(\theta) \\ &= \sum_{i=1}^{N_h}\sum_{k=1}^{P}\left(\frac{1}{2}\int_\Xi \beta^2(\theta_2)\Psi_k(\theta)\Psi_l(\theta)d\mathbb{P}_\xi(\theta)\right)\left(\int_D \phi_i'(x)\phi_j'(x)dx\right)u_{ik} \\ &= \sum_{i=1}^{N_h}\sum_{k=1}^{P} b_{kl}\left(\int_D \phi_i'(x)\phi_j'(x)dx\right)u_{ik},\end{aligned}$$

$$\begin{aligned}&\int_\Xi \int_D \alpha(\theta_1)x\left(\sum_{i=1}^{N_h}\sum_{k=0}^{P} u_{ik}\phi_i'(x)\Psi_k(\theta)\right)\phi_j(x)\Psi_l(\theta)dxd\mathbb{P}_\xi(\theta) \\ &= \sum_{i=1}^{N_h}\sum_{k=1}^{P}\left(\int_\Xi \alpha(\theta_1)\Psi_k(\theta)\Psi_l(\theta)d\mathbb{P}_\xi(\theta)\right)\left(\int_D x\phi_i'(x)\phi_j(x)dx\right)u_{ik} \\ &= \sum_{i=1}^{N_h}\sum_{k=1}^{P} a_{kl}\left(\int_D x\phi_i'(x)\phi_j(x)dx\right)u_{ik}\end{aligned}$$

and

$$\int_\Xi \int_D \phi_j(x)\Psi_l(\theta)dxd\mathbb{P}_\xi(\theta) = \left(\int_\Xi \Psi_l(\theta)d\mathbb{P}_\xi(\theta)\right)\left(\int_D \phi_j(x)dx\right) = \delta_{0l}\tilde{b}_j,$$

where a_{kl} is the element of matrix $\boldsymbol{A} \in \mathcal{M}_{P+1}(\mathbb{R})$ defined in section 5.3, b_{kl} is the element of matrix $\boldsymbol{B} \in \mathcal{M}_{P+1}(\mathbb{R})$ defined in section 5.4 and $\tilde{b}_j$ is the component of vector $\tilde{b}$ mentioned in section 5.5.1.

Let us define $k_{i,j} := \int_D \phi_i'(x)\phi_j'(x)dx$ and $m_{i,j} := \int_D x\phi_i'(x)\phi_j(x)dx$. As mentioned in section 5.5.1, the matrices $K = (k_{ij}) \in \mathcal{M}_{N_h}(\mathbb{R})$ and $M = (m_{ij}) \in \mathcal{M}_{N_h}(\mathbb{R})$ can be respectively assemblied by the element matrices in each element e_i,

$$K^i = \begin{pmatrix} 1/h & -1/h \\ -1/h & 1/h \end{pmatrix} \text{ and } M^i = z_i \begin{pmatrix} -1/2 & -1 \\ 1/2 & 1 \end{pmatrix},$$

where $z_i,\ i = 1, \dots, N_h$ are the vertices.

Let us define two block vectors $\boldsymbol{u} = (\boldsymbol{u}_0, \dots, \boldsymbol{u}_P)^T \in \mathbb{R}^{N_h(P+1)}$ with $\boldsymbol{u}_k = (u_{0k}, \dots, u_{N_h k})^T \in \mathbb{R}^{N_h}$ and $\tilde{\boldsymbol{b}} = \left(\tilde{b}, \boldsymbol{0}^{N_h}, \dots, \boldsymbol{0}^{N_h}\right)^T \in \mathbb{R}^{N_h(P+1)}$. According to the previous formulas, the internal formulation $(\mathcal{P}_{hp})$ leads to solve the following linear system,

$$(\boldsymbol{B} \otimes K + \boldsymbol{A} \otimes M)\boldsymbol{u} = \tilde{\boldsymbol{b}}.$$

As mentioned in section 4.2.2, once we get the coefficients $\boldsymbol{u}_k,\ k = 0, \dots, P$, the first order Sobol' indices can be approximated by

$$S_i\left(\mathcal{M}_2(x,\xi)\right) \approx \frac{\sum_{l \in K_i} \boldsymbol{u}_l^2(x)}{\sum_{k=1}^P \boldsymbol{u}_k^2(x)},\ i = 1, 2,$$

where $K_i = \{k \in \{1, \dots, P\} \mid \Psi_k(z) = \Psi_k(z = \xi_i)\},\ i = 1, 2$, which also leads to compute $S_{\text{inter}}\left(\mathcal{M}_2(x,\xi)\right)$ by $1 - \sum_{i=1}^2 S_i\left(\mathcal{M}_2(x,\xi)\right)$.

5.6 Numerical results

This section illustrats the numerical methods mentioned above. For all of the approaches, we choose $\mu_1 = 1, \mu_2 = 0.1, \sigma_1 = \sigma_2 = 0.05$ as the characterized parameters, $t \in [0, 10]$ as the evolution period and $x \in \bar{D} = [0, 1]$ as the spatial domain. Firstly, let us indicate in the case $\mathcal{M}_1$, that the efficiency of the MC method applied in SDE (MC SDE) depends on the size of parameter samplings n, the size of Wiener samplings m and the time stepsize Δt; the efficiency of the PC approach applied in SDE (PC SDE) depends on m, N and the dimension of the approximate polynomials space $\mathcal{Q}_{d,p}$ (or the truncated order $P = \dim(\mathcal{Q}_{d,p}) - 1$); the efficiency of the PC approach applied in PDE (PC PDE) depends on $P, \Delta t$ and the spatial stepsize Δx. Let us fix $\Delta t = \Delta x = 0.01$ in the following.

The figure 5.5 shows the evolution of the total variance $Var(y_1)$, implemented by the scheme (5.7) with $P = 9$ chosen.

