ONERA
THE FRENCH AEROSPACE LAB

INSA – Gaussian processes

Introduction

Andrés F. López-Lopera

The French Aerospace Lab ONERA, France
Information Processing and Systems Department (DTIS)
Multidisciplinary Methods, Integrated Concepts (M2CI) Research Unit

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)

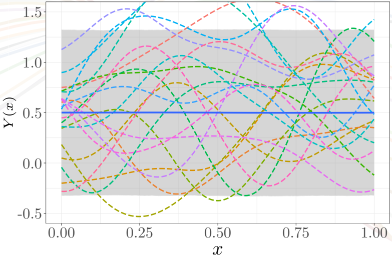
ONERA THE FRENCH AEROSPACE LAB

Research interests

- My research interests include:
  - Applied mathematics
  - Machine learning & computer science
  - Probabilistic modelling, Bayesian inference and optimisation, GPs, etc.
- With applications to:
  - Electrical engineering and signal processing
  - Risk assessment (nuclear, coastal, etc.)
  - Aerodynamics (wind tunnel test)
  - Artificial intelligence

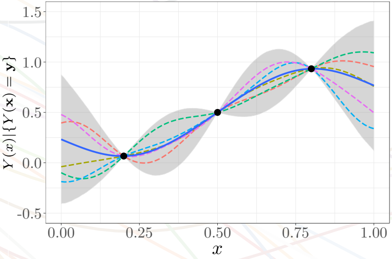
Gaussian processes (GPs) as flexible priors over functions

GP prior



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

GP posterior

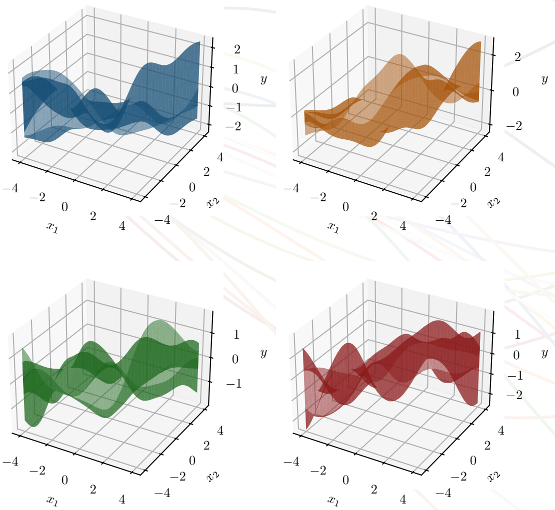


$$Y|\{Y(\boldsymbol{x}) = \boldsymbol{y}\} \sim \mathcal{GP}(m_{\text{cond}}, c_{\boldsymbol{\theta}})$$

mean function   prediction intervals $\cdots$ samples

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

Gaussian processes (GPs) as flexible priors over functions

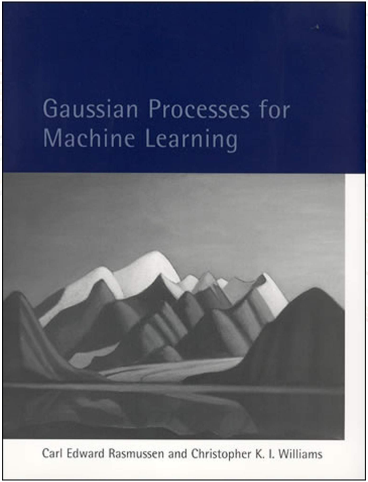


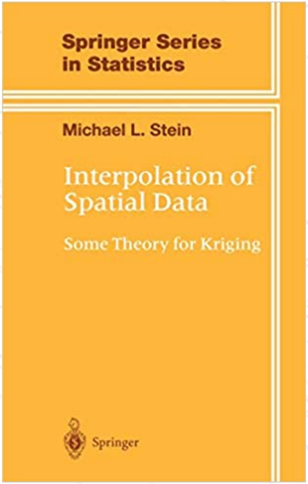
Gaussian random fields

Outline

- In these lectures:
  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 can be found at: `https://anfelopera.github.io/teaching/`

