INSA – Gaussian processes

Introduction

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Who am I?

Andrés F. López-Lopera

Colombia

2008-2013 — **Electrical Eng.**, *Universidad Tecnológica de Pereira*
· Machine learning and signal processing

2014-2015 — **M.Sc. in Electrical Eng.**, *Universidad Tecnológica de Pereira*
· Probabilistic modelling using Gaussian processes (GPs)

France

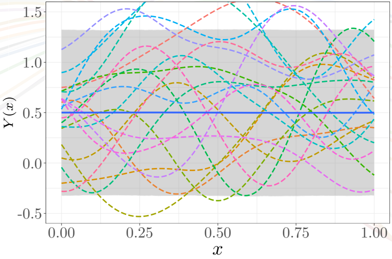
2016-2019 — **PhD in Applied Mathematics**, *Mines Saint-Étienne*
· Joint supervision: *Institut de Mathématiques de Toulouse*
· GPs under inequality constraints
· Applications: nuclear risk assessment, coastal flooding

2019-2020 — **Postdoctoral Research**, *Institut de Mathématiques de Toulouse*
· Joint supervision: *The French Geological Survey BRGM*
· Multi-output GPs & coastal flooding

2020-2021 — **Postdoctoral Research**, *The French Aerospace Lab ONERA*
· Multi-fidelity GPs & aerodynamics (wind tunnel tests)

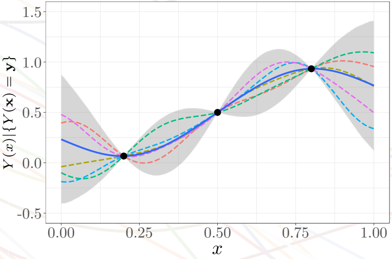
Gaussian processes (GPs) as flexible priors over functions

GP prior



$Y \sim \mathcal{GP}(m, k_{\boldsymbol{\theta}})$

GP regression



$Y|\{Y(\boldsymbol{x}) = \boldsymbol{y}\} \sim \mathcal{GP}(m_{\text{cond}}, c_{\boldsymbol{\theta}})$

■ mean function ■ prediction intervals ■ ■ ··· ■ samples

• Interpolation conditions: $(\boldsymbol{x}, \boldsymbol{y}) = (x_i, y_i)_{i=1}^{n}$

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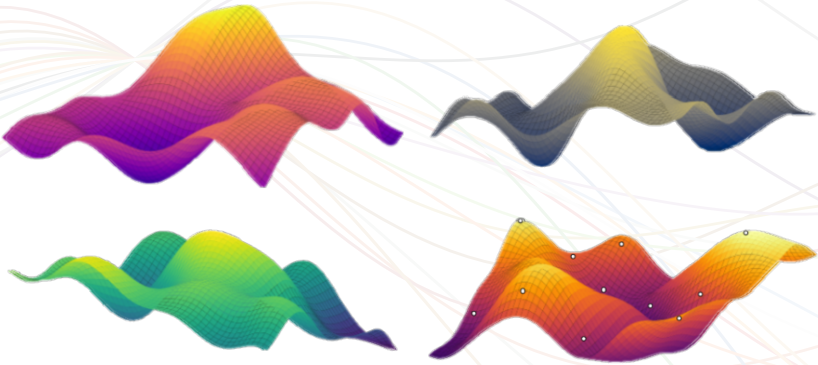
Gaussian processes (GPs) as flexible priors over functions

