

MSc thesis

# Sobol' sensitivity analysis for a parametrized diffusion process

Long LI

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Master of Science in Industrial and Applied Mathematics (MSIAM)

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# Review of SDEs

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A diffusion process  $X : [0, T] \times \Theta \rightarrow \mathbb{R}$  ( $T \in \mathbb{R}_+$ ) satisfies an autonomous SDE,

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

where  $b : \mathbb{R} \rightarrow \mathbb{R}$ ,  $\sigma : \mathbb{R} \rightarrow \mathbb{R}_+$ ,  $W_t$  defined on  $(\Theta, \mathcal{F}_\Theta, \mathbb{P}_\theta)$ .

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## Existence and uniqueness

$$\exists K \in \mathbb{R}_+ \text{ s.t. } \forall (x, y), |b(x) - b(y)| + |\sigma(x) - \sigma(y)| \leq K|y - x|.$$

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## Condition for $X_t \in L^2(\Theta, \mathbb{P}_\theta)$

$$Z \text{ is a r.v. independent of } W_t \text{ s.t. } \mathbb{E}(|Z|^2) < +\infty.$$

# Parametrized SDEs



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where  $X_t$  defined on  $(\Omega, \mathcal{F}, \mathbb{P})$ ,  $W_t$  defined on  $(\Theta, \mathcal{F}_\Theta, \mathbb{P}_\theta)$ ,  $\xi = (\xi_1, \dots, \xi_d)^T \in \mathbb{R}^d$  defined on  $(\Xi, \mathcal{B}_\Xi, \mathbb{P}_\xi)$ ,  $\xi_i$  defined on  $(\Xi_i, \mathcal{B}_{\Xi_i}, \mathbb{P}_{\xi_i})$ .



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Consequences :

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

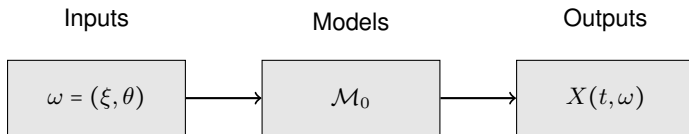
$$\Xi = \prod_{i=1}^d \Xi_i, \mathbb{P}_\Xi = \otimes_{i=1}^d \mathbb{P}_{\xi_i}, L^2(\Xi, \mathbb{P}_\Xi) = \otimes_{i=1}^d L^2(\Xi_i, \mathbb{P}_{\xi_i}).$$

# Models for SA

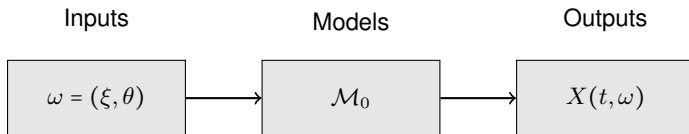


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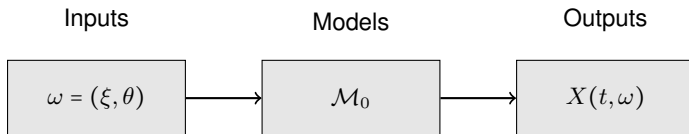
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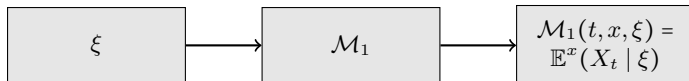
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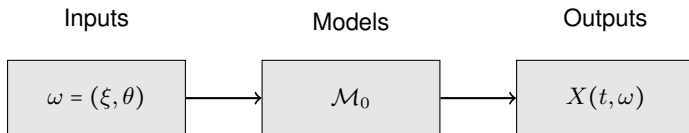


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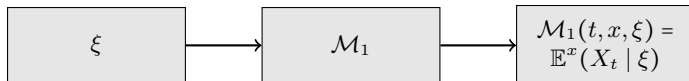


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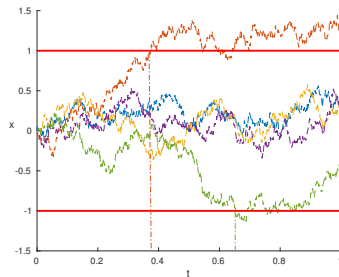


