INSA – Gaussian processes

Introduction

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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

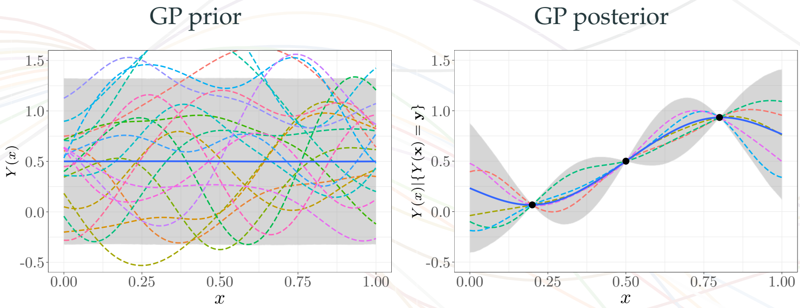
2019-2020 — **Postdoctoral Research**, *Institut de Mathématiques de Toulouse*
· Joint supervision: *The French Geological Survey BRGM*
· Multi-output GPs & coastal flooding

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

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



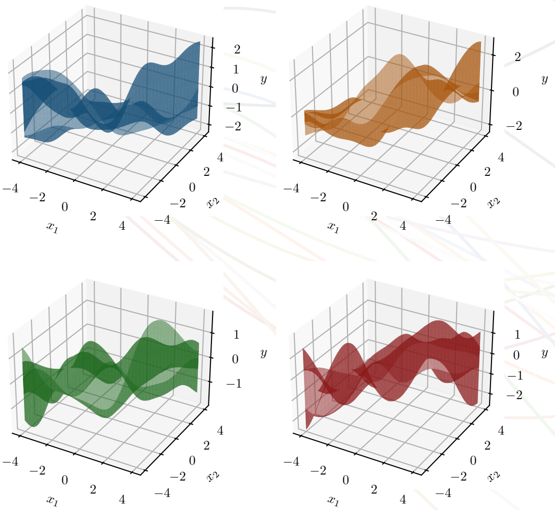
$Y \sim \mathcal{GP}(m, k_{\boldsymbol{\theta}})$

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

■ mean function ■ prediction intervals ■ ■ $\cdots$ ■ samples

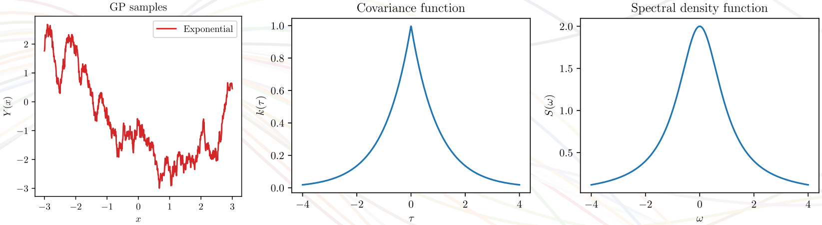
● Interpolation conditions: $(\boldsymbol{x}, \boldsymbol{y}) = (x_i, y_i)_{i=1}^{n}$

Gaussian processes (GPs) as flexible priors over functions



Gaussian random fields

Kernel functions



- Every kernel k is the **covariance function** of some centred Gaussian **stochastic process** Y: e.g. *Ornstein-Uhlenbeck process*
- Every **spectral density** $S(\omega)$ defines a (stationary) kernel
- If k is a kernel, there exists a unique **RKHS** with k as its reproducing kernel. If k is a reproducing kernel, then it is a covariance function

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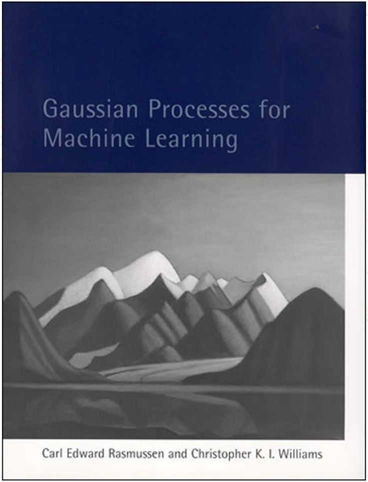
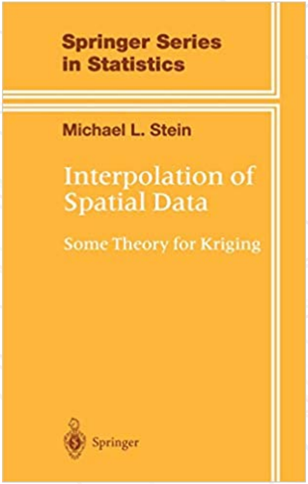
Outline