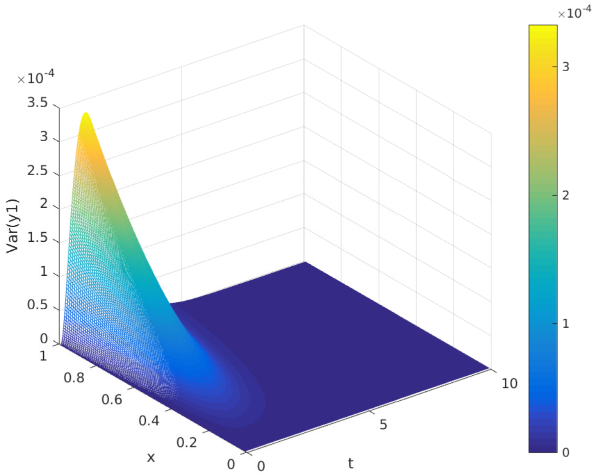


Figure 5.5: $Var\left(\mathcal{M}_1(t,x,\xi)\right)$ estimated by PC PDE for $P=9$

Let us set $X_0 = x = 0.99$, $n = 1000$, $m = 10000$ and $P = 9$, then the total variance $Var(y_1)$, estimated by various methods, has been shown in figure 5.6.

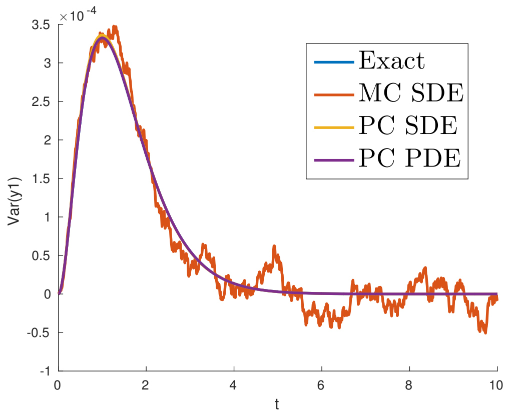


Figure 5.6: Evolution of $Var(y_1)$ obtained by various methods

We see immediately that all the curves are almost coincident, except the MC estimator. As we know, the MC samplings converge quite slowly in general, especially we perform a double MC samplings in our case.

Recall that the explicit expression of $Var(y_1)$ is given by $\mathbb{E}_2 - \mathbb{E}_1^2$ in section 5.1.3. Let us denote the total variance of model $\mathcal{M}_1(t,x,\xi)$ at the point (T,x) by $\sigma_{y_1}^{T,x}$, the estimators of the total variance at this point due to PC SDE and to PC PDE by $\hat{\sigma}_{\mathrm{SDE}}^{T,x}$ and $\hat{\sigma}_{\mathrm{PDE}}^{T,x}$ respectively. Then using the numerical schemes respect to various choices of P, we can show the approximate errors defined below as a function of P,

$$\varepsilon_{\mathrm{SDE}}^{T,x}(P) = |\hat{\sigma}_{\mathrm{SDE}}^{T,x}(P) - \sigma_{y_1}^{T,x}|, \text{ and } \varepsilon_{\mathrm{PDE}}^{T,x}(P) = |\hat{\sigma}_{\mathrm{PDE}}^{T,x}(P) - \sigma_{y_1}^{T,x}|.$$

The figure 5.7 shows that theses errors decreases as the truncated order increases, and the errors of the PDE method are much more lower than the SDE case. This result is rather logical, since we have sampled the Wiener processes in SDE case.

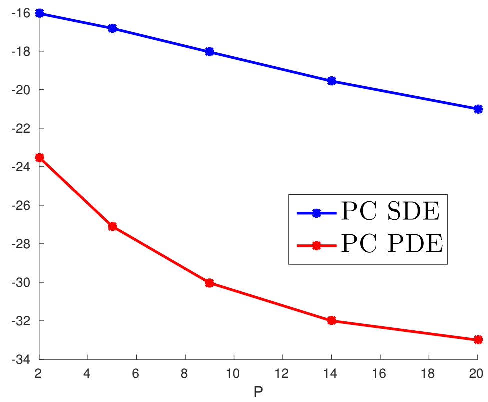


Figure 5.7: $\log\left(\varepsilon_{\text{SDE}}^{T,x}(P)\right)$ and $\log\left(\varepsilon_{\text{PDE}}^{T,x}(P)\right)$

As we know the explicit solutions of the Sobol' indices $S_1\left(\mathcal{M}_1(t,x,\xi)\right) = 1$ and $S_2\left(\mathcal{M}_1(t,x,\xi)\right) = 0$, we can show in the same way, the approximate errors of theses indices due to PC PDE :

$$\varepsilon_1^{T,x} = |1 - \hat{s}_1^{T,x}| \text{ and } \varepsilon_2^{T,x} = |\hat{s}_2^{T,x}|.$$

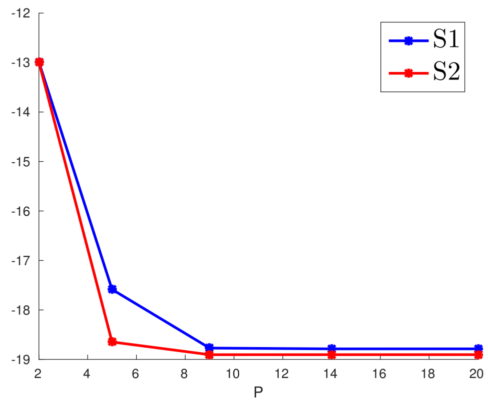


Figure 5.8: $\log\left(\varepsilon_1^{T,x}\right)$ and $\log\left(\varepsilon_2^{T,x}\right)$

We observe from the figure 5.8 that for both the two indices, the error does not decrease much when the truncated order P reach a level.

Finally, recovering $x \in \bar{D} = [0,1]$, we apply respectively the MC PDE method 5.5.2 with $n = 10000$ and the PC PDE method 5.5.3 with $P = 9$, in order to perform the estimations of $S_1\left(\mathcal{M}_2(x,\xi)\right)$ and $S_2\left(\mathcal{M}_2(x,\xi)\right)$.