# Mean exit time from an interval

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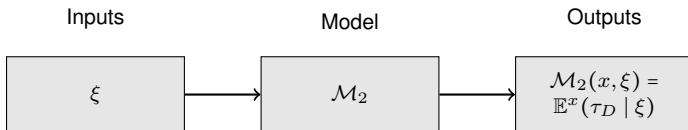
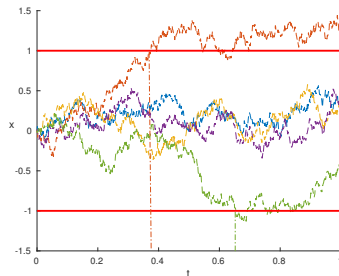
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## First order Sobol' indices

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$$\begin{cases} \mathcal{M}_1(t, x, \xi) = \mathbb{E}^x(X_t \mid \xi) \\ S_I(\mathcal{M}_1(t, x, \xi)) = \frac{\text{Var}(\mathbb{E}(\mathcal{M}_1 \mid \xi_I))}{\text{Var}(\mathcal{M}_1)}, \end{cases}$$

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# Monte Carlo estimator



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# Monte Carlo estimator

Idea :  $\xi'_{(-i)}$  independent copy of  $\xi_{(-i)}$ ,  $y = f(\xi_i, \xi_{(-i)})$ ,  $y^i = f(\xi_i, \xi'_{(-i)})$ ,  $S_i = \frac{\text{Cov}(y, y^i)}{\text{Var}(y)}$ .



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$$A = \begin{pmatrix} \xi_{1,1}^A & \cdots & \xi_{d,1}^A \\ \vdots & \vdots & \vdots \\ \xi_{1,n}^A & \cdots & \xi_{d,n}^A \end{pmatrix} \quad B = \begin{pmatrix} \xi_{1,1}^B & \cdots & \xi_{d,1}^B \\ \vdots & \vdots & \vdots \\ \xi_{1,n}^B & \cdots & \xi_{d,n}^B \end{pmatrix},$$

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4 Compute the estimator (A. Janon et al., 2014) :

$$\hat{S}_i = \frac{\frac{1}{n} \sum_{j=1}^n y_j^B y_j^{C_i} - \left( \frac{1}{n} \sum_{j=1}^n \frac{y_j^B + y_j^{C_i}}{2} \right)^2}{\frac{1}{n} \sum_{j=1}^n \frac{(y_j^B)^2 + (y_j^{C_i})^2}{2} - \left( \frac{1}{n} \sum_{j=1}^n \frac{y_j^B + y_j^{C_i}}{2} \right)^2}, \quad i = 1, \dots, d$$

# Orthogonal polynomials



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# Orthogonal polynomials

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$$-x\Psi_n(x) = A_n\Psi_{n+1}(x) - (A_n + C_n)\Psi_n(x) + C_n\Psi_{n-1}(x), \quad n \geq 1, \quad A_n, C_n \neq 0, \quad \frac{C_n}{A_{n-1}} > 0.$$



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Law	support	density function	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

Some standard distributions and classical orthogonal polynomials.



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## Multidimensional orthogonal polynomials

$$\Psi_{\alpha}(\xi) = \prod_{i=1}^d \Psi_{\alpha_i}^{(i)}(\xi_i) \text{ with } \alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d,$$

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$$\mathcal{Q}_{d,p} = \text{span}\{\xi^{\alpha} = \prod_{j=1}^d \xi_j^{\alpha_j} \mid \alpha \in \mathcal{J}_{d,p}\}, \mathcal{J}_{d,p} = \{\alpha \in \mathbb{N}^d \mid |\alpha| := \sum_{j=1}^d \alpha_j \leq p\}, \dim(\mathcal{Q}_{d,p}) = \binom{d+p}{p}.$$

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via an indexing function

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

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## Affine decomposition hypothesis

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

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.

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Classical PDEs schemes : finite differences, finite elements, spectral approach, etc.