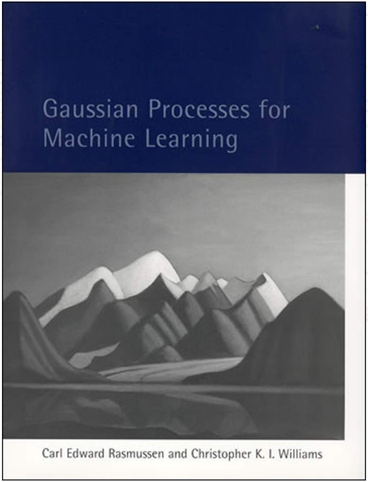


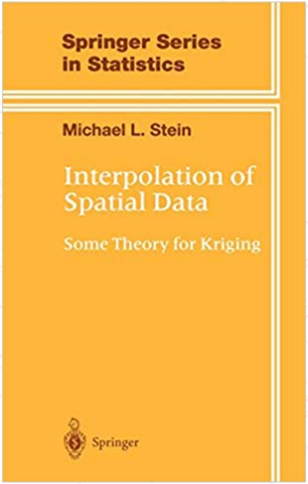
Gaussian random fields

Outline

- In this course:
    1. A recap of Gaussian processes
    2. Spectral representation and Bochner's theorem
    3. Regularity conditions (e.g. continuity, differentiability)
    4. An introduction to reproducing kernel Hilbert-spaces (RKHS)
- Material of the lectures can be found at: `https://anfelopera.github.io/`

Main references





http://www.gaussianprocess.org/gpml/

https://www.springer.com/gp/book/9780387986296

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Additional references

Alain Berlinet and Christine Thomas-Agnan. *Reproducing kernel Hilbert spaces in probability and statistics*. Springer Science & Business Media, 2011.

C. Chatfield. *The Analysis of Time Series: An Introduction, Sixth Edition*. Chapman & Hall/CRC Texts in Statistical Science. CRC Press, 2016.

Marc G. Genton. Classes of kernels for machine learning: A statistics perspective. *Journal of Machine Learning Research*, 2001.

Jochen Görtler, Rebecca Kehlbeck, and Oliver Deussen. A visual exploration of Gaussian processes. *Distill*, 2019. https://distill.pub/2019/visual-exploration-gaussian-processes.

Kevin P. Murphy. *Probabilistic Machine Learning: An introduction*. MIT Press, 2021.

Carl E. Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. MIT Press, 2005.

Arno Solin. *Machine learning with signal processing*. ICML – TUTORIAL, 2020.

Michael L. Stein. *Interpolation of Spatial Data: Some Theory for Kriging*. Springer, 1999.

Gaussian processes

· Let $\{Y(\boldsymbol{x}); \boldsymbol{x} \in \mathbb{R}^d\}$ be a GP

· Y is completely defined by its mean m and covariance (kernel) k functions:

$$Y \sim \mathcal{GP}(m, k), \tag{1}$$

where

$$\begin{aligned} &\text{(trend)} && m(\boldsymbol{x}) = \mathbb{E}\left\{Y(\boldsymbol{x})\right\}, \\ &\text{(correlation, p.s.d.)} && k(\boldsymbol{x}, \boldsymbol{x}') = \mathsf{cov}\left\{Y(\boldsymbol{x}), Y(\boldsymbol{x}')\right\}, \quad \text{for} \quad \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^d. \end{aligned} \tag{2}$$

· The operator $\mathbb{E}$ denotes the expectation of random variables (r.v's), and the covariance operator is given by

$$\mathsf{cov}\left\{Y(\boldsymbol{x}), Y(\boldsymbol{x}')\right\} = \mathbb{E}\left\{[Y(\boldsymbol{x}) - m(\boldsymbol{x})][Y(\boldsymbol{x}') - m(\boldsymbol{x}')]\right\}.$$

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· It is common to assume that Y has mean zero, i.e. $m(\cdot) = 0$. Then,

$$k(\boldsymbol{x}, \boldsymbol{x}') = \operatorname{cov}\left\{Y(\boldsymbol{x}), Y(\boldsymbol{x}')\right\} = \mathbb{E}\left\{Y(\boldsymbol{x})Y(\boldsymbol{x}')\right\}. \tag{3}$$

· If $m(\cdot) = 0$, then Y is known as a centred GP.