- In these lectures:
  1. A recap of Gaussian processes with applications
  2. Spectral representation and Bochner's theorem
  3. Regularity conditions (e.g. continuity, differentiability)
  4. An introduction to reproducing kernel Hilbert-spaces (RKHS)
- 2 practical sessions ($\sim$3.5h): Python (Jupyter) or R (Jupyter + IRkernel)
- Material can be found at: `https://anfelopera.github.io/teaching/`

Main references





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

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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

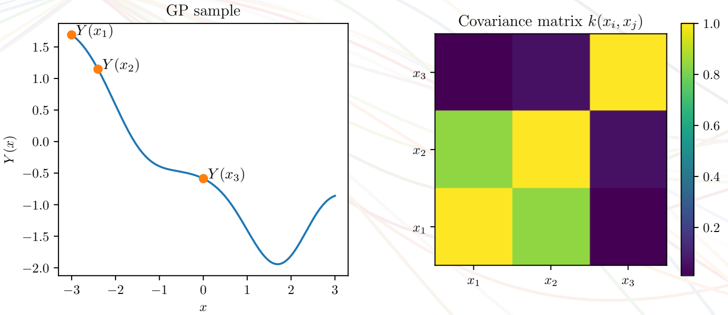
$$\begin{aligned} &\text{(trend)} && m(\boldsymbol{x}) = \mathbb{E}\left\{Y(\boldsymbol{x})\right\}, \\ &\text{(correlation)} && k(\boldsymbol{x}, \boldsymbol{x}') = \operatorname{cov}\left\{Y(\boldsymbol{x}), Y(\boldsymbol{x}')\right\}, \quad \text{for} \quad \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^d.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

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

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

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 $k(\boldsymbol{x}, \boldsymbol{x}') = 0$

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- 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 $Y \sim \mathcal{GP}(0, k)$:

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

Gaussian process regression

- Let $\{Y(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d\}$ be a centred GP with covariance function k
- Consider a set of observations $(\boldsymbol{x}_i, y_i)_{1 \leq i \leq n}$ for $n \in \mathbb{N}$
- In regression tasks, we aim at computing the distribution of the conditional process:

$$Y | \{Y(\boldsymbol{x}_1) = y_1, \dots, Y(\boldsymbol{x}_n) = y_n\}$$

- This conditional process is also GP-distributed with conditional mean and covariance functions given by

$$\mu(\boldsymbol{x}) = \boldsymbol{k}^\top(\boldsymbol{x}) \, \mathbf{K}_n^{-1} \, \boldsymbol{y},$$
$$c(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}') - \boldsymbol{k}^\top(\boldsymbol{x}) \, \mathbf{K}_n^{-1} \, \boldsymbol{k}(\boldsymbol{x}'),$$

with $\boldsymbol{k}(\boldsymbol{x}) = (\mathrm{cov}\,\{Y(\boldsymbol{x}), Y(\boldsymbol{x}_i)\})_{1 \leq i \leq n}$ and $\mathbf{K}_n = (\mathrm{cov}\,\{Y(\boldsymbol{x}_i), Y(\boldsymbol{x}_j)\})_{1 \leq i,j \leq n}$

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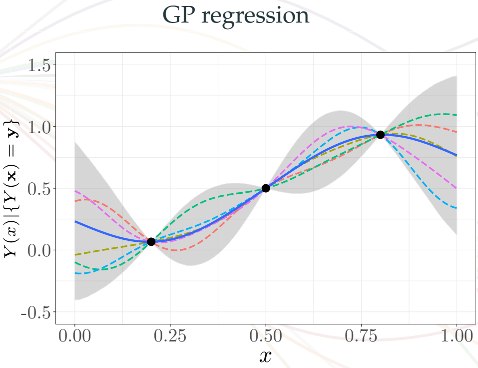
Gaussian process regression



■ conditional mean ■ confidence intervals ■ ■ $\cdots$ ■ GP realisations

● training data: $(\boldsymbol{x}, \boldsymbol{y}) = (x_i, y_i)_{i=1}^{n}$

[Link]

