

# Selected topics in statistics

## Spatial Statistics

### Course specifications

Lecturer: François Bachoc, PhD

## Practical information

### Time and Place

Time: 12am-2pm on Monday

- October 14, 21, 28,
- November 4, 11, 18, 25
- December 2, 9, 16
- January 13, 20, 27

Place:

- For **lectures** and **exams**, on 1.OG, in Seminarraum 4.
- For **lab sessions**, on 3.OG, in PC Seminarraum 07.

### Office hours

On Friday: 10am - 11am.

### Evaluation

The evaluation has three components:

- **Homeworks** (30 %). Homeworks are given at the end of a class, and are due for the following class. The homeworks can be send on paper version at the beginning of the following class, or by email (ensure that I acknowledge the receipt) before the following class.
- **Mid-term exam** (35 %). On site paper exam. No course documents and no calculators are allowed.
- **Final exam** (35 %). On site paper exam. No course documents and no calculators are allowed.

### Prerequisite

Background in probability and statistics (e.g. cdf, pdf, conditional distribution, parameter estimation, Gaussian vectors). Some notions in programming and some first notions in the use of a numerical software like R or Matlab.

## An introduction to the course

In this course, we study the field of **spatial statistics** called **geostatistics**. Geostatistics consists in observing output quantities  $Z(x_1), \dots, Z(x_n)$ , where  $x_1, \dots, x_n$  are input quantities belonging to a domain  $\mathcal{D}$ . In practical applications,  $x \in \mathcal{D}$  can represent, for instance, a point in a two-dimensional map, a position in the three-dimensional atmosphere, or a set of numerical conditions specifying a computer-based simulation of a physical system. In the three examples above, the quantity  $Z(x)$  can represent, for instance, the amount of precipitation received in a month, the concentration of a pollutant, and the result of the computer-based simulation.

In this course, we will focus on the case where  $Z$  is modeled as a trajectory of a random process. This is known as a **Kriging** model. We will also especially treat the case when the random process  $Z$  is a **Gaussian process**.

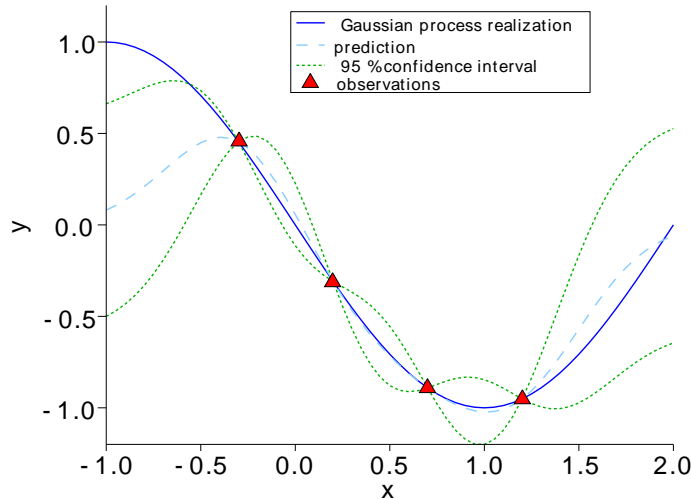


Figure 1: A Gaussian process trajectory on the domain  $\mathcal{D} = [-1, 2]$  is observed at four observation points. Thanks to Gaussian process prediction formulas, we can compute an approximation of the unknown trajectory, and an associated 95% confidence band.

Our goal will essentially be, from the observations  $Z(x_1), \dots, Z(x_n)$ , to predict the rest of the trajectory  $Z : \mathcal{D} \rightarrow \mathbb{R}$ . This consists either in **prediction**, meaning approximating the realization  $Z(x_{new})$  for any  $x_{new} \in \mathcal{D}$ , or **conditional simulation**, meaning generating trajectories  $Z : \mathcal{D} \rightarrow \mathbb{R}$  that are conditioned by the observations  $Z(x_1), \dots, Z(x_n)$ . Examples of prediction and conditional simulation are given in figures 1 and 2.

Prediction and conditional simulation necessitate to estimate the distribution of the random process  $Z$ . In the case where this process is Gaussian, the main problem is to estimate its **covariance function**. We will focus on the **Maximum Likelihood** estimation method for this problem.

