Gaussian Process Modelling under Inequality Constraints

Andrés F. López-Lopera

PhD Defense on Applied Mathematics
Mines Saint-Étienne, France

Supervisor:	Olivier Roustant	Mines Saint-Étienne (France)
Co-supervisors:	François Bachoc	Univ. Paul Sabatier (France)
	Nicolas Durrande	PROWLER.io (UK)
Jury:	Sonja Kuhnt	FH Dortmund (Germany)
	Anthony Nouy	École Centrale de Nantes (France)
	Clémentine Prieur	Univ. Grenoble Alpes (France)
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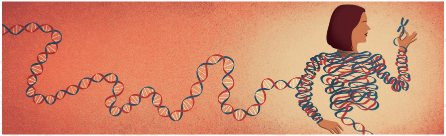
Some real-world applications satisfying inequality constraints

Regulation of gene expressions – positivity constraints (Lawrence et al., 2007).



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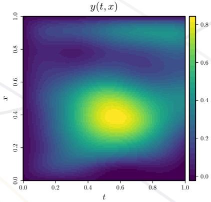
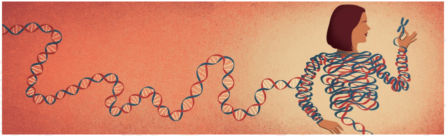


Regulation of gene expressions – positivity constraints (Lawrence et al., 2007).



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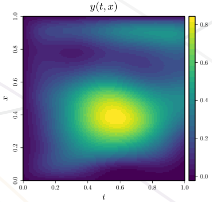
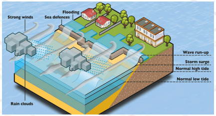


Other applications

- Coastal flooding – positivity & monotonicity (Rohmer and Idier, 2012).
- Econometrics – positivity or monotonicity (Cousin et al., 2016).
- Nuclear physics – monotonicity & convexity (Zhou et al., 2019).

⋮



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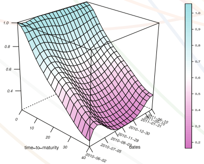
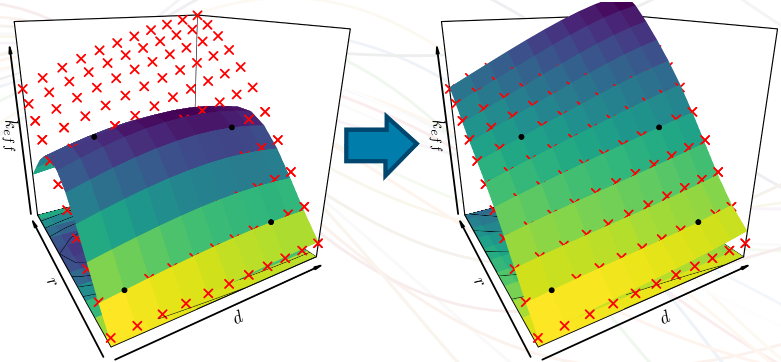


Cousin et al. (2016)

2D models for interpolating the IRSN's dataset (López-Lopera et al., 2018).