Gaussian process regression with noisy observation

· For noisy observations, we have the conditional process:

$$Y | \{Y(\boldsymbol{x}_1) + \varepsilon_1 = y_1, \dots, Y(\boldsymbol{x}_n) + \varepsilon_n = y_n\},$$

with additive noises $\varepsilon_i \sim \mathcal{N}(0, \tau^2)$, for $i = 1, \dots, n$, and noise variance τ^2

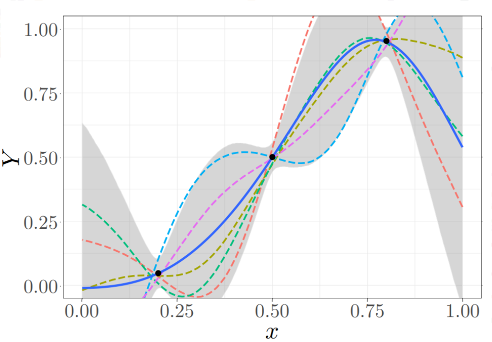
· This conditional process is also GP-distributed with conditional mean and covariance functions given by

$$\widetilde{\mu}(\boldsymbol{x}) = \boldsymbol{k}^\top(\boldsymbol{x}) \left[\mathbf{K}_n + \tau^2 \mathbf{I}\right]^{-1} \boldsymbol{y},$$
$$\widetilde{c}(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}') - \left[\mathbf{K}_n + \tau^2 \mathbf{I}\right]^{-1} \boldsymbol{k}(\boldsymbol{x}'),$$

with $\boldsymbol{k}(\boldsymbol{x}) = (\mathrm{cov}\,\{Y(\boldsymbol{x}), Y(\boldsymbol{x}_i)\})_{1 \leq i \leq n}$ and $\mathbf{K}_n = \left(\mathrm{cov}\left\{Y(\boldsymbol{x}_i), Y(\boldsymbol{x}_j)\right\}\right)_{1 \leq i,j \leq n}$

Gaussian process regression with noisy observation

GP regression



■ conditional mean ■ confidence intervals ■ ■ $\cdots$ ■ GP realisations

● training data: $(\boldsymbol{x}, \boldsymbol{y}) = (x_i, y_i)_{i=1}^n$

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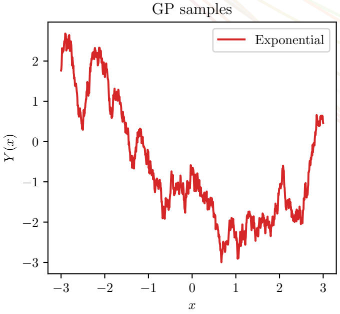
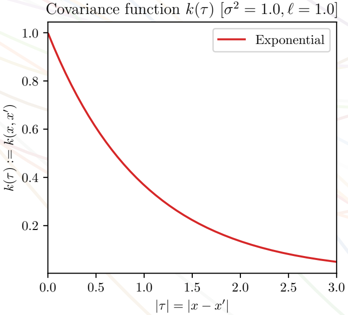
Kernel functions

Kernel functions

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

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





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.

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)

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

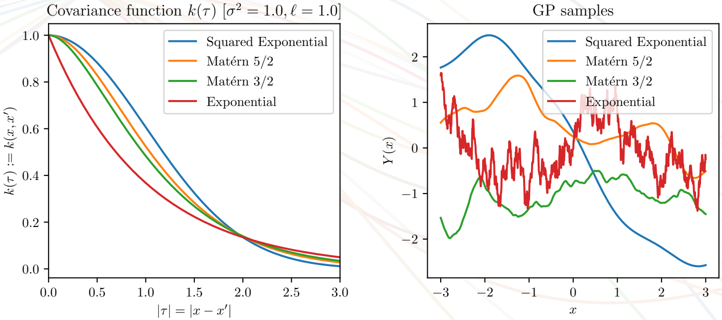
Matérn 5/2: $k_{\sigma^2,\ell}(\tau) = \sigma^2 \left(1 + \sqrt{5}\frac{|\tau|}{\ell} + \frac{5}{3}\frac{\tau^2}{\ell^2}\right) \exp\left\{-\sqrt{5}\frac{|\tau|}{\ell}\right\}$,

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.