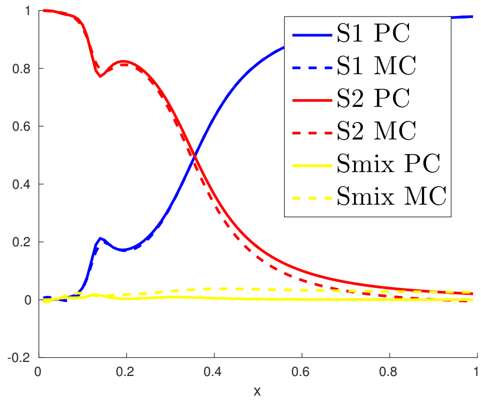


Figure 5.9: Sobol' indices of the mean exit time from the domain $[0, 1]$ of the OU process, respectively explained by ξ_1, ξ_2 and their interaction

From the figure 5.9, one can directly find a symmetrical behavior respectively explained by ξ_1 and ξ_2 in this case.

Summary and future work

This MSc thesis was meant to present the Sobol' sensitivity analysis (SA) for a parametrized diffusion process, considering the mean value relative to the intrinsic randomness as the quantity of interest. On the other hand, one can also consider the mean value relative to the uncertain parameters.

In this work, we have shown two principle tools - MC samplings and PC expansion. From an mathematical point of view, we prefer the PC apporach combined with stochastic Galerkin technique, in which one can obtain the whole information about the explicit solution, by solving the beautiful system of equations. Moreover, this method converge rather fast with a high accuracy.

One major drawback of the PC approach is that the linear systems used to compute the expansion coefficients are typically much larger than the linear systems used to solve comparable deterministic problem. This is not terribly surprising since we are essentially introducing more dimensions into the problem. But researchers are currently searching for ways to either reduce the size of these systems or devise fast and efficient methods for solving them.

Another drawback of the PC approach from an engineering point of view is that simulation codes typically have to be rewritten to solve the coupled system of equations for the coefficients. Compare this to a straightfoward MC sampling from the distribution of the random inputs and running multiple deterministic simulations, which is much more expensive in terms of CPU time but does not require new codes.

Researchers are exploring techniques such as importance sampling and stochastic collocation that could provide the accuracy of the stochastic Galerkin method using only a handful of deterministic simulations.

The key of this work is that we have established between the SA for parametrized SDEs and the SA for parametrized PDEs, via the Feymann-Kac formula. Once again, solving a high dimensional forward-backward SDEs is not immediate. We may see later some multi-dimensional exemples, such as the stochastic FitzHugh-Nagumo model which is very popular in neuroscience, and the stochastic Navier-Stokes systems which is very useful in geoscience.

Appendix A

Some classical orthogonal polynomials

In this section, we briefly review the orthogonality and the recurrence relation of some classical orthogonal polynomials. One can use theses two properties to construct an one-dimensional basis of such polynomials.

A.1 Legendre Polynomials $P_n(x)$ defined on $[-1, 1]$

Orthogonality

$$\begin{cases} W(x) = 1 \\ \langle P_n, P_m \rangle_W = \dfrac{2}{2n+1}\delta_{nm} \end{cases}$$

Recurrence

$$\begin{cases} P_0(x) = 1 \\ P_1(x) = x \\ (n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x), \ n \geq 1 \end{cases}$$

A.2 Hermite Polynomials $H_n(x)$ defined on $\mathbb{R}$

Orthogonality

$$\begin{cases} W(x) = e^{-\frac{x^2}{2}} \\ \langle H_n, H_m \rangle_W = \sqrt{2\pi} n! \delta_{nm} \end{cases}$$

Recurrence

$$\begin{cases} H_0(x) = 1 \\ H_1(x) = x \\ H_{n+1}(x) = xH_n(x) - nH_{n-1}(x), \ n \geq 1 \end{cases}$$

A.3 Laguerre Polynomials $L_n^{(\gamma)}(x), \gamma > 0$ defined on $\mathbb{R}_+$

Orthogonality

$$\begin{cases} W(x) = \dfrac{x^{\gamma-1}e^{-x}}{\Gamma(\gamma)} \\ \langle L_n, L_m \rangle_W = \dfrac{\Gamma(n+\gamma)}{n!}\delta_{nm} \end{cases}$$

Recurrence

$$\begin{cases} H_0(x) = 1 \\ H_1(x) = \gamma - x \\ (n+1)L_{n+1}^{\gamma}(x) = (2n+\gamma-x)L_n^{\gamma}(x) - (n+\gamma-1)L_{n-1}^{\gamma}(x), \ n \geq 1 \end{cases}$$

Recall that the Gamma function is defined by $\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx, Re(z) > 0$.

A.4 Jacobi Polynomials $J_n^{(\alpha,\beta)}(x), \ \alpha > 0, \beta > 0$ defined on $[-1,1]$

Orthogonality

$$\begin{cases} W(x) = \dfrac{(1+y)^{\alpha-1}(1-y)^{\beta-1}}{2^{\alpha+\beta-1}B(\alpha,\beta)} \\ \langle J_n, J_m \rangle_W = \dfrac{2^{\alpha+\beta-1}}{2n+\alpha+\beta-1}\dfrac{\Gamma(n+\alpha)\Gamma(n+\beta)}{\Gamma(n+\alpha+\beta-1)n!}\delta_{nm} \end{cases}$$

Recurrence

$$\begin{cases} J_0(x) = 1 \\ J_1(x) = \dfrac{1}{2}\left[2\alpha + (\alpha+\beta)(x-1)\right] \\ xJ_{n+1}^{\alpha,\beta}(x) = \dfrac{2(n+1)(n+\alpha+\beta-1)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)}J_{n+1}^{\alpha,\beta}(x) + \dfrac{\beta^2-\alpha^2}{(2n+\alpha+\beta-2)(2n+\alpha+\beta)}J_n^{\alpha,\beta}(x) \\ \qquad + \dfrac{2(n+\alpha-1)(n+\beta-1)}{(2n+\alpha+\beta-2)(2n+\alpha+\beta-1)}J_{n-1}^{\alpha,\beta}(x), \ n \geq 1 \end{cases}$$

Recall that the beta function is defined by $B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}$. Note that when $\alpha = \beta = 0$, the Jacobi polynomials become the Legendre polynomials.

Appendix B

Stability and consistency for the Crank-Nicholson scheme (5.5)

We study in this section about the stability and trucated error of the Crank-Nicholson scheme (5.5), in order to ensure its convergence.