k_{eff}: effective neutron multiplication factor

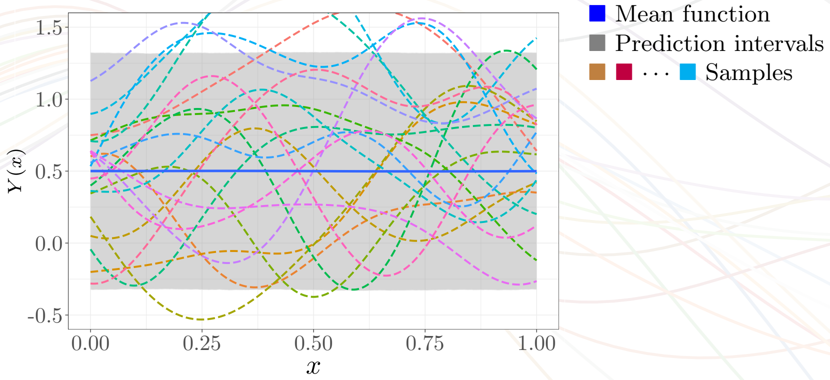


(a) unconstrained model (b) model with positivity & monotonicity

• interpolation points ($n = 4$) × test data

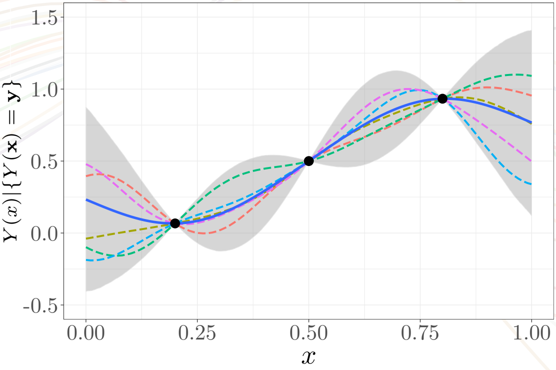
Gaussian process (GP) regression models: motivation

GPs form a flexible **prior over functions** (Rasmussen and Williams, 2005):



$$Y \sim \mathcal{GP}\left(\underbrace{\mu(x)}_{\text{mean}} = 0.5,\ \underbrace{k_\theta(x, x')}_{\text{covariance}} = \sigma^2 \exp\left\{-\frac{(x-x')^2}{2\ell^2}\right\}\right)$$

GPs form a flexible **prior over functions** (Rasmussen and Williams, 2005):



Mean function

Prediction intervals

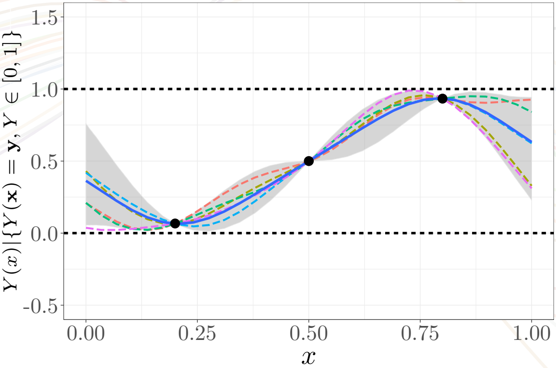
$\cdots$ Samples

- Interpolation conditions

$$\mathcal{D} = (x_i, y_i)_{i=1}^{n} = (\boldsymbol{x}, \mathbf{y})$$

$$Y|\{Y(\mathbf{x}) = \mathbf{y}\} \sim \mathcal{GP}(\underbrace{m(x)}_{\text{cond. mean}}, \underbrace{c_\theta(x, x')}_{\text{cond. covariance}})$$

GPs form a flexible **prior over functions** (Rasmussen and Williams, 2005):



- Mean function
- Prediction intervals
- ... Samples

- Interpolation conditions

$$\mathcal{D} = (x_i, y_i)_{i=1}^{n} = (\boldsymbol{x}, \mathbf{y})$$

- - Boundedness condition

$$Y \in [0,1]$$

$$Y|\{Y(\mathbf{x}) = \mathbf{y}, Y \in [0,1]\} \sim \textbf{?}$$

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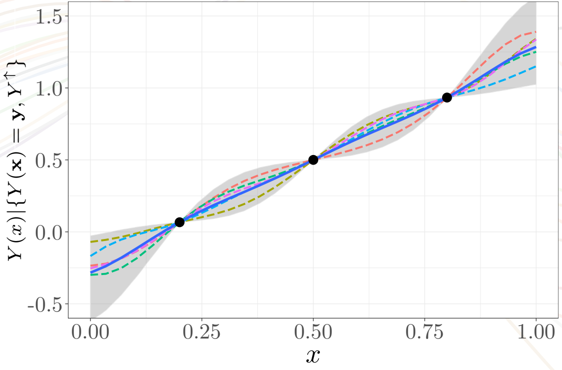

- Mean function
- Prediction intervals
- $\cdots$ Samples
- $\bullet$ Interpolation conditions

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$\uparrow$ Monotonicity condition

$$Y(x) \leq Y(x'), \quad \forall\, x \leq x'.$$

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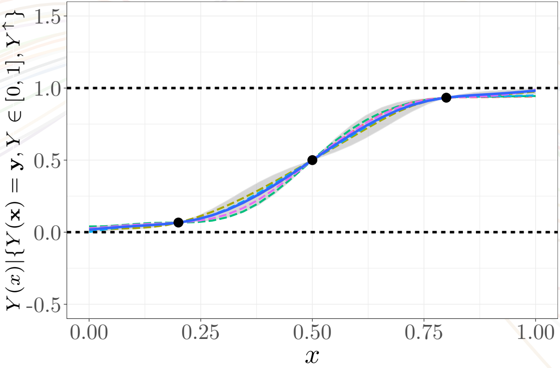

