PC EXPANSION FOR GLOBAL SENSITIVITY ANALYSIS OF NON-SMOOTH FUNCTIONALS OF UNCERTAIN STOCHASTIC DIFFERENTIAL EQUATIONS SOLUTIONS

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SAMO 2016
VIII International Conference on Sensitivity Analysis of Model Output,
30 Nov—3 Dec 2016, Le Tampon, Réunion, France.

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Center for Uncertainty Quantification

NON-INTRUSIVE PSP FOR SDES WITH PARAMETRIC UNCERTAINTY

NUMERICAL EXAMPLES

CONCLUSIONS

Non-Intrusive PSP for SDEs with parametric uncertainty

Numerical examples

Conclusions

Let (Ω, Σ, P) be a probability space in which we consider the following SDE:

$$
\begin{aligned}
dX(t,\omega) &= C(X(t,\omega))dt + D(X(t,\omega))dW(t,\omega) \\
X(t=0,\omega) &= X_{(0)}
\end{aligned}
\tag{1}
$$

where:

- $X : (t,\omega) \in T \times \Omega \mapsto \mathbb{R}$ is a **stochastic process** defined in the time interval $T = [0, T_f]$ with $T_f > 0$
- $W(t,\omega)$ is a **Wiener process**
- $C : \mathbb{R} \mapsto \mathbb{R}$ is the **drift** coefficient and $D : \mathbb{R} \mapsto \mathbb{R}$ is the **diffusion** coefficient

Note that there is only one source of randomness in SDE (1), the **Wiener process**.

We consider uncertain drift and diffusion coefficients through the introduction of **random parameters** $\xi(\omega)$

$$
\begin{aligned}
dX(t,\omega) &= C(X(t,\omega),\xi(\omega))dt + D(X(t,\omega),\xi(\omega))dW(t,\omega) \\
X(t=0,\xi(\omega)) &= X_{(0)}(\xi(\omega))
\end{aligned}
\tag{2}
$$

Note that there are two sources of randomness in SDE (2), the **Wiener process** and the **uncertain parameters**.

The **variance-based GSA of X** relies on its **Sobol-Hoeffding (SH)** decomposition:

$$X = \bar{X} + X_{\text{par}}(\boldsymbol{\xi}) + X_{\text{noise}}(W) + X_{\text{mix}}(\boldsymbol{\xi}, W), \tag{3}$$

where:

- $\bar{X} = \mathbb{E}\{X\}$
- $X_{\text{par}}(\boldsymbol{\xi}) = \mathbb{E}\{X|\boldsymbol{\xi}\} - \bar{X}$
- $X_{\text{noise}}(W) = \mathbb{E}\{X|W\} - \bar{X}$
- $X_{\text{mix}}(\boldsymbol{\xi}, W) = X - \bar{X} - \mathbb{E}\{X|\boldsymbol{\xi}\} - \mathbb{E}\{X|W\}$

Since the SH functions on the rhs of (3) are orthogonal, $\mathbb{V}\{X\}$ can be decomposed as:

$$\mathbb{V}\{X\} = V_{\text{par}} + V_{\text{noise}} + V_{\text{mix}},$$

where:

1. V_{par} is the variance due to the parametric uncertainty
2. V_{noise} is the variance due to the Wiener noise
3. V_{mix} is the variance due their interactions

Finally the **sensitivity indices (SI)** are computed:

$$S_{\text{par}} = \frac{V_{\text{par}}}{\mathbb{V}\{X\}}, \quad S_{\text{noise}} = \frac{V_{\text{noise}}}{\mathbb{V}\{X\}}, \quad S_{\text{mix}} = \frac{V_{\text{mix}}}{\mathbb{V}\{X\}}.$$

Assumptions:

1. The **Wiener noise** and the **uncertain parameters** are considered as **independent** random variables
2. The solution of SDE (2), $X(t, W, \boldsymbol{\xi})$, is a **second order** random variable for almost any trajectory of $W(t)$

$X(t, W, \boldsymbol{\xi})$ admits a truncated PC expansion of the form [1]:

$$X(t, W, \boldsymbol{\xi}) \approx \widehat{X}(t, W, \boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathscr{A}} [X_{\boldsymbol{\alpha}}](t, W)\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

where:

- $\boldsymbol{\xi}(\omega) \equiv \boldsymbol{\xi} = \{\xi_1, \cdots, \xi_N\}$ where ξ_i is a real-valued independent random variable (rv) with pdf $p_i(\xi_i)$
- $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)$ is a multi-index
- $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ are multivariate orthonormal polynomials defined through, $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) \doteq \prod_{i=1}^{N} \psi^i_{\alpha_i}(\xi_i)$, where $\{\psi^i_\alpha, \alpha \in \mathbb{N}_0\}$ is a complete orthonormal set with respect to $p_i(\xi_i)$
- The **random processes** $[X_{\boldsymbol{\alpha}}]$ are the **modes** of the expansion.