Exercise. Show that $Z \sim \mathcal{GP}(m, k)$ can be written in terms of $Y \sim \mathcal{GP}(0, k)$:

$$Z(\boldsymbol{x}) = m(\boldsymbol{x}) + Y(\boldsymbol{x}). \tag{4}$$

- If Y is a centred GP, then it is completely defined by its kernel k.
- Regularity assumptions are then encoded in k [Genton, 2001]:
  - stationarity
  - isotropy
  - periodicity
  - smoothness

Definition (Stationary kernel functions)

A kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, with $\mathcal{X} \subset \mathbb{R}^d$, is **stationary** if, for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$, $k(\boldsymbol{x}, \boldsymbol{x}')$ only depends on $\boldsymbol{x} - \boldsymbol{x}'$.

Definition (Isotropic kernel functions)

A kernel k is **isotropic** (or homogeneous) if $k(\boldsymbol{x}, \boldsymbol{x}')$ only depends on $|\boldsymbol{x} - \boldsymbol{x}'|$.

Examples of 1D stationary kernels

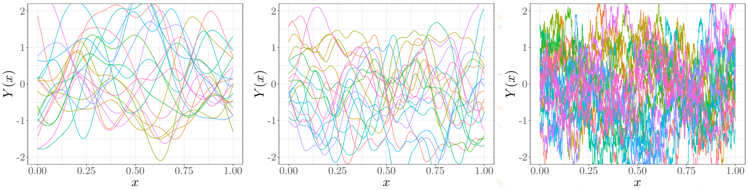
- Denote $k(\tau) := k(x, x+\tau)$ (abuse of notation)
- Some classic 1D stationary kernels are [Genton, 2001]:

Squared Exponential (SE): $$k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$$

Matérn 5/2: $$k_{\sigma^2,\ell}(\tau) = \sigma^2 \left(1 + \sqrt{5}\frac{|\tau|}{\ell} + \frac{5}{3}\frac{\tau^2}{\ell^2}\right) \exp\left\{-\sqrt{5}\frac{|\tau|}{\ell}\right\},$$

Exponential: $$k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{|\tau|}{\ell}\right\},$$

with variance parameter σ^2 and length-scale parameter ℓ.

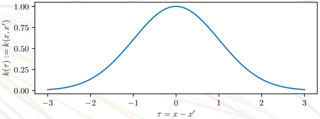


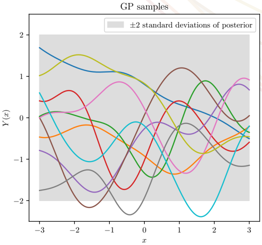
(a) Squared Exponential (b) Matérn 5/2 (c) Exponential

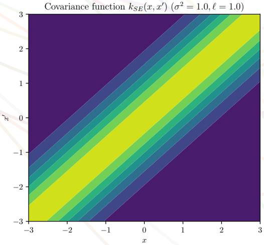
samples

Squared Exponential (SE): $k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$

$\sigma^2 = 1.0, \ell = 1.0$





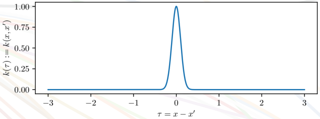


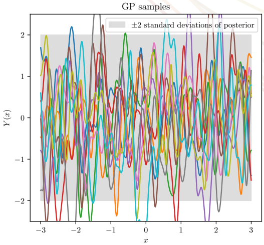
Effect of the variance σ^2 and the length-scale ℓ [Görtler et al., 2019]

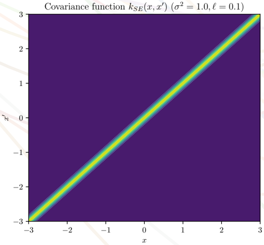
Examples of 1D stationary kernels

Squared Exponential (SE): $$k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$$