Mean function

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$\cdots$ Samples

• Interpolation conditions

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↑ Monotonicity condition

$$Y(x) \leq Y(x'), \quad \forall\, x \leq x'.$$

$$Y | \{Y(\mathbf{x}) = \mathbf{y}, Y \in [0,1], Y^{\uparrow}\} \sim \textbf{?}$$

The contributions in this thesis are threefold:

1. The improvement of the **applicability of GPs under constraints**.
   - Previous implementations: expensive and applicable up to 2D.
2. The **scalability** of constrained GPs **to high dimensions**:
   - i.e. involving hundreds of input variables.
3. **Parameter estimation under inequality constraints**.
   - Previously estimated by costly-to-evaluate cross-validation methods.

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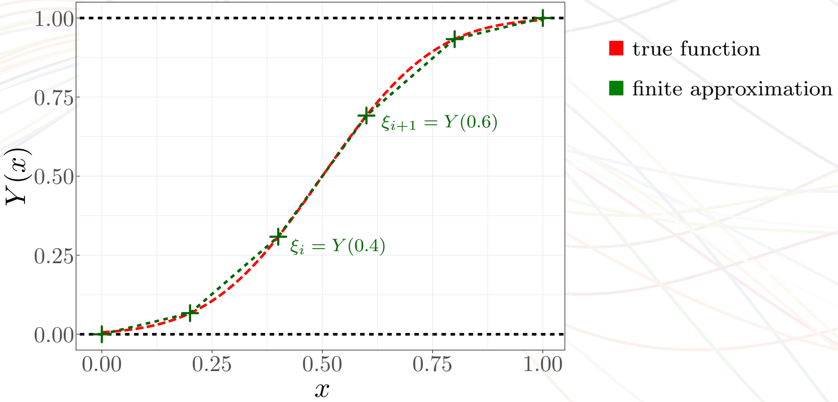
1D finite-dimensional Gaussian approximation

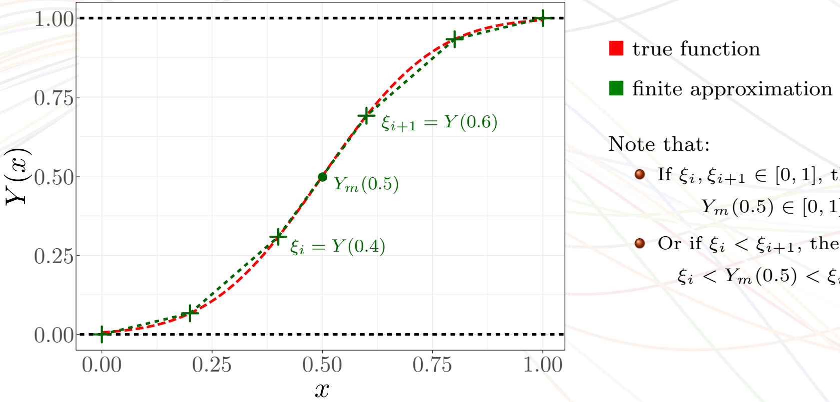
Finite-dimensional representation Y_m: also bounded & monotonic.



Imposing constraints on the knots is enough (Maatouk and Bay, 2017).

1D finite-dimensional Gaussian approximation

Finite-dimensional representation Y_m: also bounded & monotonic.



Note that:

- If $\xi_i, \xi_{i+1} \in [0, 1]$, then $Y_m(0.5) \in [0, 1]$.
- Or if $\xi_i < \xi_{i+1}$, then $\xi_i < Y_m(0.5) < \xi_{i+1}$.

Imposing constraints on the knots is enough (Maatouk and Bay, 2017).

Using the constrained GP framework in (Maatouk and Bay, 2017), allows...

