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Exercise 3: Sensitivity analysis and Random Fields in Uncertainty Quantification

Submission

Submit your code and a `.pdf` with your report on Moodle as a `.zip` file named `uq_exercise3_<groupnumber>.zip`. Please add **name** and **matriculation number** of all the group members to the report. Remember to properly describe your approach and analyze the results in the text. Submitting only code is not enough!

Sensitivity analysis

In the last worksheet, we wrote a `Python` + `chaospy` program to propagate the uncertainty in (c, k, f, y_0, y_1) through the ODE model in eq. (1) using the generalized polynomial chaos expansion. In this task, we compare these results to using a Monte Carlo approach for computing the first and total order Sobol' indices.

Assignment 1

Consider the model problem, the linear damped oscillator

$$\begin{cases} \frac{d^2y}{dt^2}(t) + c\frac{dy}{dt}(t) + ky(t) = f\cos(\omega t) \\ y(0) = y_0 \\ \frac{dy}{dt}(0) = y_1. \end{cases} \tag{1}$$

Let $t \in [0, 10]$, $\Delta t = 0.01$, and consider $y(10)$ as the output of interest. Assume that $c \sim \mathcal{U}(0.08, 0.12)$, $k \sim \mathcal{U}(0.03, 0.04)$, $f \sim \mathcal{U}(0.08, 0.12)$, $y_0 \sim \mathcal{U}(0.45, 0.55)$, $y_1 \sim \mathcal{U}(-0.05, 0.05)$ and $\omega = 1.0$.

In the paper by Saltelli et al. (2010)[1], the authors introduce Monte Carlo methods to compute the first and total order Sobol' indices. In this assignment, you are asked to choose one of the methods for this paper and compute Sobol' indices for the system eq. (1). Additionally, you need to compare this method to the pseudo-spectral approach.
To build the comparison, consider both non-sparse and sparse 5D pseudo-spectral computation of the coefficients constructed on Gaussian nodes. To generate multi-variate quadrature nodes and weights, consider $K = [3, 4]$ for the 1D quadrature rule; to construct multi-variate orthogonal polynomials, consider $N = [3, 4]$ for the 1D orthogonal polynomials.

Fill out the missing code in `assignment_1.py` and discuss your findings. Include the following points to your **report**:

- Which approach from the paper you used?
- Either plot or report in a table the results you obtain for the different method to compute the first and total order Sobol' indices. How do you explain the difference?
- Give an estimate for the computational cost (e.g., in ODE solves) for the methods you used.

Hint: You find the paper on Moodle in the literature section.
Hint: For a fair comparison the number of Monte Carlo samples should match the number of full grid points of the pseudo-spectral approach.

Covariance functions

In the lecture, we saw that the covariance function describes spatial/temporal covariance of a random field as

$$C(t, s) := \mathrm{cov}(X_t, X_s).$$

Generally, a Gaussian random field is given in terms of its mean and covariance function. If these two quantities are available we can "sample" the random field. As an example, consider a two-dimensional Gaussian random field $\mathcal{G}$ defined on $[0, 1]^2$ having mean function $m(\boldsymbol{x})$ and covariance function $C(\boldsymbol{x}, \boldsymbol{y})$. To sample this random field, we can apply the following procedure:

[1] Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index, *Andrea Saltelli et al.*, Computer Physics Communications, 2010.

- Discretize the domain $[0, 1]^2$ using an $N \times N$ grid. Put each discretization point in, e.g., the middle of one discretization cell.
- Evaluate $m(\boldsymbol{x})$ and $C(\boldsymbol{x}, \boldsymbol{y})$ at all grid points, i.e., obtain mean vector $\hat{m} \in \mathbb{R}^{N^2}$ and the covariance matrix $\hat{C} \in \mathbb{R}^{N^2 \times N^2}$.
- Perform a Cholesky decomposition to obtain $\hat{C} = LL^T$, where L is a lower triangular matrix.
- Obtain samples from $\mathcal{G}$ as $\mathcal{G}_i = \hat{m} + L\Psi$, where $\Psi \sim \mathcal{N}(\mathbf{0}_{N^2}, \boldsymbol{I}_{N^2})$, and $\boldsymbol{I}_{N^2}$ is the identity matrix of size $N^2 \times N^2$.

Assignment 2

In this assignment, we will work with a Gaussian random field described above. For the mean function, use $m(\boldsymbol{x}) = 0.1$, and consider two options for the covariance function:

- Exponential covariance function

$$C_1(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-||\boldsymbol{x} - \boldsymbol{y}||_2 / l\right), \quad l \in \mathbb{R}.$$

- Squared exponential covariance function

$$C_2(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-||\boldsymbol{x} - \boldsymbol{y}||_2^2 / \left(2 * l^2\right)\right), \quad l \in \mathbb{R}.$$

Your task is to generate and visualize three samples from each field.

Fill out the missing code in `assignment_2.py` and discuss your findings. Include the following points to your **report**:

- Show three samples of each field. What difference can you observe between the two?
- How could this difference be used in modelling?