B.1 Stability in L^2 norm

We apply the Fourier transform of x on $U(t,x)$,

$$\mathcal{F}[U(t,x)] = \int_{\mathbb{R}} U(t,x)e^{-i2k\pi x}dx := \hat{U}(t,k) \in \mathbb{R}^{P+1}.$$

We deduce then

$$\mathcal{F}[U(t,x-\Delta x)] = \int_{\mathbb{R}} U(t,x-\Delta x)e^{-i2k\pi x}dx = \int_{\mathbb{R}} U(t,y)e^{-i2k\pi(y+\Delta x)}dy = e^{-i2k\pi\Delta x}\hat{U}(t,k).$$

Similarly, $\mathcal{F}[U(t,x+\Delta x)] = e^{i2k\pi\Delta x}\hat{U}(t,k)$. Replcaing them in the scheme (5.5),

$$\begin{aligned}
&\frac{1}{\Delta t}\hat{U}^{i+1}(k) + \frac{1}{4\Delta x}\boldsymbol{A}x_j\left(e^{i2k\pi\Delta x} - e^{-i2k\pi\Delta x}\right)\hat{U}^{i+1}(k) - \frac{1}{2(\Delta x)^2}\boldsymbol{B}\left(e^{-i2k\pi\Delta x} - 2 + e^{i2k\pi\Delta x}\right)\hat{U}^{i+1}(k)\\
&= \frac{1}{\Delta t}\hat{U}^{i}(k) - \frac{1}{4\Delta x}\boldsymbol{A}x_j\left(e^{i2k\pi\Delta x} - e^{-i2k\pi\Delta x}\right)\hat{U}^{i}(k) + \frac{1}{2(\Delta x)^2}\boldsymbol{B}\left(e^{-i2k\pi\Delta x} - 2 + e^{i2k\pi\Delta x}\right)\hat{U}^{i}(k).
\end{aligned}$$

Using the following formulas

$$\begin{cases} e^{-i2k\pi\Delta x} - 2 + e^{i2k\pi\Delta x} = 2(\cos(2k\pi\Delta x) - 1) = -4\sin^2\left(\dfrac{2k\pi\Delta x}{2}\right) \\ e^{i2k\pi\Delta x} - e^{-i2k\pi\Delta x} = 2i\sin(2k\pi\Delta x), \end{cases}$$

we can show that

$$\hat{U}^{i+1}(k) = S(k)\hat{U}^{i}(k),$$

where $S(k)$ is the amplification function defined by

$$S(k) = \frac{I^{P+1} - \frac{2\Delta t}{(\Delta x)^2}\boldsymbol{B}\sin^2(k\pi\Delta x) - i\frac{\Delta t}{2\Delta x}\boldsymbol{A}x_j\sin(2k\pi\Delta x)}{I^{P+1} + \frac{2\Delta t}{(\Delta x)^2}\boldsymbol{B}\sin^2(k\pi\Delta x) + i\frac{\Delta t}{2\Delta x}\boldsymbol{A}x_j\sin(2k\pi\Delta x)}.$$

As we konw, the stability in L^2 norm is assured **if and only if** $|S(k)| \le 1$, which is equivalent to

$$\left(I^{P+1} - \frac{2\Delta t}{(\Delta x)^2}\boldsymbol{B}\sin^2(k\pi\Delta x)\right)^2 \le \left(I^{P+1} + \frac{2\Delta t}{(\Delta x)^2}\boldsymbol{B}\sin^2(k\pi\Delta x)\right)^2,$$

hence it requires that each element of matrix $\boldsymbol{B}$ is non-negatif. Indeed, this is equivalent to show that the inner products $\langle\Psi_2\Psi_i,\Psi_j\rangle$ and $\langle\Psi_2\Psi_2\Psi_i,\Psi_j\rangle$ are both non-negatif. One can prove them using the tensor product notation of the 2D Legendre polynomials, the recurrence and the orthogonality of the 1D Legendre polynomials,

$$\begin{aligned}
\langle\Psi_{(0,1)}\Psi_{(r_1,r_2)},\Psi_{(s_1,s_2)}\rangle &= \int_0^1\int_0^1 \Psi_1^{(2)}(\xi_2)\Psi_{r_1}^{(1)}(\xi_1)\Psi_{r_2}^{(2)}(\xi_2)\Psi_{s_1}^{(1)}(\xi_1)\Psi_{s_2}^{(2)}(\xi_2)d\xi_1 d\xi_2\\
&= \left(\int_0^1 \Psi_{r_1}^{(1)}(\xi_1)\Psi_{s_1}^{(1)}(\xi_1)d\xi_1\right)\left(\int_0^1 \Psi_1^{(2)}(\xi_2)\Psi_{r_2}^{(2)}(\xi_2)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\right)\\
&= \delta_{r_1 s_1}\int_0^1 (2\xi_2-1)\Psi_{r_2}^{(2)}(\xi_2)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\\
&= \delta_{r_1 s_1}\int_0^1 \left(\frac{r_2+1}{2r_2+1}\Psi_{r_2+1}^{(2)}(\xi_2) + \frac{r_2}{2r_2+1}\Psi_{r_2-1}^{(2)}(\xi_2)\right)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\\
&= \delta_{r_1 s_1}\left(\frac{r_2+1}{2r_2+1}\int_0^1 \Psi_{r_2+1}^{(2)}(\xi_2)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2 + \frac{r_2}{2r_2+1}\int_0^1 \Psi_{r_2-1}^{(2)}(\xi_2)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\right)\\
&= \delta_{r_1 s_1}\left(\frac{r_2+1}{2r_2+1}\delta_{(r_2+1)s_2} + \frac{r_2}{2r_2+1}\delta_{(r_2-1)s_2}\right) \ge 0.
\end{aligned}$$