Main references





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

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

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

· A GP $\{Y(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d\}$ is a collection of random variables, any finite number of which have a joint Gaussian distribution [Rasmussen and Williams, 2005]

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

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

where

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

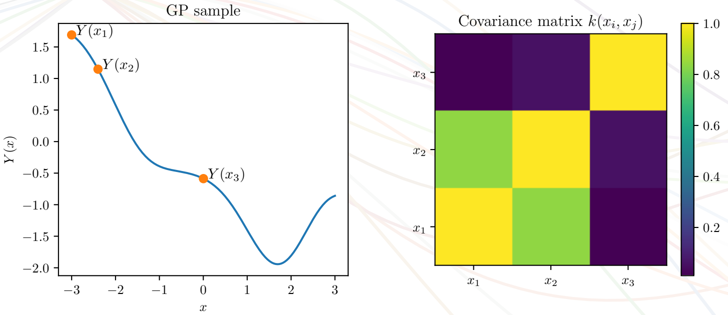
· The operator $\mathbb{E}$ denotes the expectation of random variables (r.v's), and the covariance operator is given by

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

ONERA
THE FRENCH AEROSPACE LAB

Note. Independence between $Y(\boldsymbol{x}), Y(\boldsymbol{x}')$ implies $k(\boldsymbol{x}, \boldsymbol{x}') = 0$.

Squared Exponential (SE) kernel



- If $Y(\boldsymbol{x}), Y(\boldsymbol{x}')$ are correlated, then $k(\boldsymbol{x}, \boldsymbol{x}') \neq 0$
- If $Y(\boldsymbol{x}), Y(\boldsymbol{x}')$ are non-correlated, then $k(\boldsymbol{x}, \boldsymbol{x}') = 0$

- It is common to assume that Y is centred, i.e. $m(\cdot) = 0$.
- Then, Y is completely defined by its kernel k:

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

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

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

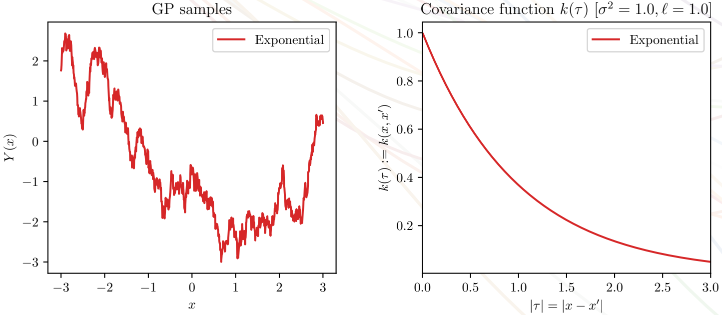
ONERA
THE FRENCH AEROSPACE LAB

Kernel functions

Kernel functions

· In previous lectures, the exponential (Ornstein-Uhlenbeck) kernel function has been studied:

$$k(x, x') = \sigma^2 \exp\left\{ -\frac{|x - x'|}{\ell} \right\}.$$



ONERA
THE FRENCH AEROSPACE LAB

Kernel functions

Definition (Symmetry)

Let $\mathcal{X}$ be a non-empty set (e.g. $\mathcal{X} \subset \mathbb{R}^d$). A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is symmetric if, for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$:

$$k(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}', \boldsymbol{x}).$$

Definition (Positive semi-definiteness, p.s.d)

k is p.s.d. if for all $n \in \mathbb{N}$, and for all $a_1, \ldots, a_n \in \mathbb{R}$, $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathcal{X}$:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(\boldsymbol{x}_i, \boldsymbol{x}_j) \geq 0.$$

Definition (Covariance functions)

k is a valid covariance function (or kernel) on $\mathcal{X}$ if it is symmetric and p.s.d.

ONERA
THE FRENCH AEROSPACE LAB

Kernel functions

· **Remember.** Every kernel k is the covariance function of some centred (Gaussian) stochastic process.

