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)

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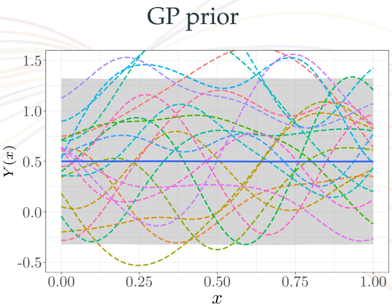
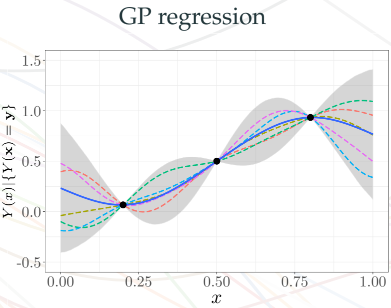
Gaussian processes (GPs) as flexible priors over functions



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

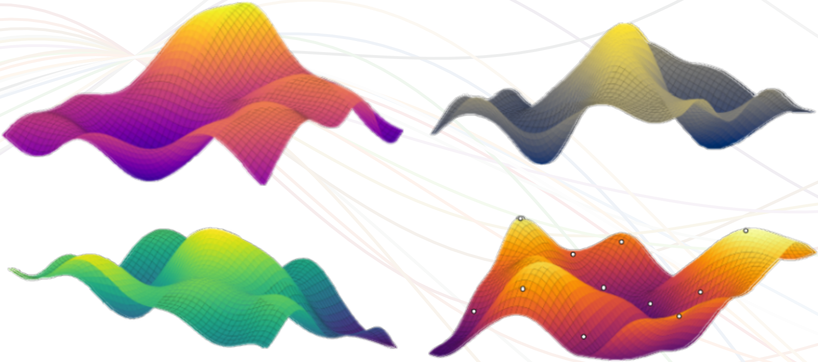


$Y|\{Y(\boldsymbol{x}) = \boldsymbol{y}\} \sim \mathcal{GP}(m_{\text{cond}}, c_{\boldsymbol{\theta}})$

■ 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

Outline

- In this course:

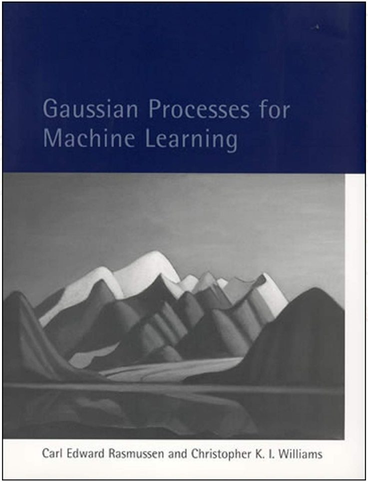
  1. A recap of Gaussian processes

  2. Spectral representation and Bochner's theorem

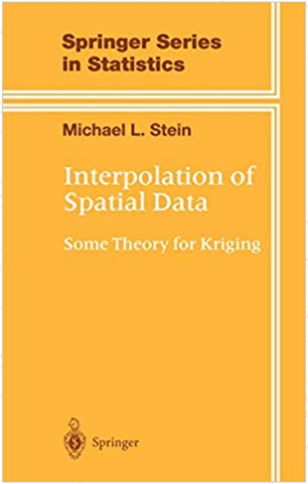
  3. Regularity conditions (e.g. continuity, differentiability)

  4. An introduction to reproducing kernel Hilbert-spaces (RKHS)

Main references



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



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

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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

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

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

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

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

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

· 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 $Y \sim \mathcal{GP}(0, k)$:

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

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

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

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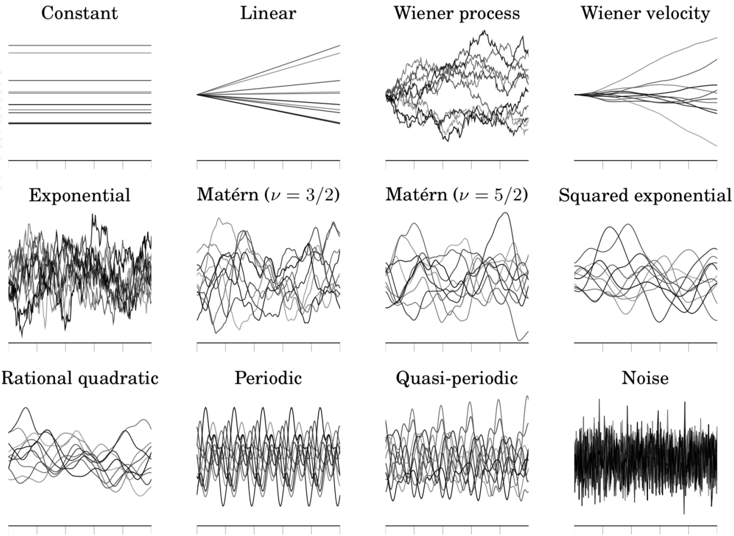
Examples of 1D kernels