# Parabolic case

## Feymann-Kac formula

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

where  $b$  and  $\sigma$  are bounded and satisfy the lipschitz condition. Assume moreover  $0 < m \leq \sigma^2(x)$ ,  $\forall x \in \mathbb{R}$ .

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

where  $f, g, k : \mathbb{R} \rightarrow \mathbb{R}$  are continuous bounded,  $f \in L^2(\mathbb{R})$  s.t.  $\lim_{|x| \rightarrow \infty} |f(x)| = 0$ , the operator  $\mathcal{A}$  acting on functions in  $\varphi \in C^2(\mathbb{R})$  by

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

Then  $u(t, x) \in C^{1,2}([0, T] \times \mathbb{R}; \mathbb{R})$  and satisfies

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



# Parametrized parabolic PDE

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Setting  $k = g \equiv 0$  and  $f(x) = x$ ,  $\forall x \in \mathbb{R}$ ,

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

is the solution of the parametrized PDE,

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

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In practice, we work in a bounded open domain  $D = (l, r) \subset \mathbb{R}$ ,

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

# PC expansion and Sobol' SA

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PC expansion of  $u(t, x, \xi)$  in the approximate space  $\mathcal{S}_P$  :

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

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

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



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# Elliptic case

## Feymann-Kac formula

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

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  $b, \sigma$  are bounded s.t.

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

Assuming also  $k \geq 0, g \in \mathcal{C}^2(\bar{D}; \mathbb{R})$ . Then  $u \in \mathcal{C}^2(\bar{D}; \mathbb{R})$  and satisfies

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

# Parametrized parabolic PDE, PC expansion and Sobol' SA

Setting  $f = k \equiv 0$  and  $g \equiv 1$ ,

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

becomes the solution of the parametrized PDE,

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

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# Numerical exemple : parametrized OU process



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## Proprities of the OU process

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

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

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- exact scheme :

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

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

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

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$$\begin{cases} \alpha(\xi_1) = \mu_1 \Psi_0(\xi) + \sigma_1 \Psi_1(\xi) \\ \beta(\xi_2) = \mu_2 \Psi_0(\xi) + \sigma_2 \Psi_2(\xi) \end{cases}$$

# Parabolic case



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# Parabolic case

## Model and Sobol' indices

$$\begin{cases} \mathcal{M}_1(t, x, \xi) = \mathbb{E}^x(X_t \mid \xi) \\ S_i(\mathcal{M}_1(t, x, \xi)) = \frac{\text{Var}(\mathbb{E}(\mathcal{M}_1 \mid \xi_i))}{\text{Var}(\mathcal{M}_1)} \\ S_{12}(\mathcal{M}_1(t, x, \xi)) = 1 - \sum_{i=1}^2 S_i(\mathcal{M}_1(t, x, \xi)) \end{cases}$$

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## Explicit solutions

$$E_2 := \mathbb{E} \left[ \left( \mathbb{E}^x(X_t \mid \xi) \right)^2 \right] = x^2 \mathbb{E} \left( e^{-2\alpha(\xi_1)t} \right) = x^2 e^{-2\mu_1 t} \frac{\sinh(2\sqrt{3}\sigma_1 t)}{2\sqrt{3}\sigma_1 t},$$

# Parabolic case

## Model and Sobol' indices

$$\begin{cases} \mathcal{M}_1(t, x, \xi) = \mathbb{E}^x(X_t | \xi) \\ S_i(\mathcal{M}_1(t, x, \xi)) = \frac{\text{Var}(\mathbb{E}(\mathcal{M}_1 | \xi_i))}{\text{Var}(\mathcal{M}_1)} \\ S_{12}(\mathcal{M}_1(t, x, \xi)) = 1 - \sum_{i=1}^2 S_i(\mathcal{M}_1(t, x, \xi)) \end{cases}$$