· Then, it is possible to design dedicated kernels for encoding regularity assumptions in GPs [Genton, 2001], e.g.:

- smoothness (continuity & differentiability)
- periodicity, quasi-periodicity
- stationarity
- isotropy (homogeneity)

ONERA
THE FRENCH AEROSPACE LAB

Kernel functions

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 $\boldsymbol{x} - \boldsymbol{x}'$.

- We denote $k(\boldsymbol{\tau}) := k(\boldsymbol{x} - \boldsymbol{x}')$ (abuse of notation)

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 kernels

· Some classic 1D stationary kernels are [Genton, 2001]:

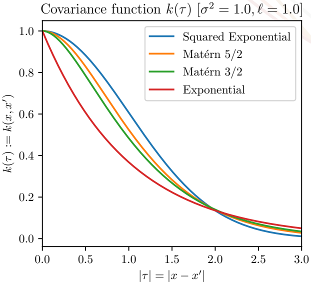
Squared Exponential (SE): $k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\},$

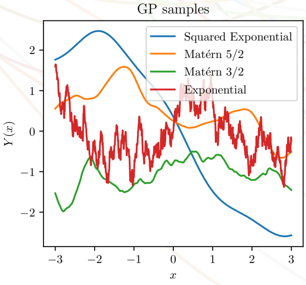
Matérn 5/2: $k_{\sigma^2,\ell}(\tau) = \sigma^2 \left(1 + \sqrt{5}\frac{|\tau|}{\ell} + \frac{5}{3}\frac{\tau^2}{\ell^2}\right) \exp\left\{-\sqrt{5}\frac{|\tau|}{\ell}\right\},$

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

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

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

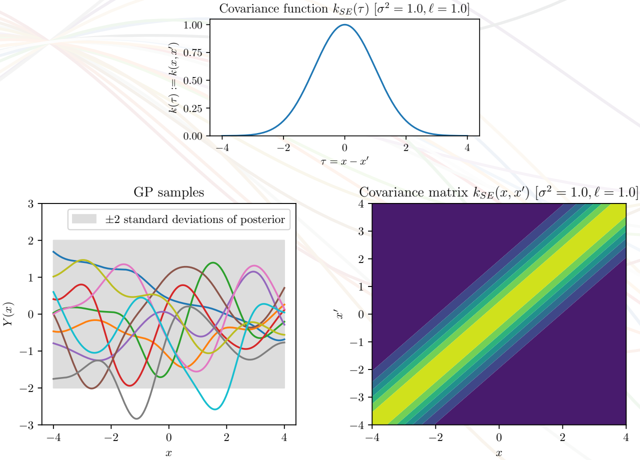




ONERA
THE FRENCH AEROSPACE LAB

Examples of 1D kernels

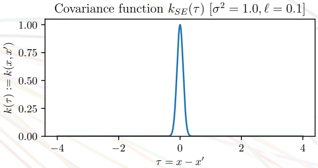
Squared Exponential (SE): $k_{\sigma^2,\ell}(\tau) = \sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\}$

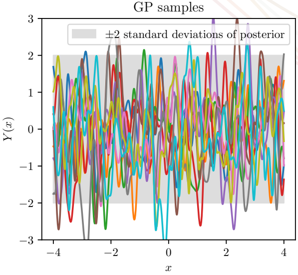


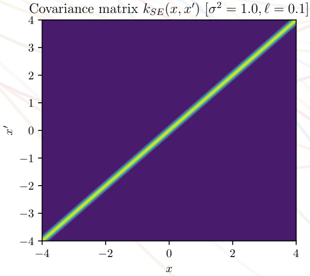
Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

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



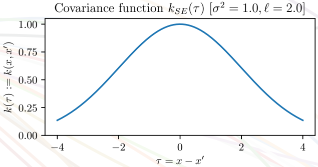


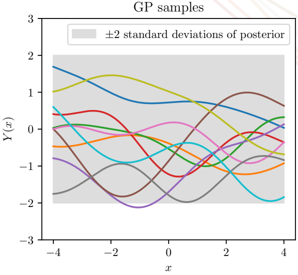


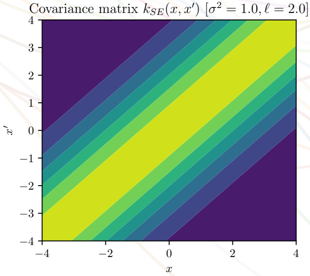
Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