Examples of 1D kernels



Examples of 1D kernels

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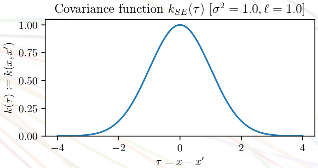
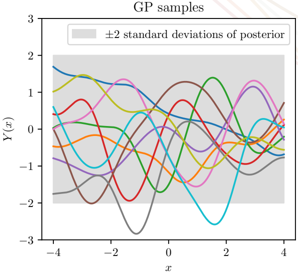
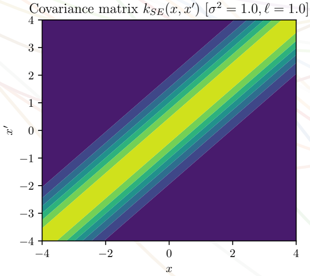


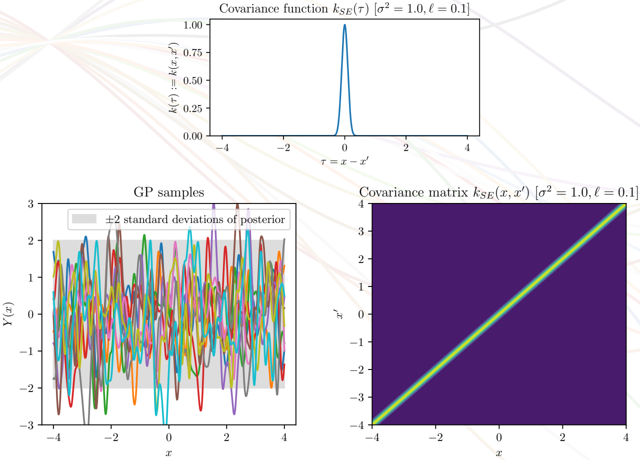




Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

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



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

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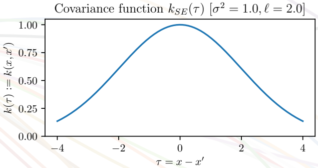
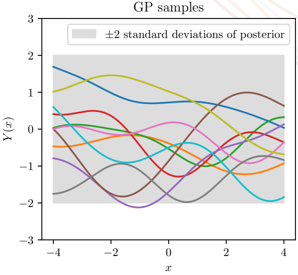
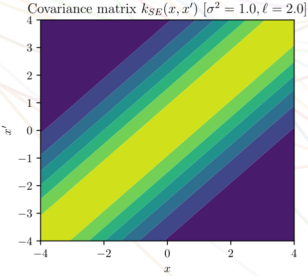
Examples of 1D kernels

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



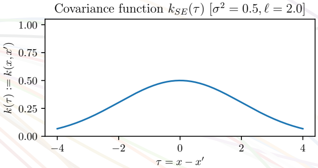


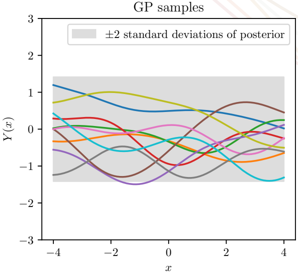


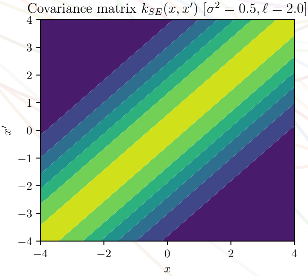
Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

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



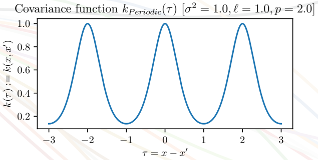


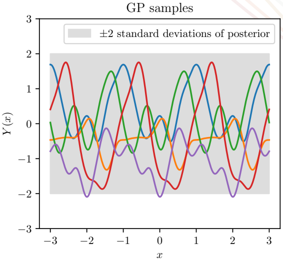


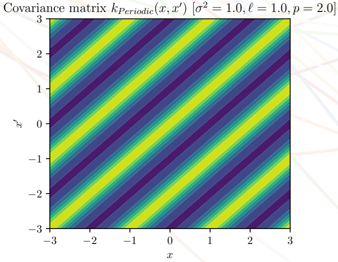
Effect of the variance σ^2 and the length-scale ℓ on GP samples