## Explicit solutions

$$E_2 := \mathbb{E} \left[ \left( \mathbb{E}^x(X_t | \xi) \right)^2 \right] = x^2 \mathbb{E} \left( e^{-2\alpha(\xi_1)t} \right) = x^2 e^{-2\mu_1 t} \frac{\sinh(2\sqrt{3}\sigma_1 t)}{2\sqrt{3}\sigma_1 t},$$

$$\text{Var}(\mathcal{M}_1) = \text{Var}(\mathbb{E}^x(X_t | \xi)) = E_2 - E_1^2,$$

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$$S_1(\mathcal{M}_1(t, x, \xi)) = 1, \quad S_2(\mathcal{M}_1(t, x, \xi)) = 0 \text{ and } S_{12}(\mathcal{M}_1(t, x, \xi)) = 0.$$

# Parametrized parabolic PDE

- Feymann-Kac formula :  $u(t, x, \xi) = \mathbb{E}^x[X_t(\omega, \xi) \mid \xi]$  is the solution of

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

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- Stochastic Galerkin projection in  $\mathcal{S}_P$  :

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



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where  $U = (u_0, \dots, u_P)^T$ ,  $\mathbf{A} = (a_{ij})$ ,  $\mathbf{B} = (b_{ij}) \in \mathcal{M}_{P+1}(\mathbb{R})$  s.t.

$$\begin{cases} a_{ij} = \mu_1 \delta_{ij} + \sigma_1 \langle \Psi_1 \Psi_i, \Psi_j \rangle \\ b_{ij} = \frac{1}{2} \mu_2^2 \delta_{ij} + \mu_2 \sigma_2 \langle \Psi_2 \Psi_i, \Psi_j \rangle + \frac{1}{2} \sigma_2^2 \langle \Psi_2^2 \Psi_i, \Psi_j \rangle \end{cases}$$

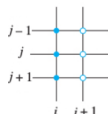


# Crank-Nicholson scheme

Consider  $0 = t_0 < t_1 < \dots < t_N = T, \Delta t = \frac{T}{N}$ ,  $0 = x_0 < x_1 < \dots < x_M = 1, \Delta x = \frac{1}{M}$  and  $U(t_i, x_j) \approx U^{i,j}, \forall (t_i, x_j)$ .

# Crank-Nicholson scheme

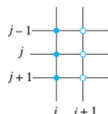
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$$\begin{aligned} \frac{U^{i+1,j} - U^{i,j}}{\Delta t} = & \frac{1}{2} \left( -Ax_j \frac{U^{i,j+1} - U^{i,j-1}}{2\Delta x} + B \frac{U^{i,j-1} - 2U^{i,j} + U^{i,j+1}}{(\Delta x)^2} \right) \dots \\ & + \frac{1}{2} \left( -Ax_j \frac{U^{i+1,j+1} - U^{i+1,j-1}}{2\Delta x} + B \frac{U^{i+1,j-1} - 2U^{i+1,j} + U^{i+1,j+1}}{(\Delta x)^2} \right), \end{aligned}$$

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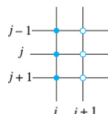


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$$LU^{i+1} = RU^i + (F^{i+1} + F^i), \quad i = 0, \dots, N-1$$

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Avantage : unconditionally stable in  $L^2$  norm and second order both in time and in space.



# Numerical results

$$\mu_1 = 1, \mu_2 = 0.1, \sigma_1 = \sigma_2 = 0.05, t \in [0, 10], x \in [0, 1], \Delta t = \Delta x = 0.01.$$