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





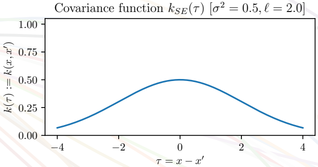


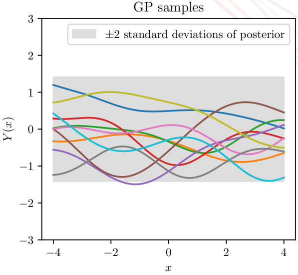
Effect of the variance σ^2 and the length-scale ℓ on GP samples

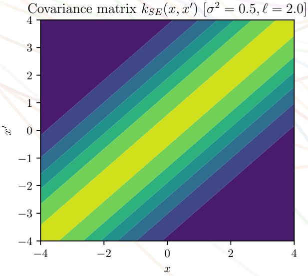
ONERA
THE FRENCH AEROSPACE LAB

Examples of 1D kernels

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



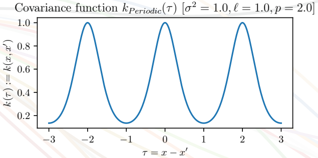


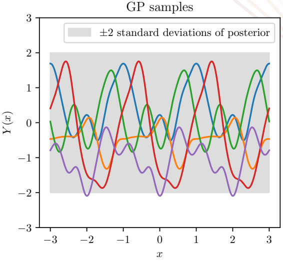


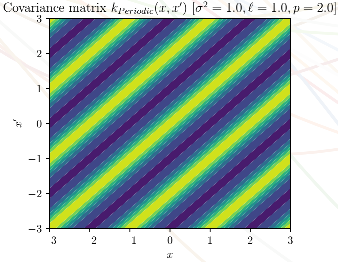
Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

Periodic kernel: $$k_{\sigma^2,\ell,p}(\tau) = \sigma^2 \exp\left\{-\frac{2}{\ell^2}\sin^2\left[\frac{\pi}{p}\tau\right]\right\}$$

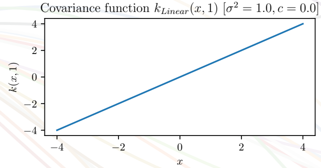


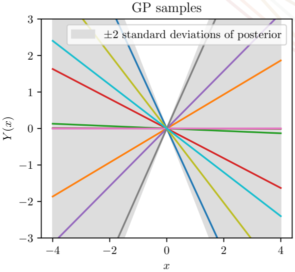


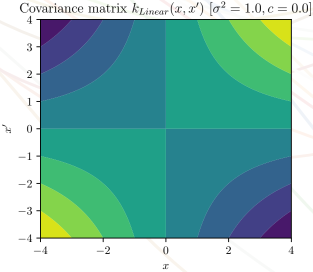


Examples of 1D kernels

Linear kernel: $$k_{\sigma^2,c}(x,x') = \sigma^2(x-c)(x'-c)$$

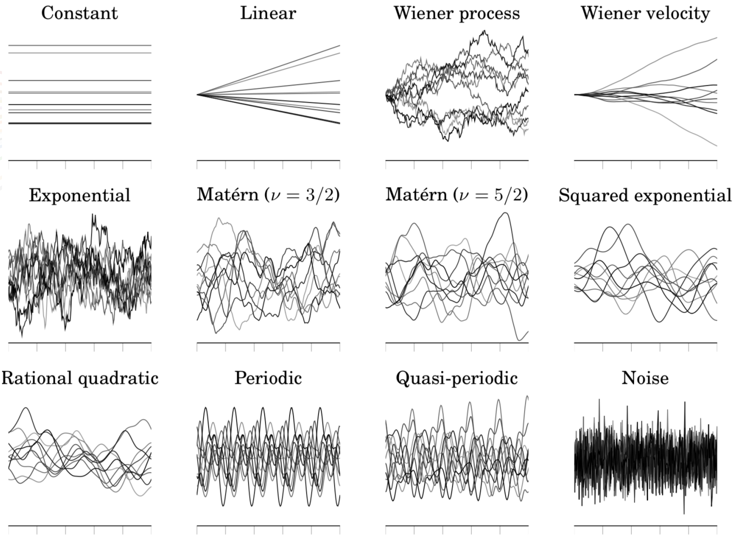






ONERA
THE FRENCH AEROSPACE LAB

Examples of 1D kernels



Examples of GP samples [Solin, 2020]