Hint: You can use `np.linalg.cholesky` for Cholesky decomposition. If you face numerical issues when doing Cholesky decomposition because the covariance function might not be strictly positive definite, try to add some small numbers to the diagonal entries.
Hint: In the end, you will get a random vector of size N^2. To visualize the random field realization, transform this vector into an $N \times N$ matrix.

The Wiener process

In the lecture, we saw that the Brownian motion/Wiener process is defined as a stochastic process $\{W_t : t \in \mathbb{T}\}$ such that

- $W_0 = 0$;
- W_t is continuous in t;
- the increments $W_1 - W_0, W_2 - W_1, \ldots$ are (stochastically) independent;
- $W_{t+u} - W_t \sim \mathcal{N}(0, u) \Leftrightarrow W_t - W_s \sim \mathcal{N}(0, t-s)$;
- $C(t, s) = \min(t, s)$.

For simplicity, assume that $\mathbb{T} = [0, 1]$. The Karhunen-Loève expansion of the Wiener process reads

$$W_t = \sum_{m=1}^{\infty} \sqrt{\lambda_m}\phi_m(t)\zeta_m \approx \sqrt{2}\sum_{m=1}^{M} \frac{\sin((m+0.5)\pi t)}{(m+0.5)\pi}\zeta_m, \quad \zeta_m \sim \mathcal{N}(0,1)$$

given its eigenvalues λ_m and eigenfunctions $\phi_m(t)$ as

$$\lambda_m = \frac{1}{(m-0.5)^2\pi^2}, \quad \phi_m(t) = \sqrt{2}\sin\left(\pi t\left(m - \frac{1}{2}\right)\right). \tag{2}$$

Assignment 3.1

In this exercise, we want to look at the convergence of the Karhunen-Loève expansion for the Wiener process described above. Your task is to generate a realization of the Wiener process for $N = 1000$ points and compare it to the Karhunen-Loève expansion approximation for the same points.
First, we want to look at the eigenvalues of the Karhunen-Loève expansion. For this, consider $M = 1000$ and compute the eigenvalues from eq. (2). Next, employ the Karhunen-Loève expansion approximation with $M = [10, 100, 1000]$ samples (to qualitatively observe the "convergence" of the Karhunen-Loève approximation, use the same seed for all values of M!). Afterwards, use the definition of the Wiener process to generate its realization and compare it to the approximations.

Fill out the missing code in `assignment_3.1.py` and discuss your findings. Include the following points to your **report**:

- The number of samples N and M refer to discretizations of different spaces. What spaces each of these parameters discretize?
- Plot the eigenvalues for $M = 1000$. What do you observe? What to the results imply?
- Visualize three Karhunen-Loève approximations with $M = [10, 100, 1000]$. Can you see the convergence?
- Visualize a random process generated by the definition. What do you observe? What could be the reason for this?

Hint: To generate a realization of the Wiener process using its definition, use the property $W_t - W_s \sim \mathcal{N}(0, t-s)$. Therefore, we have

$$dW := W_{t+dt} - W_{dt} \sim \mathcal{N}(0, dt)$$

for an increment dt.

Assignment 3.2

The KL terms for the Wiener process for an arbitrary time period $t \in [0, T]$ are given by

$$\phi_n(t) = \sqrt{\frac{2}{T}} \sin\left(\frac{(n+\frac{1}{2})\pi t}{T}\right)$$

and

$$\lambda_n = \frac{T^2}{(n+\frac{1}{2})^2\pi^2}$$

for $n \in [1, \infty]$, see [2].

We decide now to model the source term f as a Wiener process in our oscillator model

$$\begin{cases} \frac{d^2y}{dt^2}(t) + c\frac{dy}{dt}(t) + ky(t) = f(t)\cos(\omega t) \\ y(0) = y_0 \\ \frac{dy}{dt}(0) = y_1. \end{cases} \tag{3}$$

Propagate the uncertainty of f through the model in eq. (3) using the Wiener process definition and Karhunen-Loève expansion from the previous assignment. Use the deterministic values

$$c = 0.5, \quad k = 2.0, \quad y_0 = 0.5, \quad y_1 = 0, \quad \omega = 1.0,$$

[2] http://www.maths.lth.se/matstat/staff/georg/Publications/lecture2004.pdf, page 94

and set the mean value of f to $\mu_f = 0.5$. Consider the time period $t \in [0, 10]$ and $dt = 0.01$. For the Monte Carlo sampling, use $N = 1000$ with $M = [5, 10, 100]$ KL terms and compute the mean and variance over time.

Fill out the missing code in `assignment_3.2.py` and discuss your findings. Include the following points to your **report**:

- Show in a table the solutions that you get for mean and variance of $y_0(10)$ for the Wiener process and its different Karhunen-Loève discretizations of $M = [5, 10, 100]$. What do you observe?
- Which methods other than Monte Carlo could be employed to compute the mean and variance of the solution? How would you employ them?