Examples of 1D kernels

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

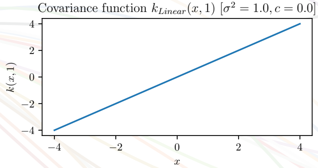


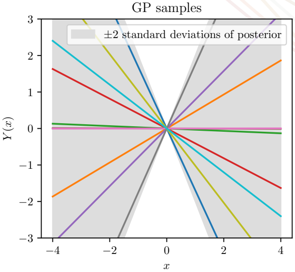


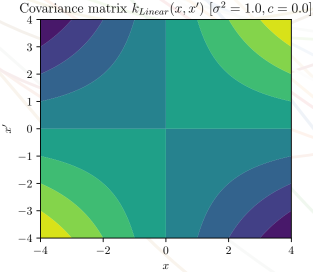


Examples of 1D kernels

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







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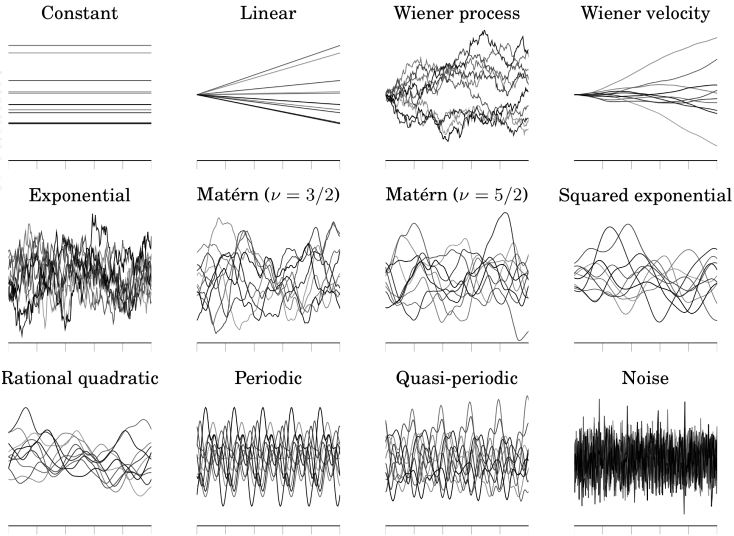
Examples of 1D kernels



Examples of GP samples [Solin, 2020]

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Building new kernels from other ones

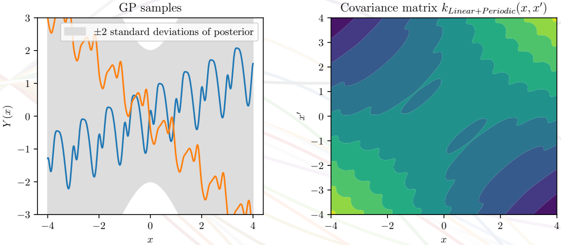
· We can also create new kernels by combining predefined ones, e.g.:

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

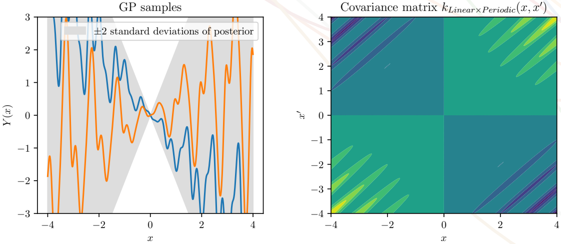
Exercise. Show that all the previous operations preserve the p.s.d.

Building new kernels from other ones

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



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



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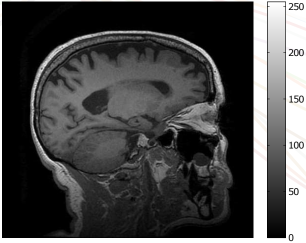
A visual exploration of GPs

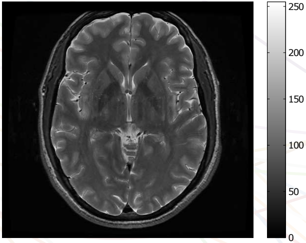
- **Durrande [2017]**: Gaussian process playground **[Link]**
- **Görtler et al. [2019]**: A visual exploration of Gaussian processes **[Link]**
- **Damianou [2016]:** A Python notebook on Gaussian processes **[Link]**