Building new kernels from other ones

- We can also create new kernels by combining predefined ones, e.g.:

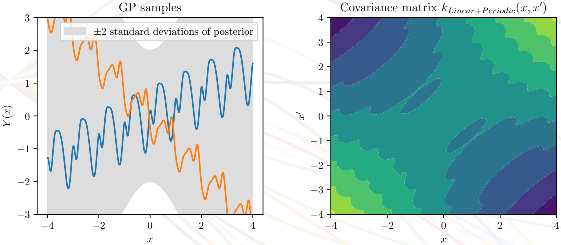
$$
\begin{array}{ll}
\text{Sum of kernels:} & k(\boldsymbol{x}, \boldsymbol{x}') = k_1(\boldsymbol{x}, \boldsymbol{x}') + k_2(\boldsymbol{x}, \boldsymbol{x}') \\
\text{Product of kernels:} & k(\boldsymbol{x}, \boldsymbol{x}') = k_1(\boldsymbol{x}, \boldsymbol{x}') \times k_2(\boldsymbol{x}, \boldsymbol{x}') \\
\text{Composed with a function:} & k(\boldsymbol{x}, \boldsymbol{x}') = k_1(\phi(\boldsymbol{x}), \phi(\boldsymbol{x}'))
\end{array}
$$

- All the previous operations preserve the p.s.d.

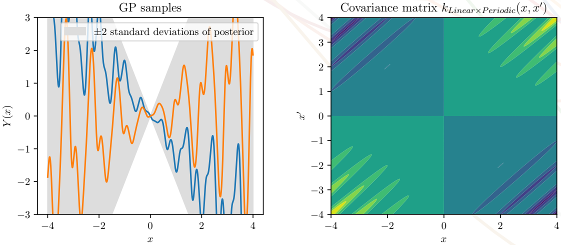
ONERA
THE FRENCH AEROSPACE LAB

Building new kernels from other ones

$$k(x,x') = k_{\text{Linear}}(x,x') + k_{\text{Periodic}}(x,x')$$



$$k(x,x') = k_{\text{Linear}}(x,x') \times k_{\text{Periodic}}(x,x')$$

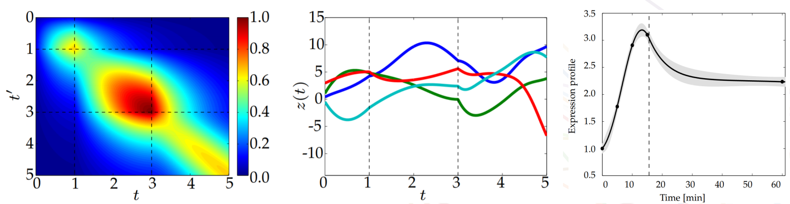


ONERA
THE FRENCH AEROSPACE LAB

- **Durrande [2017]**: Gaussian process playground **[Link]**
- **Görtler et al. [2019]**: A visual exploration of Gaussian processes **[Link]**
- **Damianou [2016]:** A Python notebook on Gaussian processes **[Link]**

Applications of Gaussian processes

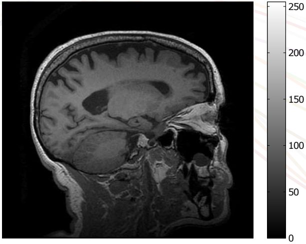
Biology: prediction of protein concentrations