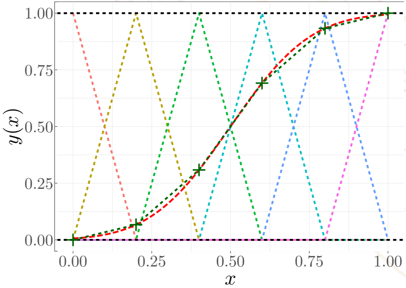
1. To impose either **boundedness**, **monotonicity** or **convexity**.
   - Other GP models deal with only one of those conditions (e.g. log GPs, Vanhatalo and Vehtari, 2007).
2. To ensure the **inequalities everywhere in the input space**.
   - Other frameworks satisfy constraints only over a finite number of evaluations (e.g. Riihimäki and Vehtari, 2010).
3. To approximate the constrained process by **sampling methods**.
   - Other approaches can lead to expensive or intractable computations.

- Let the (constrained) finite-dimensional GP Y_m be defined as

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x), \text{ s.t. } \begin{cases} Y_m(x_i) = y_i & \text{(interpolation conditions)}, \\ \boldsymbol{l} \leq \boldsymbol{\Lambda\xi} \leq \boldsymbol{u} & \text{(linear inequality conditions)}, \end{cases} \tag{1}$$

where $x_i \in [0, 1]$, $y_i \in \mathbb{R}$ for $i = 1, \dots, n$; and

- $\boldsymbol{\xi} = [\xi_1, \dots, \xi_m]^\top \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma}_\theta)$ with covariance matrix $\boldsymbol{\Gamma}_\theta$,
- $(\boldsymbol{\Lambda}, \boldsymbol{l}, \boldsymbol{u})$ defines the inequality conditions, and
- $\phi_j : [0, 1] \mapsto \mathbb{R}$ are hat basis functions:



- Since the **Gaussianity** is preserved for *linear operations*:

$$\boldsymbol{\Lambda}\boldsymbol{\xi} | \{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}\} \sim \mathcal{N}\left(\boldsymbol{\Lambda}\boldsymbol{\mu}, \boldsymbol{\Lambda}\boldsymbol{\Sigma}\boldsymbol{\Lambda}^\top\right), \quad \text{(conditional distribution)} \tag{2}$$

with conditional parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ given by

$$\mathbf{K} = \boldsymbol{\Phi}\boldsymbol{\Gamma}\boldsymbol{\Phi}^\top, \quad \boldsymbol{\mu} = \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top\mathbf{K}^{-1}\mathbf{y}, \quad \boldsymbol{\Sigma} = \boldsymbol{\Gamma} - \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top\mathbf{K}^{-1}\boldsymbol{\Phi}\boldsymbol{\Gamma}.$$

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- Then, *quantifying uncertainty* on $Y_m(x) = \sum_{j=1}^m \xi_j \phi_j(x)$ relies on simulating the **truncated Gaussian vector** $\boldsymbol{\xi}$:

$$\boldsymbol{\Lambda}\boldsymbol{\xi}|\{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\} \sim \mathcal{TN}(\boldsymbol{\Lambda}\boldsymbol{\mu}, \boldsymbol{\Lambda}\boldsymbol{\Sigma}\boldsymbol{\Lambda}^\top, \boldsymbol{l}, \boldsymbol{u}). \qquad (3)$$

(3) is computed via *Monte Carlo* (MC) or *Markov Chain MC* (MCMC):

- **e.g. *Hamiltonian MC* (HMC) (Pakman and Paninski, 2014).**

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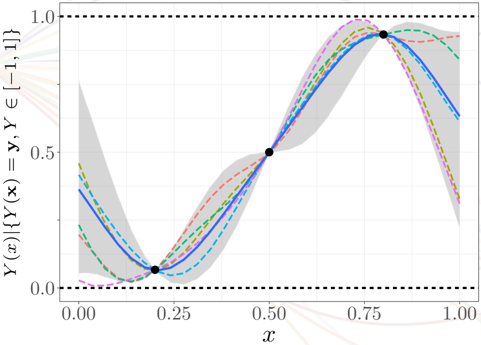
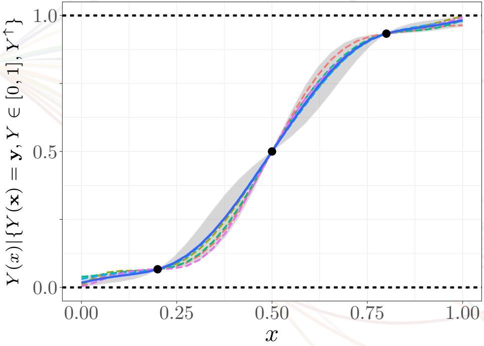
1D example with **boundedness** constraints via HMC