## Tentative course programm

- **Class 1 (lecture):** General introduction, stochastic processes. *Homework.*
- **Class 2 (lecture):** Stochastic processes. *Homework.*
- **Class 3 (lecture):** Gaussian processes. *Homework.*
- **Class 4 (lecture):** A focus on the covariance function. *Homework.*
- **Class 5 (lecture):** Classical covariance functions. *Homework.*
- **Class 6 (lecture):** Gaussian conditioning, prediction. *No homework.*
- **Class 7: mid-term exam.** *No homework.*
- **Class 8 (lab-session):** Unconditional simulation, prediction, conditional simulation. *Homework: finish the lab-session and write a report.*
- **Class 9 (lecture):** Covariance function estimation, Maximum Likelihood. *Homework.*
- **Class 10 (lab-session):** Maximum Likelihood. *Homework: finish the lab-session and write a report.*
- **Class 11 (lecture):** Universal Kriging. *Homework.*
- **Class 12 (lecture):** Some additional topics. *No homework.*
- **Class 13: final exam.** *No homework.*

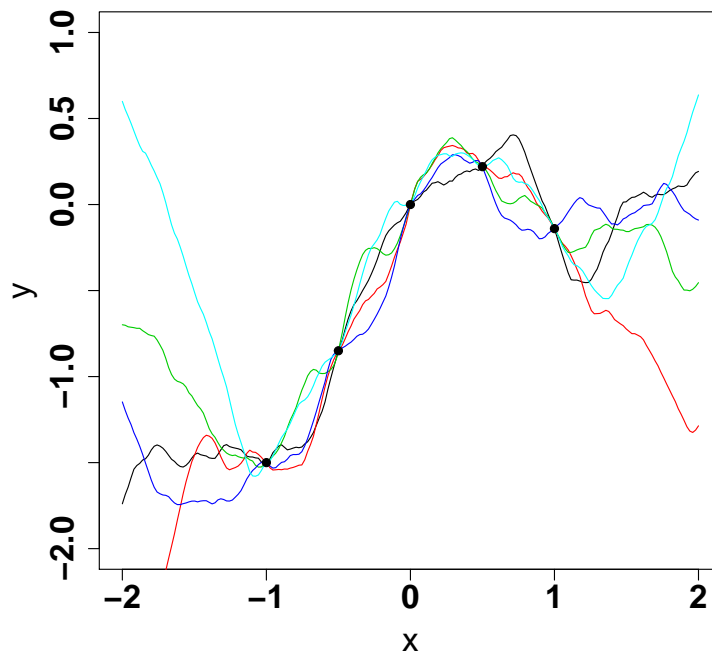


Figure 2: Plot of realizations of a Gaussian process on  $[-2, 2]$ , that are conditioned by five observations. These realizations are obtained thanks to Gaussian process conditioning formulas.

## Some further references

- Books:

[SWN03] On Kriging models for computer experiments.

[RW06] On Gaussian process modeling.

[Ste99] On asymptotic theory for Kriging models.

- Articles:

[SWMW89] On Kriging models for computer experiments.

[JSW98] On the use of Kriging models for global optimization.

[BGL<sup>+</sup>12] On the use of Kriging models for estimating a probability of failure.

[BBP<sup>+</sup>07] On the use of Kriging models for computer model validation (from experimental data).

- The Gaussian process website: <http://www.gaussianprocess.org/>.
- The R packages KrigInv (Kriging-based inversion), MuFiCokriging (Kriging for multi-fidelity computer models), DiceKriging (Kriging methods) and DiceOptim (Kriging-based inversion).

## References

- [BBP<sup>+</sup>07] M. J. Bayarri, J.O. Berger, R. Paulo, J. Sacks, J.A. Cafeo, J. Cavendish, C.H. Lin, and J. Tu. A framework for validation of computer models. *Technometrics*, 49(2):138–154, 2007.
- [BGL<sup>+</sup>12] J Bect, D Ginsbourger, L Li, V Picheny, and E Vazquez. Sequential design of computer experiments for the estimation of a probability of failure. *Statistics and Computing*, 22:773–793, 2012.
- [JSW98] D.R. Jones, M. Schonlau, and W.J. Welch. Efficient global optimization of expensive black box functions. *Journal of Global Optimization*, 13:455–492, 1998.
- [RW06] C.E. Rasmussen and C.K.I. Williams. *Gaussian Processes for Machine Learning*. The MIT Press, Cambridge, 2006.

- [Ste99] M.L Stein. *Interpolation of Spatial Data: Some Theory for Kriging*. Springer, New York, 1999.
- [SWMW89] J. Sacks, W.J. Welch, T.J. Mitchell, and H.P. Wynn. Design and analysis of computer experiments. *Statistical Science*, 4:409–423, 1989.
- [SWN03] T.J Santner, B.J Williams, and W.I Notz. *The Design and Analysis of Computer Experiments*. Springer, New York, 2003.