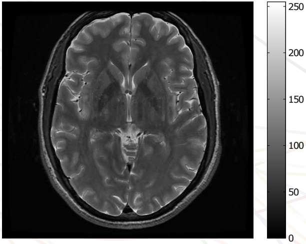


- **A. F. López-Lopera and M. A. Alvarez:**
Switched latent force models for reverse-engineering transcriptional regulation in genes
IEEE/ACM Transaction on Computational Biology and Bioinformatics, 2017

Applications of Gaussian processes

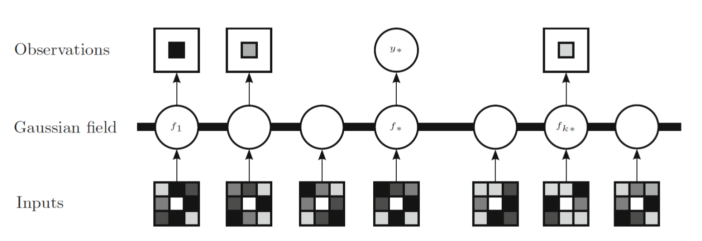
Neuroscience: magnetic resonance imaging (MRI)





- **H. Vargas, A. López-Lopera, M. A. lvarez, A. Orozco, J. Hernández and N. Malpica:**
Gaussian processes for slice-based super-resolution MR images
Lecture Notes in Computer Science (LNCC), 2015

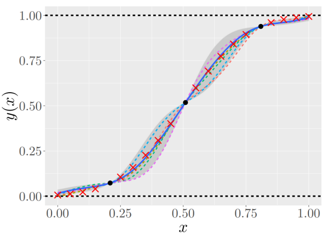
Neuroscience: magnetic resonance imaging (MRI)

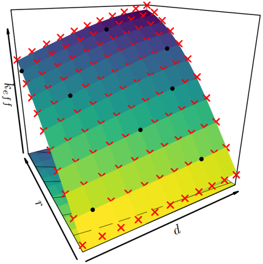


- **H. Vargas, A. López-Lopera, M. A. lvarez, A. Orozco, J. Hernández and N. Malpica:**
Gaussian processes for slice-based super-resolution MR images
Lecture Notes in Computer Science (LNCC), 2015

ONERA
THE FRENCH AEROSPACE LAB

Risk assessment: nuclear safety

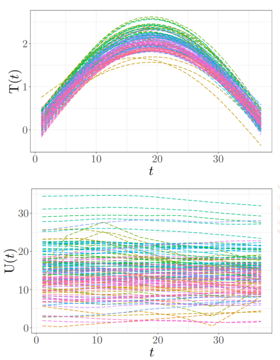


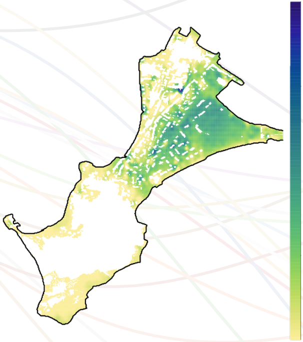


- **A. F. López-Lopera, N. Durrande, F. Bachoc and O. Roustant:**
Finite-dimensional Gaussian approximation with linear inequality constraints
SIAM/ASA Journal on Uncertainty Quantification, 2018

ONERA
THE FRENCH AEROSPACE LAB

Risk assessment: coastal flooding



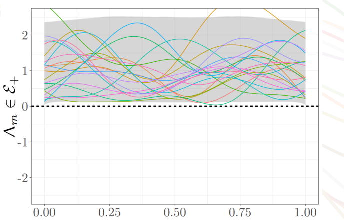


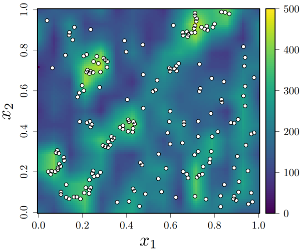
- **A. F. López-Lopera, D. Idier, J. Rohmer and F. Bachoc:**
Multi-output Gaussian processes with functional data: A study on coastal flood hazard assessment
Submitted, 2020

ONERA
THE FRENCH AEROSPACE LAB

Applications of Gaussian processes

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

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
    - stationarity, isotropy, periodicity, smoothness...