Futhermore it is positive **if and only if** $\begin{cases} r_1 = s_1 \\ |r_2 - s_2| = 1 \end{cases}$ On the other hand,

$$\begin{aligned}
&\langle\Psi_{(0,1)}\Psi_{(0,1)}\Psi_{(r_1,r_2)},\Psi_{(s_1,s_2)}\rangle\\
&= \int_0^1\int_0^1 \Psi_1^{(2)}(\xi_2)\Psi_1^{(2)}(\xi_2)\Psi_{r_1}^{(1)}(\xi_1)\Psi_{r_2}^{(2)}(\xi_2)\Psi_{s_1}^{(1)}(\xi_1)\Psi_{s_2}^{(2)}(\xi_2)d\xi_1 d\xi_2\\
&= \left(\int_0^1 \Psi_{r_1}^{(1)}(\xi_1)\Psi_{s_1}^{(1)}(\xi_1)d\xi_1\right)\left(\int_0^1 \Psi_1^{(2)}(\xi_2)\Psi_{r_2}^{(2)}(\xi_2)\Psi_1^{(2)}(\xi_2)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\right)\\
&= \delta_{r_1 s_1}\int_0^1 (2\xi_2-1)\Psi_{r_2}^{(2)}(\xi_2)(2\xi_2-1)\Psi_{s_2}^{(2)}(\xi_2)d\xi_2\\
&= \delta_{r_1 s_1}\int_0^1 \left(\frac{r_2+1}{2r_2+1}\Psi_{r_2+1}^{(2)}(\xi_2) + \frac{r_2}{2r_2+1}\Psi_{r_2-1}^{(2)}(\xi_2)\right)\left(\frac{s_2+1}{2s_2+1}\Psi_{s_2+1}^{(2)}(\xi_2) + \frac{s_2}{2s_2+1}\Psi_{s_2-1}^{(2)}(\xi_2)\right)d\xi_2\\
&= \frac{\delta_{r_1 s_1}}{(2s_1+1)(2r_2+1)}\left(c_1\delta_{(r_2+1)(s_2+1)} + c_2\delta_{(r_2+1)(s_2-1)} + c_3\delta_{(r_2-1)(s_2+1)} + c_4\delta_{(r_2-1)(s_2-1)}\right) \ge 0,
\end{aligned}$$

where $c_1 = (r_2+1)(s_2+1)$, $c_2 = (r_2+1)s_2$, $c_3 = r_2(s_2+1)$, $c_4 = r_2 s_2$. Futhermore it is positive **if and only if** $\left(\begin{cases} r_1 = s_1 \\ r_2 = s_2 \end{cases} \text{ or } \begin{cases} r_1 = s_1 \\ |r_2 - s_2| = 2 \end{cases}\right)$

Therefore, the Crank-Nicholson scheme (5.5) is unconditionally stable in L^2 norm.

B.2 Consistency

We derive then the truncation error for the Crank–Nicolson scheme. We say that $f = o(g)$ if for all $\delta \in \mathbb{R}_+$ as small as it is, we have $|f(h)| \le C\delta|g(h)|$ as soon as $|h|$ is small enough. For $k = 0,\dots,P$, we apply the Taylor-Young formula on $u_k(t,x)$, $\forall t \in [0,T]$, $\forall x \in [0,1]$,

- $$\frac{u_k(t+\Delta t,x)-u_k(t,x)}{\Delta t} = \partial_t u_k(t,x) + \frac{\Delta t}{2}\partial^2_{tt}u_k(t,x) + \frac{(\Delta t)^2}{6}\partial^3_{ttt}u_k(t,x) + o\big((\Delta t)^2\big)$$
- $$\frac{u_k(t,x+\Delta x)-u_k(t,x-\Delta x)}{2\Delta x} = \partial_x u_k(t,x) + \frac{(\Delta x)^2}{6}\partial^3_{xxx}u_k(t,x) + o\big((\Delta t)^2+(\Delta x)^2\big)$$
- $$\frac{u_k(t+\Delta t,x+\Delta x)-u_k(t+\Delta t,x-\Delta x)}{2\Delta x} = \partial_x u_k(t,x) + \Delta t\partial^2_{xt}u_k(t,x) + \frac{(\Delta t)^2}{2}\partial^3_{ttx}u_k(t,x)\ \ldots$$
$$+\ \frac{(\Delta x)^2}{6}\partial^3_{xxx}u_k(t,x) + o\big((\Delta t)^2+(\Delta x)^2\big)$$
- $$\frac{u_k(t,x-\Delta x)-2u_k(t,x)+u_k(t,x+\Delta x)}{(\Delta x)^2} = \partial^2_{xx}u_k(t,x) + \frac{(\Delta x)^2}{12}\partial^4_{xxxx}u_k(t,x) + o\big((\Delta x)^2\big)$$
- $$\frac{u_k(t+\Delta t,x-\Delta x)-2u_k(t+\Delta t,x)+u_k(t+\Delta t,x+\Delta x)}{(\Delta x)^2} = \partial^2_{xx}u_k(t,x) + \frac{(\Delta x)^2}{12}\partial^4_{xxxx}u_k(t,x)\ \ldots$$
$$+\ \Delta t\partial^3_{xxt}u_k(t,x) + \frac{(\Delta t)^2}{2}\partial^4_{xxtt}u_k(t,x) + o\big((\Delta t)^2+(\Delta x)^2\big)$$

Replacing respectively these formulas in the equation

$$\partial_t u_k = -\frac{1}{2}\sum_{l=0}^{P} a_{kl}x\,(\partial_x u_l + \partial_x u_l) + \frac{1}{2}\sum_{l=0}^{P} b_{kl}\,(\partial_{xx}u_l + \partial_{xx}u_l),$$