Examples of GP samples [Solin, 2020]

Examples of 1D stationary kernels

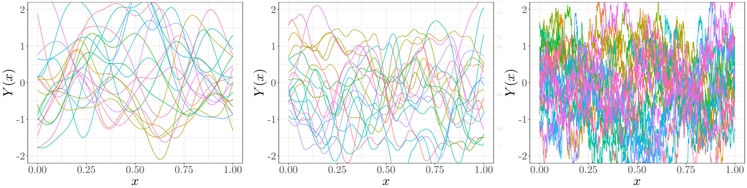
- Denote $k(\tau) := k(x, x+\tau)$ (abuse of notation)
- Some classic 1D stationary kernels are [Genton, 2001]:

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

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

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

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



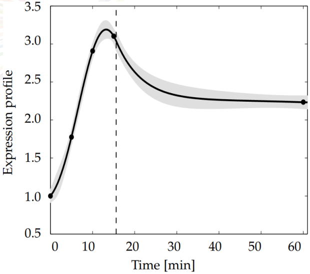
(a) Squared Exponential (b) Matérn 5/2 (c) Exponential

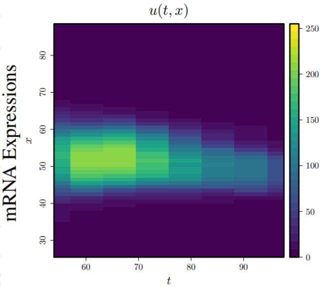
■ ■ · · · ■ samples

[A visual exploration of GPs]

Applications of Gaussian processes

Biology: prediction of protein concentrations





- **A. F. López-Lopera, N. Durrande and M. A. Alvarez:**
Physically-inspired Gaussian process models for post-transcriptional regulation in Drosophila
IEEE/ACM Transaction on Computational Biology and Bioinformatics, 2019

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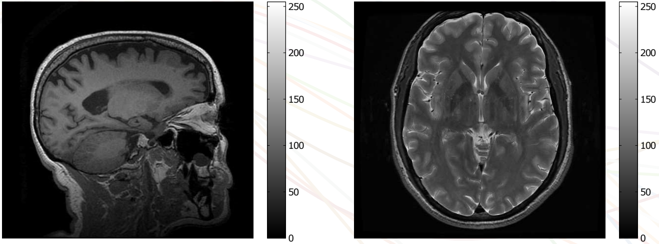
Switched latent force models for reverse-engineering transcriptional regulation in genes
IEEE/ACM Transaction on Computational Biology and Bioinformatics, 2017

Applications of Gaussian processes

Neuroscience: magnetic resonance imaging (MRI)



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Gaussian processes for slice-based super-resolution MR images
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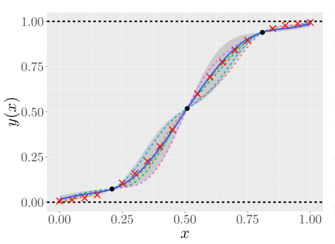
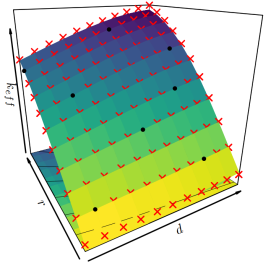
Risk assessment: nuclear safety





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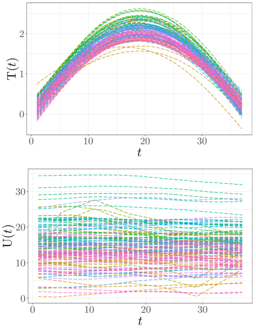
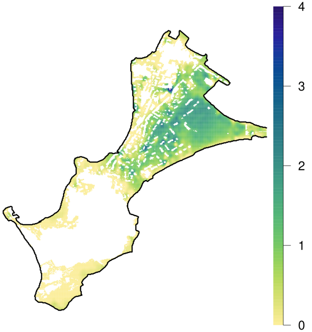
Finite-dimensional Gaussian approximation with linear inequality constraints
SIAM/ASA Journal on Uncertainty Quantification, 2018

Risk assessment: coastal flooding





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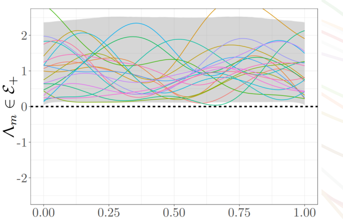
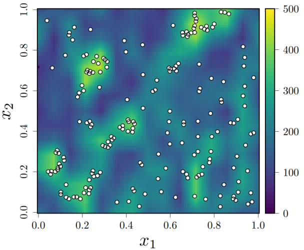
Multi-output Gaussian processes with functional data: A study on coastal flood hazard assessment
Submitted, 2020

Geostatistics: spatial distribution of tree species





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Gaussian process modulated Cox processes under linear inequality constraints
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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, ...