Applications of Gaussian processes

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

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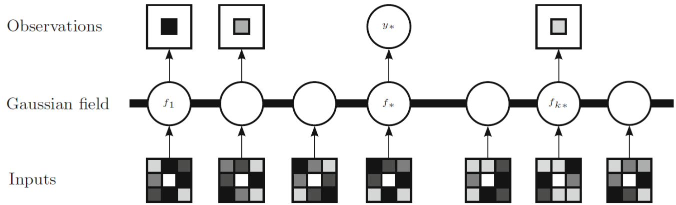
Applications of Gaussian processes

Neuroscience: magnetic resonance imaging (MRI)



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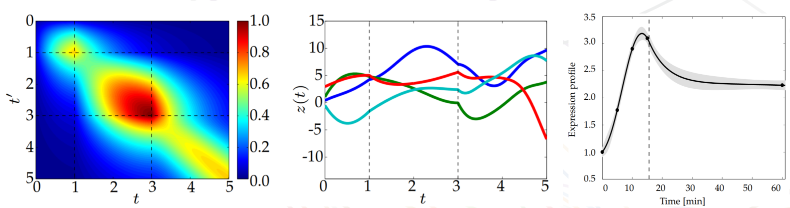
Applications of Gaussian processes

Biology: prediction of protein concentrations



We considered a system of coupled differential equations:

$$\frac{dy_d(t)}{dt} + \gamma_d y_d(t) = B_d + \sum_{r=1}^{R} S_{r,d} u_r(t),$$

with $u_1, \ldots, u_R$ being independent GPs

- **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

· Consider the first-order differential equation given by

$$\frac{dY(t)}{dt} + \gamma Y(t) = SU(t), \tag{5}$$

with $\gamma \in \mathbb{R}^+, S \in \mathbb{R}^+$

· By assuming the initial condition $Y(0) = 0$, we obtain

$$Y(t) = Sc(t) \int_0^t U(\tau) \exp(\gamma\tau) d\tau, \quad \text{avec} \quad c(t) = \exp(-\gamma t)$$

· If $U \sim \mathcal{GP}(0, k_{u,u})$, we can show that Y is also GP-distributed with covariance function given by:

$$\begin{aligned} k_{y,y}(t,t') &:= \operatorname{cov}\left\{Y(t), Y(t')\right\} \left(= \mathbb{E}\left\{Y(t)Y(t')\right\}\right) \\ &= S^2 c(t) c(t') \int_0^t \exp(\gamma\tau) \int_0^{t'} \exp(\gamma\tau') \underbrace{k_{u,u}(\tau,\tau')}_{\mathbb{E}\{U(\tau),U(\tau')\}} d\tau' d\tau \end{aligned}$$

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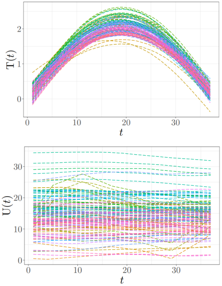
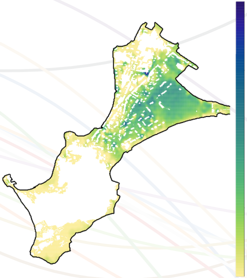
Risk assessment: coastal flooding





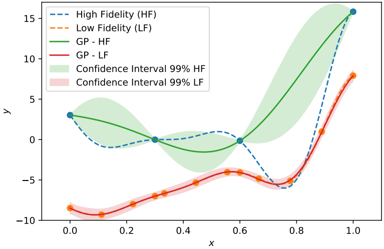
We considered a separable kernel given by

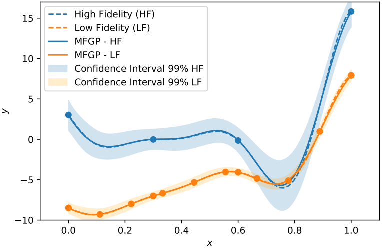
$$k((\boldsymbol{\mathcal{F}}, \boldsymbol{x}), (\boldsymbol{\mathcal{F}}', \boldsymbol{x}')) = k_f(\boldsymbol{\mathcal{F}}, \boldsymbol{\mathcal{F}}')k_x(\boldsymbol{x}, \boldsymbol{x}'),$$

with $k_f : \mathcal{F}(\mathcal{T}, \mathbb{R})^Q \times \mathcal{F}(\mathcal{T}, \mathbb{R})^Q \to \mathbb{R}$ (kernel for the functional inputs) and $k_x : \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}$ (spatial kernel)

- **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

Aerodynamics: multi-fidelity Gaussian processes





· We considered the autoregressive model:

$$Y_1(x) = \rho Y_0(x) + \delta(x),$$

with Y_0 and δ independent (centred) GPs and $\rho \in \mathbb{R}$.