we compute the truncation error at point (t,x),

$$\begin{aligned}
\mathcal{E}(u_k) &= \frac{\Delta t}{2}\partial^2_{tt}u_k + \frac{(\Delta t)^2}{6}\partial^3_{ttt}u_k + \sum_{l=0}^{P} a_{kl}x\left(\frac{(\Delta x)^2}{6}\partial^3_{xxx}u_l + \frac{\Delta t}{2}\partial^2_{xt}u_l + \frac{(\Delta t)^2}{4}\partial^3_{ttx}u_l\right)\ \ldots\\
&- \sum_{l=0}^{P} b_{kl}\left(\frac{(\Delta x)^2}{12}\partial^4_{xxxx}u_l + \frac{\Delta t}{2}\partial^3_{xxt}u_l + \frac{(\Delta t)^2}{4}\partial^4_{xxtt}u_l\right) + o\big((\Delta t)^2+(\Delta x)^2\big)\\
&= \frac{\Delta t}{2}\left(\partial^2_{tt}u_k + \sum_{l=0}^{P} a_{kl}x\partial^2_{xt}u_l - b_{kl}\partial^3_{xxt}u_l\right) + \frac{(\Delta t)^2}{12}\left(2\partial^3_{ttt}u_k + \sum_{l=0}^{P} 3a_{kl}x\partial^3_{ttx}u_l - 3b_{kl}\partial^4_{xxtt}u_l\right)\ \ldots\\
&+ \frac{(\Delta x)^2}{12}\left(\sum_{l=0}^{P} 2a_{kl}x\partial^3_{xxx}u_l - b_{kl}\partial^4_{xxxx}u_l\right) + o\big((\Delta t)^2+(\Delta x)^2\big)\\
&= \frac{\Delta t}{2}\left[\partial_t(\partial_t u_k) + \sum_{l=0}^{P} a_{kl}x\partial_x(\partial_t u_l) - b_{kl}\partial^2_{xx}(\partial_t u_l)\right]\ \ldots\\
&+ \frac{(\Delta t)^2}{12}\left[3\left(\partial_t(\partial^2_{tt}u_k) + \sum_{l=0}^{P} a_{kl}x\partial_x(\partial^2_{tt}u_l) - b_{kl}\partial^2_{xx}(\partial^2_{tt}u_l)\right) - \partial^3_{ttt}u_k\right] + \frac{(\Delta x)^2}{12}\ \ldots\\
&\left[2\left(\partial_t(\partial^2_{xx}u_k) + \sum_{l=0}^{P} a_{kl}x\partial_x(\partial^2_{xx}u_l) - b_{kl}\partial^2_{xx}(\partial^2_{xx}u_l)\right) - 2\partial^3_{xxt}u_k + \sum_{l=0}^{P} b_{kl}\partial^4_{xxxx}u_l\right] + o\big((\Delta t)^2+(\Delta x)^2\big)\\
&= \frac{(\Delta x)^2}{12}\left(\sum_{l=0}^{P} b_{kl}\partial^4_{xxxx}u_l - 2\partial^3_{xxt}u_k\right) - \frac{(\Delta t)^2}{12}\partial^3_{ttt}u_k + o\big((\Delta t)^2+(\Delta x)^2\big)
\end{aligned}$$

Therefore the Crank-Nicholson scheme (5.5) is second order both in time and in space.

Appendix C

An alternative stochastic Galerkin solver for the parametrized PDE

Different to the discussion in section 5.4, we present here how to solve the parametrized PDE $(\mathcal{P}_u)$ in another way, where we firstly discretise $(\mathcal{P}_u)$ and then we project the discretized scheme in the space $\mathcal{Q}_{d,p}$.

C.1 Method development

Firstly, let us consider a Crank-Nicholson scheme for $(\mathcal{P}_u)$,

$$\left(\frac{1}{\Delta t}I^{M-1}+\frac{\alpha(\xi_1)}{4\Delta x}DA-\frac{\beta(\xi_2)^2}{4(\Delta x)^2}B\right)u^{i+1}(\xi)=\left(\frac{1}{\Delta t}I^{M-1}-\frac{\alpha(\xi_1)}{4\Delta x}DA+\frac{\beta(\xi_2)^2}{4(\Delta x)^2}B\right)u^{i}(\xi)+\left(f^{i+1}(\xi)+f^{i}(\xi)\right),$$

where the matrices A, B, D are the same ones in 5.4 and $f^i(\xi)=\left(f^{i,1}(\xi),0,\dots,0,f^{i,M-1}(\xi)\right)^T\in\mathbb{R}^{M-1}$ with

$$\begin{cases} f^{i,1}(\xi)=\dfrac{\alpha(\xi_1)}{4\Delta x}x_1u^{i,0}(\xi)+\dfrac{\beta(\xi_2)^2}{4(\Delta x)^2}u^{i,0}(\xi)=0\\ f^{i,M-1}(\xi)=-\dfrac{\alpha(\xi_1)}{4\Delta x}x_{M-1}u^{i,M}(\xi)+\dfrac{\beta(\xi_2)^2}{4(\Delta x)^2}u^{i,M}(\xi).\end{cases}$$

In this case, the solution u and the source terms f depend both on ξ.

Denoting

$$\begin{cases} L(\xi)=\dfrac{1}{\Delta t}I^{M-1}+\dfrac{\alpha(\xi_1)}{4\Delta x}DA-\dfrac{\beta(\xi_2)^2}{4(\Delta x)^2}B\\ R(\xi)=\dfrac{1}{\Delta t}I^{M-1}-\dfrac{\alpha(\xi_1)}{4\Delta x}DA+\dfrac{\beta(\xi_2)^2}{4(\Delta x)^2}B,\end{cases}$$

a strong formulation at the deterministic level has been given : find a random variable $u^i(\xi)\in\mathbb{R}^{M-1}$, $i=0,\dots,N$ verifying almost surely,

$$L(\xi)u^{i+1}(\xi)=R(\xi)u^i(\xi)+\left(f^{i+1}(\xi)+f^i(\xi)\right).$$

Then decomposing the solution u^i, $i=0,\dots,N$ by PC expansion in the approximate space $\mathcal{Q}_{d,p}$,

$$u^i(\xi)\approx\sum_{k=0}^{P}\tilde{u}_k^i\Psi_k(\xi),\ \tilde{u}_k^i\in\mathbb{R}^{M-1},$$

and following an Galerkin projection in the same space, we get a weak formulation at stochastic level : $\forall k = 0, \dots, P$,

$$\langle L(\xi)\left(\sum_{l=0}^{P} \tilde{u}_l^{i+1}\Psi_l(\xi)\right), \Psi_k(\xi)\rangle = \langle R(\xi)\left(\sum_{l=0}^{P} \tilde{u}_l^{i}\Psi_l(\xi)\right), \Psi_k(\xi)\rangle + \langle f^{i+1}(\xi), \Psi_k(\xi)\rangle + \langle f^{i}(\xi), \Psi_k(\xi)\rangle,$$

which leads to

$$\sum_{l=0}^{P} \langle L(\xi)\Psi_l(\xi), \Psi_k(\xi)\rangle \tilde{u}_l^{i+1} = \sum_{l=0}^{P} \langle R(\xi)\Psi_l(\xi), \Psi_k(\xi)\rangle \tilde{u}_l^{i} + \langle f^{i+1}(\xi), \Psi_k(\xi)\rangle + \langle f^{i}(\xi), \Psi_k(\xi)\rangle.$$