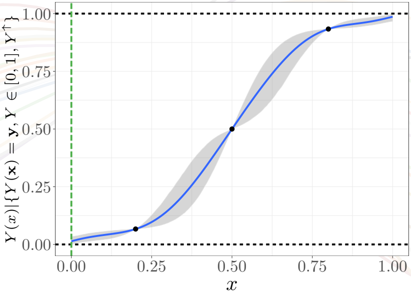
$$\underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}}_{\boldsymbol{\Lambda}} \underbrace{\begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \vdots \\ \xi_{m-1} \\ \xi_m \end{bmatrix}}_{\boldsymbol{\xi}} \leq \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}}_{\boldsymbol{u}}$$

1D example with **boundedness** & **monotonicity** constraints via HMC

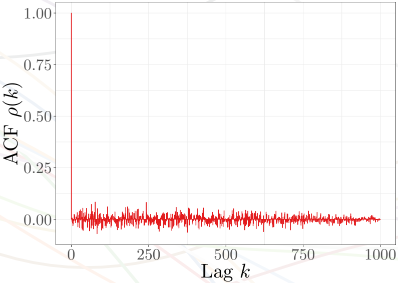


$$
\underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}}_{\boldsymbol{\Lambda}} \underbrace{\begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \vdots \\ \xi_{m-1} \\ \xi_m \end{bmatrix}}_{\boldsymbol{\xi}} \leq \underbrace{\begin{bmatrix} 1 \\ \infty \\ \infty \\ \vdots \\ \infty \\ 1 \end{bmatrix}}_{\boldsymbol{u}}
$$

boundedness & **monotonicity** constraints



$m = 100,\ N = 10^3$



MC/MCMC Sampler	CPU Time [s]
(Maatouk and Bay, 2016)	-
(Botev, 2017)	73.7
Gibbs – (Taylor and Benjamini, 2016)	29.0
HMC – (Pakman and Paninski, 2014)	**12.6**

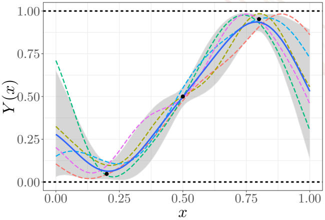
Considering noisy observations

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x), \text{ s.t. } \begin{cases} Y_m(x_i) + \varepsilon_i = y_i & \text{(interpolation conditions)}, \\ \boldsymbol{l} \leq \boldsymbol{\Lambda\xi} \leq \boldsymbol{u} & \text{(linear inequality conditions)}, \end{cases} \quad (4)$$

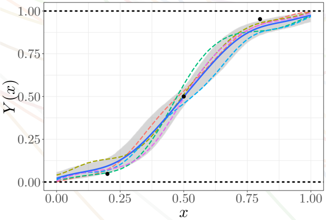
where $\varepsilon_i \sim \mathcal{N}\left(0, \tau^2\right)$ with noise variance τ^2.

Modification: $\mathbf{K} = \mathbf{\Phi\Gamma\Phi}^\top \quad \rightarrow \quad \mathbf{K} = \mathbf{\Phi\Gamma\Phi}^\top + \tau^2\mathbf{I}$.

boundedness

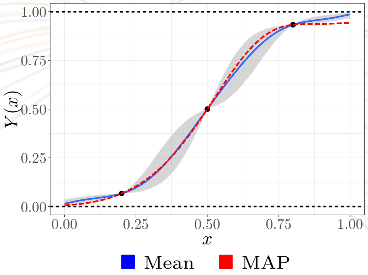


boundedness & **monotonicity**



Adding $\boldsymbol{\varepsilon}$ leads to more flexible GP models and less restrictive sample spaces for MC/MCMC algorithms (López-Lopera et al., 2019).