Exercise. Considering $Y_0 \sim \mathcal{GP}(0, k_{y_0,y_0})$ and $\delta \sim \mathcal{GP}(0, k_{\delta,\delta})$, compute the covariance function of Y_1.

- **A. F. López-Lopera, N. Bartoli, T. Lefèbvre and S. Mouton:**
Data fusion with multifidelity Gaussian processes for aerodynamic experimental and numerical databases. Work in progress

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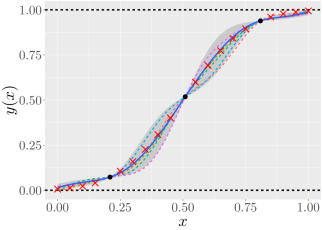
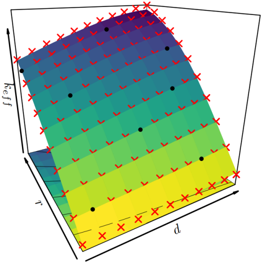
Risk assessment: nuclear safety



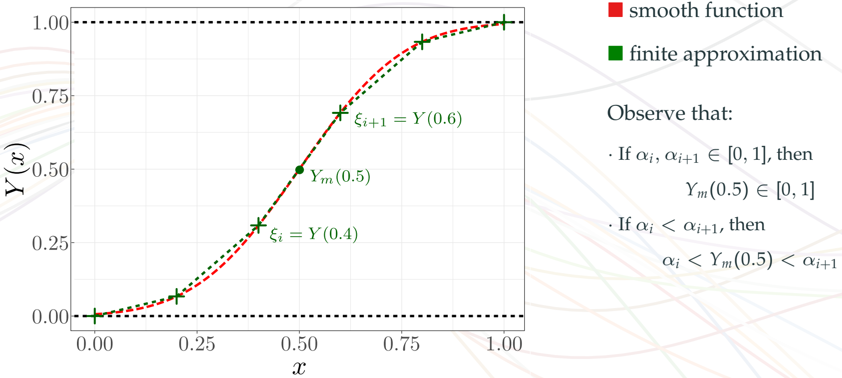


We considered the piecewise-linear approximation given by

$$Y_m(x) = \sum_{j=1}^{m} \phi_j(x) Y(t_j), \text{ s.t. } \begin{cases} Y_m(x_i) = y_i, \text{ for } i = 1, \dots, n & \text{(interpolation constraints)} \\ Y_m \in \mathcal{E} & \text{(inequality constraints)} \end{cases}$$

with $[Y(t_1), \dots, Y(t_m)] \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma})$, and $\phi_i, \dots, \phi_m$ hat basis functions

- **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



Observe that:

- If $\alpha_i, \alpha_{i+1} \in [0, 1]$, then
$$Y_m(0.5) \in [0, 1]$$
- If $\alpha_i < \alpha_{i+1}$, then
$$\alpha_i < Y_m(0.5) < \alpha_{i+1}$$

Advantage : It is enough imposing the inequality constraints over the knots

- Assuming that $\boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma})$, such that $\boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}$, then we have

$$\boldsymbol{\xi} \sim \mathcal{TN}(\mathbf{0}, \boldsymbol{\Lambda}\boldsymbol{\Gamma}\boldsymbol{\Lambda}^\top, \boldsymbol{l}, \boldsymbol{u})$$

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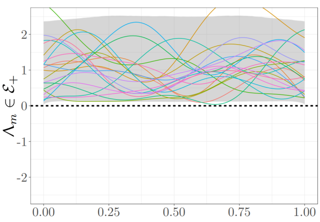
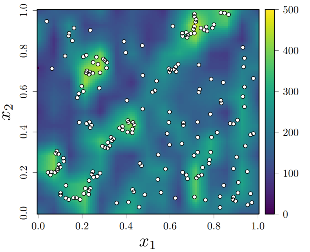
Applications of Gaussian processes

Geostatistics: spatial distribution of tree species





We considered a Poisson process with stochastic intensity function $\Lambda \sim \mathcal{GP}(0, k)$ subject to Λ being positive

- **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...