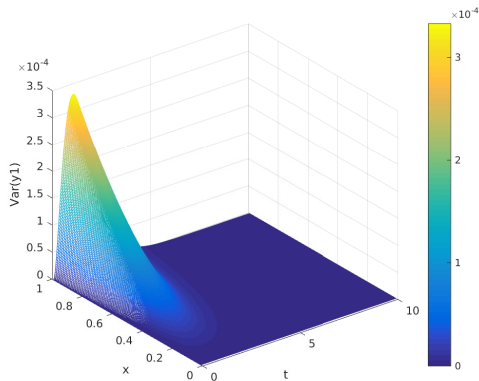


Figure:  $Var(\mathcal{M}_1(t, x, \xi))$  estimated by PC PDE for  $P = 9$

# Numerical results

$$X_0 = x = 0.99, n = 1000, m = 10000, P = 9.$$

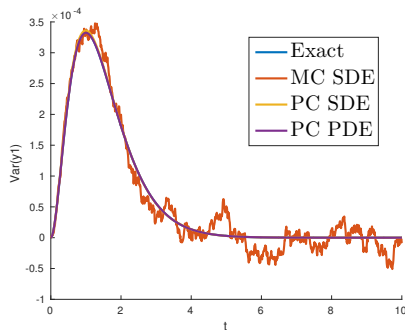


Figure: Evolution of  $Var(\mathcal{M}_1)$  obtained by various methods

# Numerical results

$$\sigma_{y_1}^{T,x} := \text{Var}(\mathcal{M}_1(T, x, \xi)), \quad x = 0.99$$

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

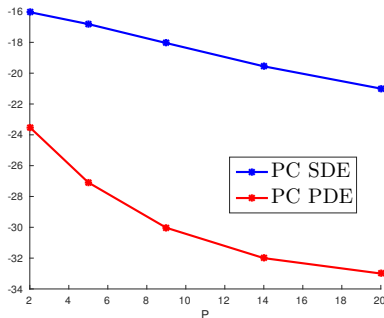


Figure:  $\log(\varepsilon_{\text{SDE}}^{T,x}(P))$  and  $\log(\varepsilon_{\text{PDE}}^{T,x}(P))$



# Numerical results

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

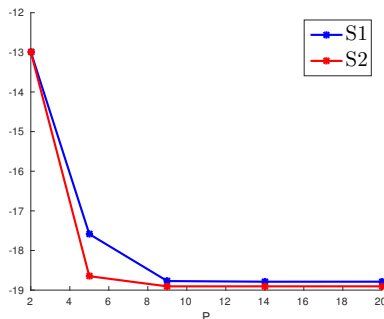


Figure:  $\log(\varepsilon_1^{T,x})$  and  $\log(\varepsilon_2^{T,x})$

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$$\begin{cases} \mathcal{M}_2(x, \xi) = \mathbb{E}^x(\tau_D \mid \xi) \\ S_i(\mathcal{M}_2(x, \xi)) = \frac{\text{Var}(\mathbb{E}(\mathcal{M}_2 \mid \xi_i))}{\text{Var}(\mathcal{M}_2)} \\ S_{12}(\mathcal{M}_2(x, \xi)) = 1 - \sum_{i=1}^2 S_i(\mathcal{M}_2(x, \xi)) \end{cases}$$

# Elliptic case

## Model and Sobol' indices

$$\begin{cases} \mathcal{M}_2(x, \xi) = \mathbb{E}^x(\tau_D \mid \xi) \\ S_i(\mathcal{M}_2(x, \xi)) = \frac{\text{Var}(\mathbb{E}(\mathcal{M}_2 \mid \xi_i))}{\text{Var}(\mathcal{M}_2)} \\ S_{12}(\mathcal{M}_2(x, \xi)) = 1 - \sum_{i=1}^2 S_i(\mathcal{M}_2(x, \xi)) \end{cases}$$

## Feymann-Kac formula

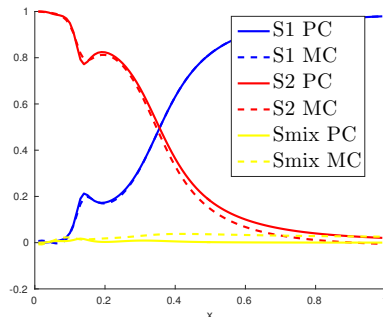
$$u(x, \xi) = \mathbb{E}^x[\tau_D \mid \xi] = \mathcal{M}_2(x, \xi)$$

is the solution of the parametrized PDE,

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

# Numerical results

$$n = 10000, P = 9.$$



**Figure:** Sobol' indices of the mean exit time from the domain  $[0, 1]$  of the OU process, respectively explained by  $\xi_1$ ,  $\xi_2$  and their interaction

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# Thanks for your attentions !