We developpe then the terms for $k = 0, \dots, P$,

$$\begin{aligned}
\sum_{l=0}^{P} \langle R(\xi)\Psi_l(\xi), \Psi_k(\xi)\rangle\, \tilde{u}_l^{i} &= \sum_{l=0}^{P} \langle \left(\frac{1}{\Delta t} I^{M-1} - \frac{\alpha(\xi_1)}{4\Delta x} DA + \frac{\beta(\xi_2)^2}{4(\Delta x)^2} B\right) \Psi_l(\xi), \Psi_k(\xi)\rangle \tilde{u}_l^{i} \\
&= \sum_{l=0}^{P} \{ \frac{1}{\Delta t} I^{M-1}\delta_{lk} - \frac{1}{4\Delta x}\left(\mu_1\delta_{lk} + \sigma_1\langle\Psi_1\Psi_l, \Psi_k\rangle\right) DA \ \dots \\
&\quad + \frac{1}{2(\Delta x)^2}\left(\frac{1}{2}\mu_2^2\delta_{lk} + \mu_2\sigma_2\langle\Psi_2\Psi_l, \Psi_k\rangle + \frac{1}{2}\sigma^2\langle\Psi_2^2\Psi_l, \Psi_k\rangle\right) B\} \tilde{u}_l^{i} \\
&= \sum_{l=0}^{P} \left(\frac{1}{\Delta t} I^{M-1}\delta_{lk} - \frac{1}{4\Delta x} a_{kl} DA + \frac{1}{2(\Delta x)^2} b_{kl} B\right) \tilde{u}_l^{i}
\end{aligned}$$

Denoting the block vector $\tilde{U}^i = \left(\tilde{u}_0^i, \dots, \tilde{u}_P^i\right)^T \in \mathbb{R}^{(M-1)(P+1)}$, $i = 0, \dots, N$, the formula above becomes a product of a block matrix of size $(M-1)(P+1) \times (M-1)(P+1)$ and the block vector $\tilde{U}^i$,

$$\left(\frac{1}{\Delta t} I^{(P+1)} \otimes I^{(M-1)} - \frac{1}{4\Delta x} \boldsymbol{A} \otimes (DA) + \frac{1}{2(\Delta x)^2} (\boldsymbol{B} \otimes B)\right) \tilde{U}^i := \tilde{\boldsymbol{R}}\tilde{U}^i.$$

For a similar reason, we have

$$\left(\frac{1}{\Delta t} I^{(P+1)} \otimes I^{(M-1)} + \frac{1}{4\Delta x} \boldsymbol{A} \otimes (DA) - \frac{1}{2(\Delta x)^2} (\boldsymbol{B} \otimes B)\right) \tilde{U}^{i+1} := \tilde{\boldsymbol{L}}\tilde{U}^{i+1},\ i = 0, \dots, N-1.$$

In particular for $i = 0$, we have $u^0(\xi) = \sum_{l=0}^{P} \tilde{u}_l^0 \Psi_l(\xi)$, $\tilde{u}_l^0 \in \mathbb{R}^{M-1}$, i.e. $\forall l = 0, \dots, P$,

$$\tilde{u}_l^0 = \langle \left(u^{0,1}(\xi), \dots, u^{0,M-1}(\xi)\right)^T, \Psi_l(\xi)\rangle = \langle (x_1, \dots, x_{M-1})^T, \Psi_l(\xi)\rangle = (x_1, \dots, x_{M-1})^T \delta_{0l}$$

We can construct then the initial condition by $\tilde{U}^0 = \left(\tilde{u}_0^0, \dots, \tilde{u}_P^0\right)^T \in \mathbb{R}^{(M-1)(P+1)}$. We compute next the boundary condition : for $i = 0, \dots, N$, $k = 0, \dots, P$,

$$\tilde{f}_k^{i,1} := \langle f^{i,1}(\xi), \Psi_k(\xi)\rangle = 0,$$

$$\begin{aligned}
\tilde{f}_k^{i,M-1} := \langle f^{i,M-1}(\xi), \Psi_k(\xi)\rangle &= \langle \left(-\frac{\alpha(\xi_1)}{4\Delta x} x_{M-1} + \frac{\beta(\xi_2)^2}{4(\Delta x)^2}\right) u^{i,M}(\xi), \Psi_k(\xi)\rangle \\
&= \langle \left(-\frac{\alpha(\xi_1)}{4\Delta x} x_{M-1} + \frac{\beta(\xi_2)^2}{4(\Delta x)^2}\right) e^{-\alpha(\xi_1)t_i}, \Psi_k(\xi)\rangle
\end{aligned}$$

For $i = 0, \dots, N$ denoting $\tilde{F}^i = \left(\tilde{f}_0^{i,1}\ 0\ \dots\ 0\ \tilde{f}_0^{i,M-1}\ ,\ \dots\ ,\ \tilde{f}_P^{i,1}\ 0\ \dots\ 0\ \tilde{f}_P^{i,M-1}\right)^T \in \mathbb{R}^{(M-1)(P+1)}$, the final linear system writes,

$$\begin{cases} \tilde{\boldsymbol{L}}\tilde{U}^{i+1} = \tilde{\boldsymbol{R}}\tilde{U}^i + \tilde{F}^{i+1} + \tilde{F}^i,\ i = 0, \dots, N-1 \\ \tilde{U}^0 = (x_1, \dots, x_{M-1}, 0, \dots, 0)^T \in \mathbb{R}^{(M-1)(P+1)}. \end{cases} \tag{C.1}$$