$\sigma^2 = 1.0, \ell = 0.1$





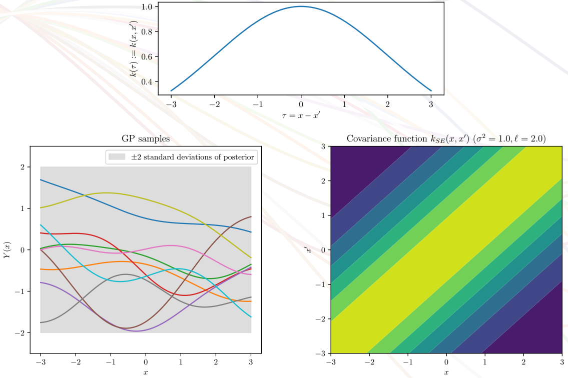


Effect of the variance σ^2 and the length-scale ℓ [Görtler et al., 2019]

Examples of 1D stationary kernels

Squared Exponential (SE): $$k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$$

$\sigma^2 = 1.0, \ell = 2.0$

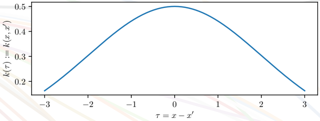


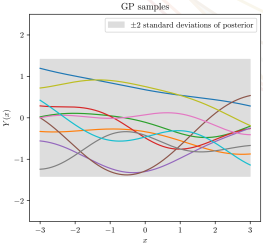
Effect of the variance σ^2 and the length-scale ℓ [Görtler et al., 2019]

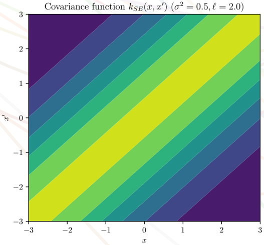
Examples of 1D stationary kernels

Squared Exponential (SE): $\quad k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$

$\sigma^2 = 0.5, \ell = 2.0$

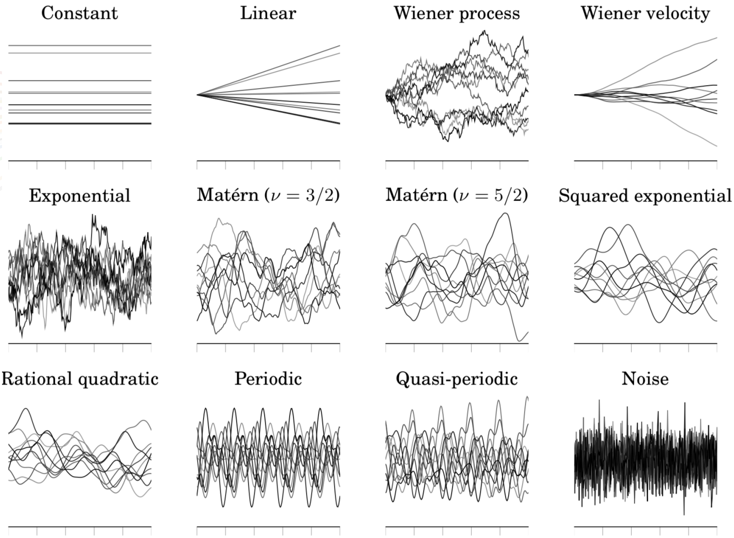






Effect of the variance σ^2 and the length-scale ℓ [Görtler et al., 2019]

Other examples of 1D kernels

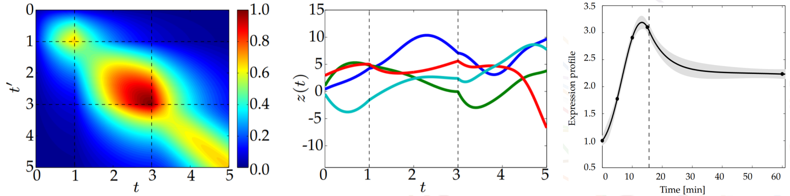


Examples of GP samples [Solin, 2020]

- **Görtler et al. [2019]**: A visual exploration of Gaussian processes **[Link]**
- **Damianou [2016]:** A Python notebook on Gaussian processes **[Link]**