Maximum a posteriori (MAP) estimate



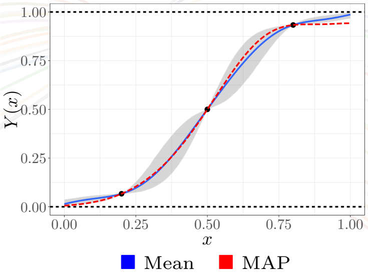
- Let $\boldsymbol{\mu}^*$ be the mode that maximises the pdf of $\boldsymbol{\xi}|\{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\}$:

$$\boldsymbol{\mu}^* = \underset{\boldsymbol{\xi} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}}{\arg\max} \{-[\boldsymbol{\xi}-\boldsymbol{\mu}]^\top \boldsymbol{\Sigma}^{-1}[\boldsymbol{\xi}-\boldsymbol{\mu}]\}. \tag{5}$$

- The *MAP estimate* of Y_m is given by

$$Y_m^{\mathrm{MAP}}(x) = \sum_{j=1}^{m} \mu_j^* \phi_j(x), \tag{6}$$

Maximum a posteriori (MAP) estimate



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- The *MAP estimate* of Y_m is given by

$$Y_m^{\text{MAP}}(x) = \sum_{j=1}^{m} \mu_j^* \phi_j(x), \tag{6}$$

Benefits:

- **Easy** and **fast calculations**.
- **Convergence to the spline solution** as $m \to \infty$ (Bay et al., 2016).
- **Starting point for MCMC** aiming for *fast convergence*.

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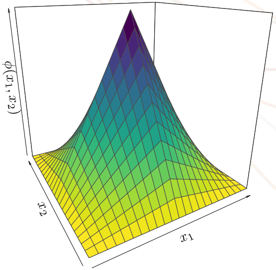
Finite-dimensional approximation in d dimensions

- The extension to d dimensions is obtained by **tensorisation**:

$$Y_m(\boldsymbol{x}) = \sum_{j_1,\ldots,j_d=1}^{m_1,\ldots,m_d} \left[\prod_{p=1,\ldots,d} \phi_{j_p}^{(p)}(x_p) \right] \xi_{j_1,\cdots,j_d}, \text{ s.t. } \begin{cases} Y_m(\boldsymbol{x}_i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi} \in \mathcal{C}, \end{cases} \tag{7}$$

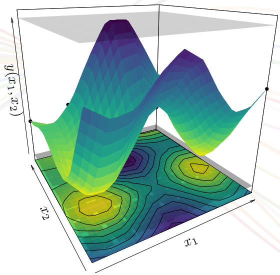
where $\boldsymbol{x}_i \in [0,1]^d$, $y_i \in \mathbb{R}$, $\varepsilon_i \sim \mathcal{N}(0, \tau^2)$, for $i = 1, \ldots, n$; and

- $\boldsymbol{\xi} = [\xi_{1,\ldots,1}, \ldots, \xi_{m_1,\ldots,m_d}]^\top \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}_\theta)$,
- $\mathcal{C}$ is a convex set of linear inequality constraints, and
- $\phi_{j_i}^{(i)} : [0,1] \mapsto \mathbb{R}$ are hat basis functions.

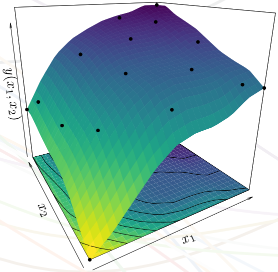


2D numerical illustration

boundedness in 2D



monotonicity in 2D.



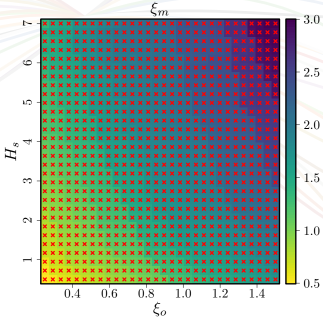
● interpolation points ■ predictive mean ■ bounds

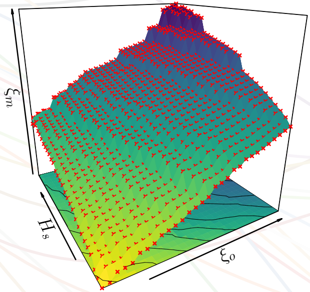
MC/MCMC Method	2D boundedness example CPU Time $[s]$	2D monotonicity example CPU Time $[s]$
(Maatouk and Bay, 2016)	-	-
(Botev, 2017)	0.9	1488.3
(Taylor and Benjamini, 2016)	9.7	-
(Pakman and Paninski, 2014)	**0.6**	**8.6**

$$m_1 = m_2 = 10, N = 10^3$$

2D coastal flooding application

ξ_m: maximum water level, ξ_0: offshore water level, H_s: wave height.