To compute the modes, $[X_{\boldsymbol{\alpha}}](t, W)$ for $\boldsymbol{\alpha} \in \mathscr{A}$, we rely on **non-intrusive PSP**

$$[X_{\boldsymbol{\alpha}}](t, W) = \sum_{j=1}^{N_Q} \mathscr{P}^{\mathrm{PSP}}_{\boldsymbol{\alpha} j} X(t, W, \boldsymbol{\xi}_j),$$

where:

- $\mathscr{P}^{\mathrm{PSP}}$ is a non-intrusive operator that uses sparse tensorization of one-dimensional projection operators at different levels
- N_Q is the number of sparse grids points
- $\boldsymbol{\xi}_j$ are the quadrature points

In particular, one SDE at each N_Q is solved for a particular trajectory $W^{(i)} = W(\omega_i)$. The **expansion coefficients** of the corresponding trajectory of $X(t)$ are finally obtained through:

$$[X_{\boldsymbol{\alpha}}]^{(i)}(t) = \sum_{j=1}^{N_Q} \mathscr{P}^{\mathrm{PSP}}_{\boldsymbol{\alpha} j} X^{(i)}(t, \boldsymbol{\xi}_j)$$

PC expansion of X:

$$X(t,W,\xi) \approx \widehat{X}(t,W,\xi) = \sum_{\alpha \in \mathscr{A}} [X_\alpha](t,W)\Psi_\alpha(\xi)$$

The approximated **expressions of the statistic** of the SDE solution can be obtained **using the PC coefficients**:

- $\bar{X} \approx \sum_{\alpha \in \mathscr{A}} \mathbb{E}\{[X_\alpha](W)\}\,\mathbb{E}\{\Psi_\alpha\} = \mathbb{E}\{[X_0](W)\}$
- $\mathbb{V}\{X\} = \mathbb{E}\{X^2\} - \bar{X}^2 \approx \sum_{\alpha \in \mathscr{A}} \mathbb{E}\left\{[X_\alpha]^2\right\} - \mathbb{E}\{[X_0]\}^2$
- $S_{\mathrm{par}} = \frac{V_{\mathrm{par}}}{\mathbb{V}\{X\}}$ and $V_{\mathrm{par}} = \sum_{\alpha \in \mathscr{A} \setminus \mathbf{0}} \mathbb{E}\{[X_\alpha]\}^2$
- $S_{\mathrm{noise}} = \frac{V_{\mathrm{noise}}}{\mathbb{V}\{X\}}$ and $V_{\mathrm{noise}} = \mathbb{V}\{[X_0]\}$
- $S_{\mathrm{mix}} = \frac{V_{\mathrm{mix}}}{\mathbb{V}\{X\}}$ and $V_{\mathrm{mix}} = \sum_{\alpha \in \mathscr{A} \setminus \mathbf{0}} \mathbb{V}\{[X_\alpha]\}$

For a detailed proof see [2]

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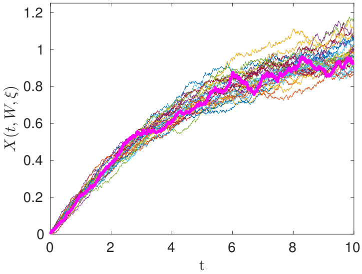
Let us consider the process governed by the following SDE

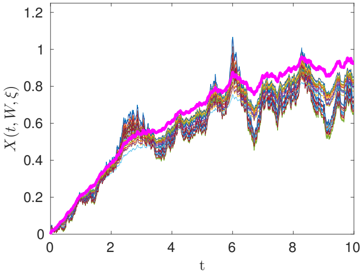
$$
\begin{aligned}
& dX(W,\boldsymbol{\xi}) = (\xi_1 - X(W,\boldsymbol{\xi}))dt + (\nu X(W,\boldsymbol{\xi}) + 1)\xi_2 dW \\
& X(t=0) = 0 \text{ almost surely}
\end{aligned} \tag{4}
$$

where:

- ξ_1 and ξ_2 are independent and uniformly distributed random variables $\xi_1 \sim \mathscr{U}([0.95, 1.15])$ and $\xi_2 \sim \mathscr{U}([0.02, 0.22])$
- $\nu = 0.2$ so the problem has multiplicative noise
- Note that for $\nu = 0$, X is the Ornstein-Uhlenbeck (OU) process



(A) Sampling W

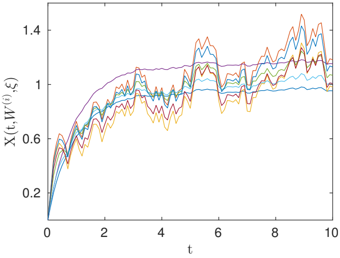


(B) Sampling $\boldsymbol{\xi}$

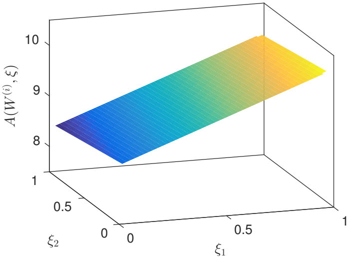
FIGURE: Samples trajectories of X computed using the PC expansion. (A) Trajectories for samples of W at a fixed value of the parameters $\xi_1 = 1.05$ and $\xi_2 = 0.12$. (B) Trajectories for samples of $\boldsymbol{\xi}$ and a fixed realization of W. $\xi_1 \sim \mathscr{U}[0.95, 0.15]$ and $\xi_2 \sim \mathscr{U}[0.02, 0.22]$.

Assuming that we are not interested in $X(t, W, \boldsymbol{\xi})$, but in some **derived quantity** such as the **integral of X over $t \in [0, 10]$:**

$$A(W, \boldsymbol{\xi}) \doteq \int_0^{10} X(t, W, \boldsymbol{\xi}) dt.$$



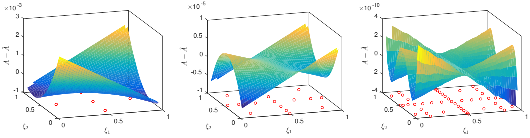
(A) Trajectories of $X(W^{(i)}, \boldsymbol{\xi})$



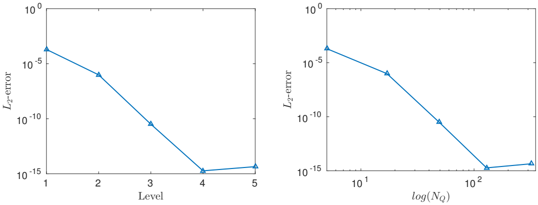
(B) Response surface of $A(W^{(i)}, \boldsymbol{\xi})$

FIGURE: (A) Different trajectories of X, for a fixed noise $W^{(i)}$ and different realizations of $\boldsymbol{\xi}$. (b) $A^{(i)}(\boldsymbol{\xi})$ versus ξ_1 and ξ_2 for fixed $W^{(i)}$.

Convergence of the direct NI projection



(A) Approximation error in $\hat{A}$.



(B) L_2-norm of approximation error.

FIGURE: (A) $A - \hat{A}$ versus $\boldsymbol{\xi}$ for fixed $W^{(i)}$. Plotted are 2D surfaces for $\ell = 1, 2$ and 3 arranged from left to right. (B) Normalized L_2 error versus ℓ (left) and $\log(N_Q)$ (right).