C.2 Comparison with the method in 5.4

In order to compare the linear systems (5.6) and (C.1), we follow a linear transformation

$$U^i = Q\tilde{U}^i, \ \forall i = 0, \dots, N,$$

where

$$\begin{cases} U^i = \left(u_0^{i,1}, \dots, u_P^{i,1}, \dots, u_0^{i,M-1}, \dots, u_P^{i,M-1}\right)^T \in \mathbb{R}^{(M-1)(P+1)} \\ \tilde{U}^i = \left(u_0^{i,1}, \dots, u_0^{i,M-1}, \dots, u_P^{i,1}, \dots, u_P^{i,M-1}\right)^T \in \mathbb{R}^{(M-1)(P+1)} \end{cases}$$

and Q is a permutation matrix of size $(M-1)(P+1) \times (M-1)(P+1)$ with the following column representation,

$$Q = \left[\mathbf{e}_{\pi(1)}, \dots, \mathbf{e}_{\pi((M-1)(P+1))}\right]^T = \left[\mathbf{e}_1, \dots, \mathbf{e}_{1+P(M-1)}, \dots, \mathbf{e}_{M-1}, \dots, \mathbf{e}_{M-1+P(M-1)}\right]^T,$$

where π is a permutation of $(M-1)(P+1)$ elements and $\mathbf{e}_l$ is a standard basis vector, denotes a row vector of length $(M-1)(P+1)$ with 1 in the l-th position and 0 in every other position.

Then the system (5.6) becomes,

$$\boldsymbol{L}Q\tilde{U}^{i+1} = \boldsymbol{R}Q\tilde{U}^i + F^{i+1} + F^i.$$

By the orthogonality of matrix Q, we have

$$Q^T\boldsymbol{L}Q\tilde{U}^{i+1} = Q^T\boldsymbol{R}Q\tilde{U}^i + Q^T(F^{i+1} + F^i).$$

Note that for any two squared reel matrices M and N, we have $M \otimes N$ and $N \otimes M$ are permutation equivalent, i.e. there exist a permutation matrix Q s.t.

$$M \otimes N = Q^T(N \otimes M)Q.$$

We deduce by this property,

$$\begin{aligned} Q^T\boldsymbol{L}Q &= Q^T\left(\frac{1}{\Delta t}I^{(M-1)} \otimes I^{(P+1)} + \frac{1}{4\Delta x}(DA) \otimes \boldsymbol{A} - \frac{1}{2(\Delta x)^2}B \otimes \boldsymbol{B}\right)Q \\ &= \frac{1}{\Delta t}I^{(P+1)} \otimes I^{(M-1)} + \frac{1}{4\Delta x}\boldsymbol{A} \otimes (DA) - \frac{1}{2(\Delta x)^2}(\boldsymbol{B} \otimes B) = \tilde{\boldsymbol{L}}. \end{aligned}$$

Similarly, we have also $Q^T\boldsymbol{R}Q = \tilde{\boldsymbol{R}}$.

Note that one can approximate the terms $\tilde{f}_k^{i,M-1}$ by $f_k^{i,M-1}$ for $i = 0, \dots, N,\ k = 0, \dots, P$. Indeed, decomposing also the boundary condition by PC expansion in the space $\mathcal{Q}_{d,p}$,

$$u^{i,M}(\xi) \approx \sum_{k=0}^{P} u_k^{i,M}\Psi_k(\xi), \ u_k^{i,M} \in \mathbb{R},$$

and following a Galerkin projection in the same sapce, we deduce then

$$\begin{aligned}
\tilde{f}_k^{i,M-1} &= \langle\left(-\frac{\alpha(\xi_1)}{4\Delta x}x_{M-1} + \frac{\beta(\xi_2)^2}{4(\Delta x)^2}\right)u^{i,M}(\xi), \Psi_k(\xi)\rangle \\
&\approx \langle\left(-\frac{\alpha(\xi_1)}{4\Delta x}x_{M-1} + \frac{\beta(\xi_2)^2}{4(\Delta x)^2}\right)\sum_{l=0}^{P} u_l^{i,M}\Psi_l(\xi), \Psi_k(\xi)\rangle \\
&= \sum_{l=0}^{P}\left[-\frac{x_{M-1}}{4\Delta x}\left(\mu_1\delta_{lk} + \sigma_1\langle\Psi_1\Psi_l, \Psi_k\rangle\right) + \frac{1}{2(\Delta x)^2}\left(\frac{1}{2}\mu_2^2\delta_{lk} + \mu_2\sigma_2\langle\Psi_2\Psi_l, \Psi_k\rangle + \frac{1}{2}\sigma^2\langle\Psi_2^2\Psi_l, \Psi_k\rangle\right)\right]u_l^{i,M} \\
&\approx \sum_{l=0}^{P}\left(-\frac{x_{M-1}}{4\Delta x}a_{kl} + \frac{1}{2(\Delta x)^2}b_{kl}\right)\langle e^{-\alpha(\xi_1)t_i}, \Psi_l(\xi)\rangle = f_k^{i,M-1}.
\end{aligned}$$

According to this, we can show that

$$Q^T F^i \approx \tilde{F}^i, \ \forall i = 0, \dots, N.$$

Therefore, the final linear systems (5.6) and (C.1) are permutation equivalent with approximations of boundary conditions.

To see the difference between $f_k^{i,M-1}$ and $\tilde{f}_k^{i,M-1}$, we can compute the variables

$$\varepsilon^i(P) := \left[\sum_{k=0}^{P}\left(\tilde{f}_k^{i,M-1} - f_k^{i,M-1}\right)^2\right]^{1/2},$$

as a function of the truncated order P, for serveral instant $t_i, i = 0, \dots, N$. The figure C.1 shows that the value of ε^i decreases as the truncated order P increases.

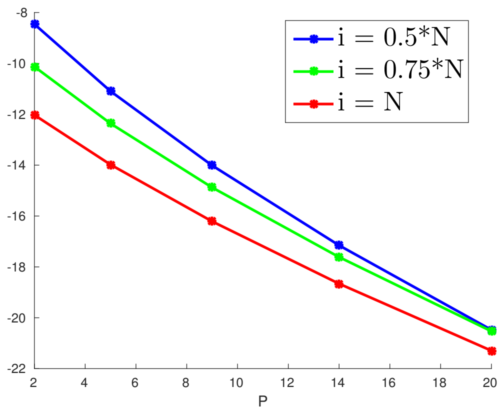


Figure C.1: $\log(\varepsilon^i(P))$ with $N = 1000$

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