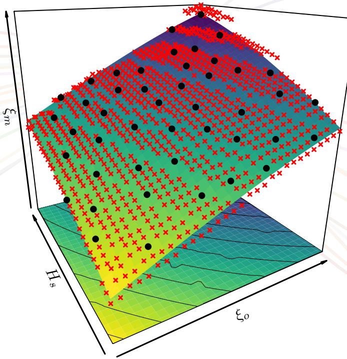




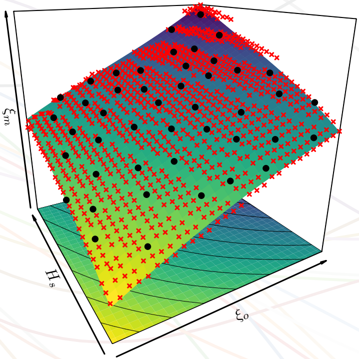
× coastal flooding data

2D coastal flooding application in (Rohmer and Idier, 2012).

Prediction using 5% of data ($n = 45$)



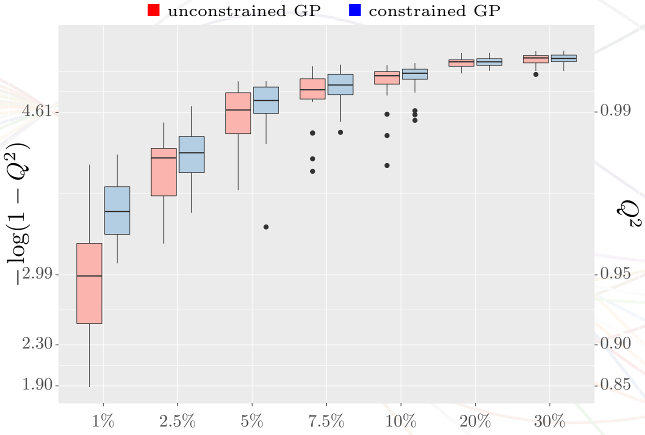
(a) Unconstr. GP: $Q^2 = 0.98$



(b) Constr. GP: $Q^2 = 0.99$

• training data × test data

Accurate predictions are obtained when $Q^2 \to 1$.

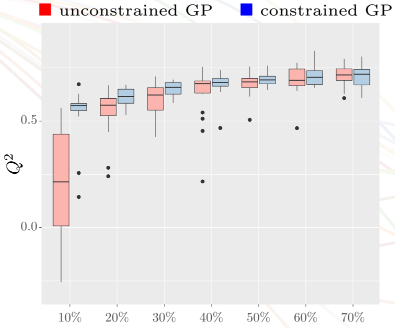


Q^2 performance using 20 replicates

Accurate predictions are obtained when $Q^2 \to 1$.

5D coastal flooding application

- Coastal flooding induced by overflow on the Atlantic coast, focusing on the **inland flooded surface** (Azzimonti et al., 2019).



Q^2 performance using 20 replicates

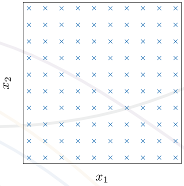
For small values of n, the constrained GP is more accurate.

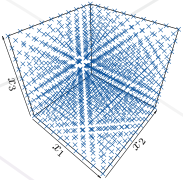
Main contributions

1. The improvement of the **applicability of GPs under constraints**: ✓
   - applicable up to 5D without further assumptions.
2. The scalability of constrained GPs to high dimensions.
3. Parameter estimation under inequality constraints.

Curse of dimensionality

- The cost of Y_m increases as d (or $m = m_1 \times \cdots \times m_d$) increases.





Curse of dimensionality

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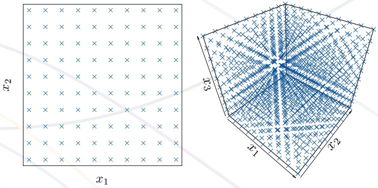
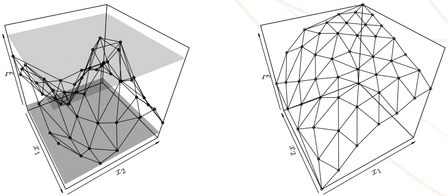
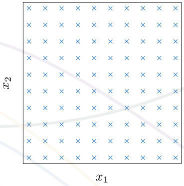
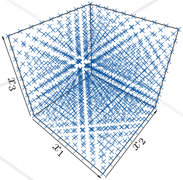


This downside can be partially mitigated in different ways...