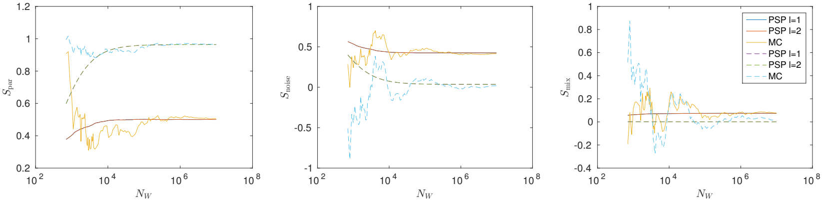
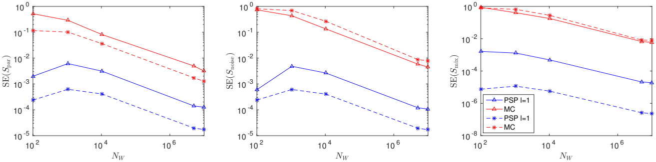
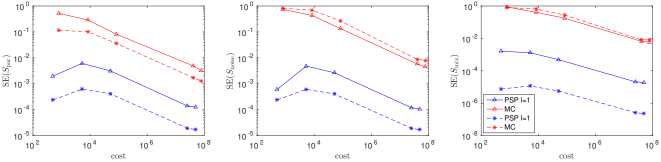


FIGURE: S_{par}, S_{noise} and S_{mix} versus N_W for different PSP levels. Also shown for comparison are the estimators for a direct MC approach (without PSP approximation, labeled MC). The solid lines correspond to the settings of the *Test problem*, whereas dashed lines correspond to results obtained using PSP with a reduced diffusion coefficient $\xi_2 \sim \mathscr{U}[0.02, 0.03]$.



(A) SE (bootstrapping) versus N_W.

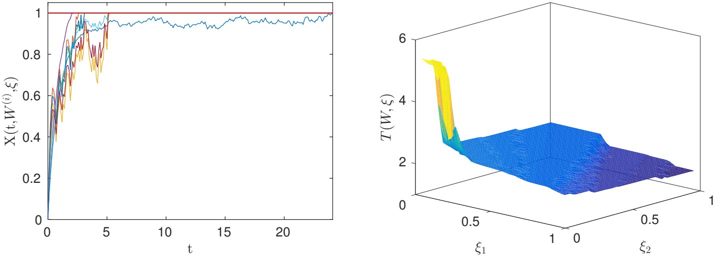


(B) SE versus computational cost which is estimated as $N_Q \times N_W$.

FIGURE: Standard Errors in the sensitivity indices of A, using the direct PSP with $N_Q = 5$ and standard MC methods. The solid lines correspond to the settings of *Test problem*, whereas the dashed lines correspond to the reduced diffusion coefficient $\xi_2 \sim \mathscr{U}[0.02, 0.03]$.

We continue to consider the solution, X, of the SDE in (4), but focus on the variance decomposition of the **exit time, T, corresponding to the exit boundary $X = c$:**

$$T(W, \boldsymbol{\xi}) = \min_{t>0}\{X(t, W, \boldsymbol{\xi}) > c\} \quad \text{we set } c = 1.$$



(A) Trajectories of $X(W^{(i)}, \boldsymbol{\xi})$ (B) Response surface of $T(W^{(i)}, \boldsymbol{\xi})$

FIGURE: (A) Different trajectories of X, for a fixed noise $W^{(i)}$ and different realizations of $\boldsymbol{\xi}$. (B) $T^{(i)}(\boldsymbol{\xi})$ versus ξ_1 and ξ_2 for fixed $W^{(i)}$.

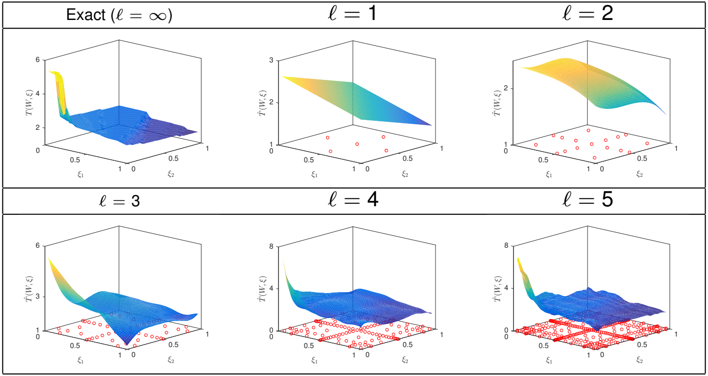


FIGURE: Direct PSP approximation of $T(W^{(i)}, \boldsymbol{\xi})$ for different levels ℓ as indicated. Also shown as circles are the sparse grid points used in the PSP constructions.