Applications of Gaussian processes

Biology: prediction of protein concentrations



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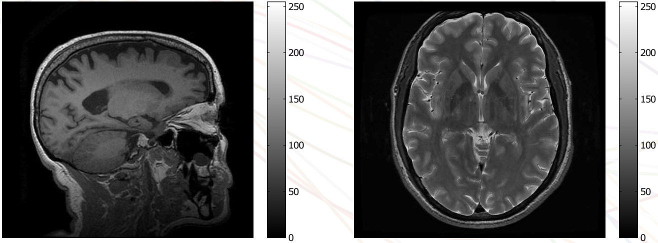
Switched latent force models for reverse-engineering transcriptional regulation in genes
IEEE/ACM Transaction on Computational Biology and Bioinformatics, 2017

Neuroscience: magnetic resonance imaging (MRI)



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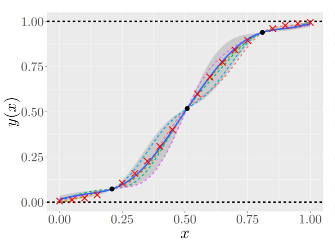
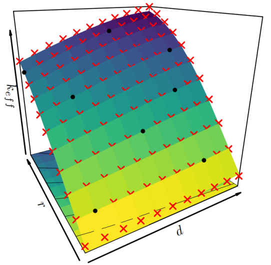
Gaussian processes for slice-based super-resolution MR images
Lecture Notes in Computer Science (LNCC), 2015

Risk assessment: nuclear safety





- **A. F. López-Lopera, N. Durrande, F. Bachoc and O. Roustant:**
Finite-dimensional Gaussian approximation with linear inequality constraints
SIAM/ASA Journal on Uncertainty Quantification, 2018

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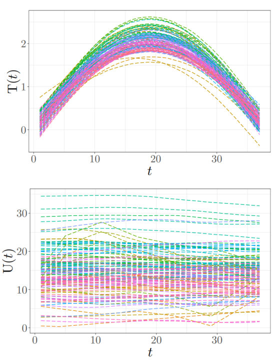
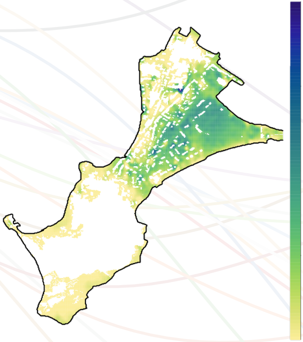
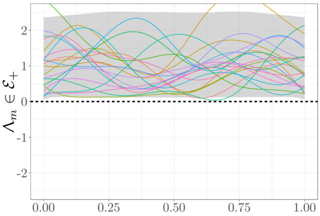
Risk assessment: coastal flooding

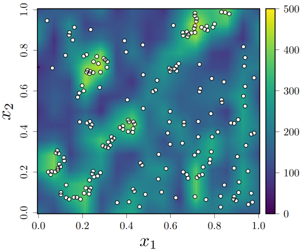




- **A. F. López-Lopera, D. Idier, J. Rohmer and F. Bachoc:**
Multi-output Gaussian processes with functional data: A study on coastal flood hazard assessment
Submitted, 2020

Geostatistics: spatial distribution of tree species





- **A. F. López-Lopera, S. John and N. Durrande:**
Gaussian process modulated Cox processes under linear inequality constraints
International Conference on Artificial Intelligence and Statistics (AISTATS), 2019

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Conclusions

Conclusions

- GPs provide a well-founded non-parametric (Bayesian) framework
- They have been successfully applied in diverse applications:
  - Geostatistics, physics, chemistry
  - Neuroscience, biology and medicine
  - Engineering fields
  - Econometrics
  - ...
- Regularity assumptions are encoded in kernel functions
  - smoothness, periodicity, stationarity, isotropy, ...