KEY IDEA: the exact exit time T (or its direct non-intrusive approximation) is substituted with the surrogate $\tilde{T} = T(\hat{X})$, *indirectly* constructed through

$$T(W, \xi) \approx \tilde{T}(W, \xi) = \min_{t>0}\{\hat{X}(t, W, \xi) > c = 1\},$$

where:

- $\hat{X}(t, W, \xi) = \sum_{\alpha \in \mathscr{A}} [X_\alpha](t, W)\Psi_\alpha(\xi)$

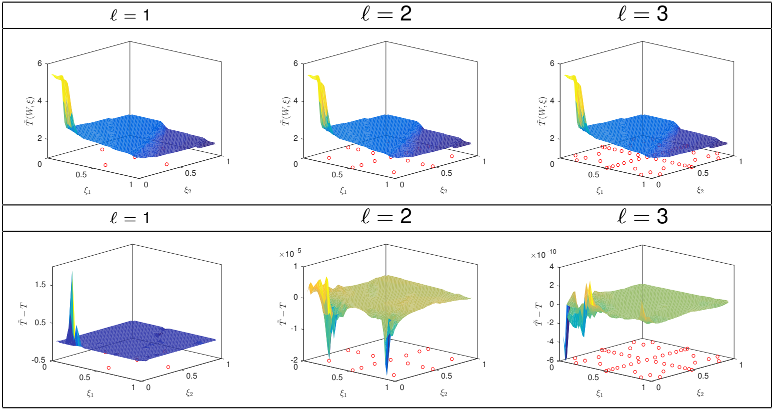


FIGURE: Indirect approximation $\tilde{T}$ of the exit time (top row) and absolute indirect approximation error $T - \tilde{T}$ (bottom row). The plots correspond to a fixed trajectory W of the noise and different PSP levels ℓ as indicated.

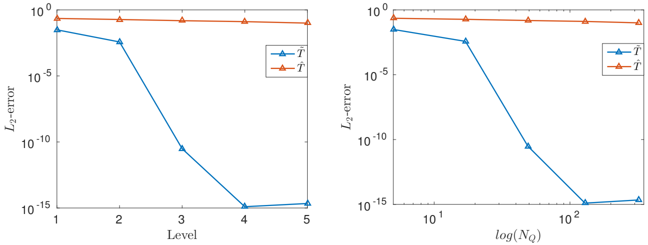


FIGURE: L_2 error norms of the direct and indirect PSP approximations of T.

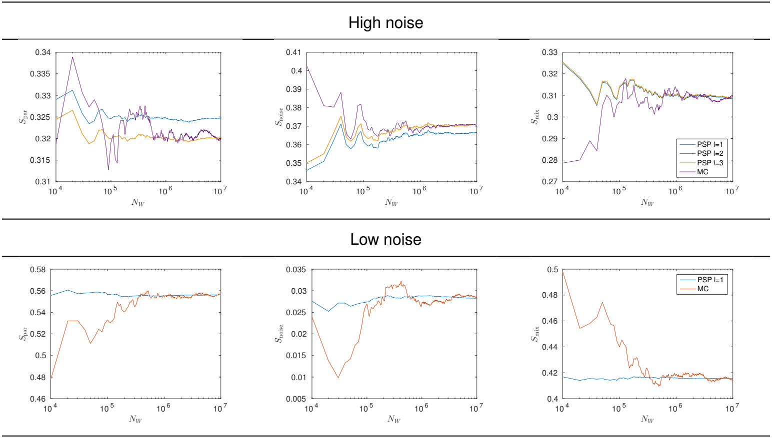


FIGURE: Sensitivity indices S_{par}, S_{noise} and S_{mix} versus the number, N_W, of noise samples for different PSP levels. Also shown for comparison are the standard MC estimators (labeled MC). High noise: $\xi_1 \sim \mathscr{U}[0.95, 1.05]$, $\xi_2 \sim \mathscr{U}[0.02, 0.22]$ and $\nu = 0.2$. Low noise: $\xi_1 \sim \mathscr{U}[0.95, 1.05]$, $\xi_2 \sim \mathscr{U}[0.02, 0.03]$ and $\nu = 0.0$

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CONCLUSIONS

- Very efficient for large S_{par} or smooth QoIs with respect to ξ
- It is trivially implemented in parallel (see [4])
- It can be generalized to any sensitivity indices
- Extension to complex problems and acceleration to MLMC
- Extension to stochastic simulators (see [3])

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