- Using a **"smarter" construction of rectangular grids** of knots.
- Considering **further assumptions for complexity simplification**:
  - e.g. inactive dimensions, additive conditions.
- Using other types of designs of knots: e.g. **Delaunay triangulations**.







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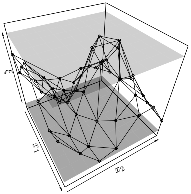
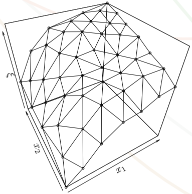
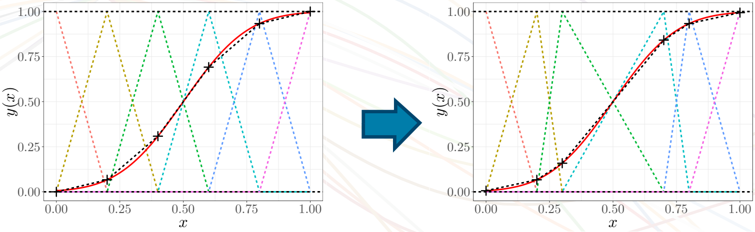




Free-knot finite-dimensional approximation of GPs

- Consider the **asymmetric hat basis functions**:



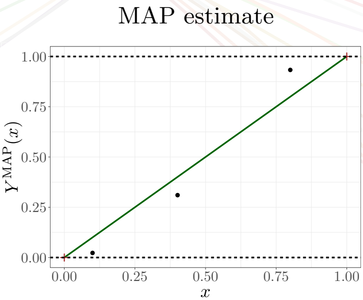
Standard hat basis functions. Asymmetric hat basis functions.

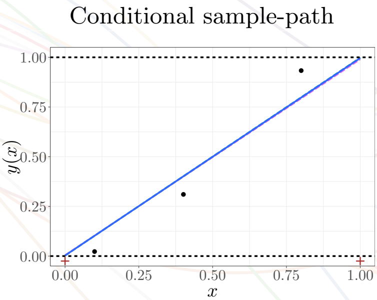
This allows sequentially refining (rectangular) grids of knots:

- **In highly variable regions.**
- **Along more active dimensions.**

- The "optimal" knot insertion is achieved by maximising the **integrated MAP squared error (iMAP-SE)** criterion:

$$t_*^{\text{opt}} = \underset{t_* \in [0,1]}{argmax} \int_0^1 [Y^{\text{MAP}}_{m_{i+1}, t_*}(x) - Y^{\text{MAP}}_{m_i}(x)]^2 dx. \quad (8)$$



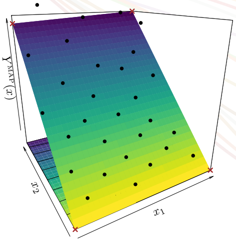


• training points + knots ■ MAP estimate
■ predictive mean ■ 90% confidence intervals

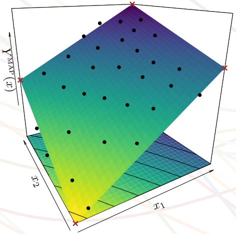
- In d dimensions, the **iMAP-SE** criterion is given by

$$t_*^{j_*,\mathrm{opt}} = \underset{j_* \in \{1,\cdots,d\},\ t_* \in [0,1]}{argmax} \int_{\boldsymbol{x} \in [0,1]^d} [Y^{\mathrm{MAP}}_{m_{i+1},j_*,t_*}(\boldsymbol{x}) - Y^{\mathrm{MAP}}_{m_i}(\boldsymbol{x})]^2 d\boldsymbol{x}. \quad (9)$$

Toy 1



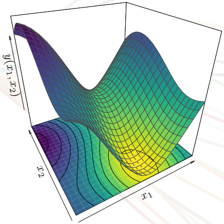
Toy 2

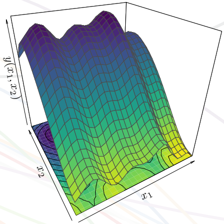


• training points + knots ■ MAP estimate

This construction has been tested up to 5D applications.

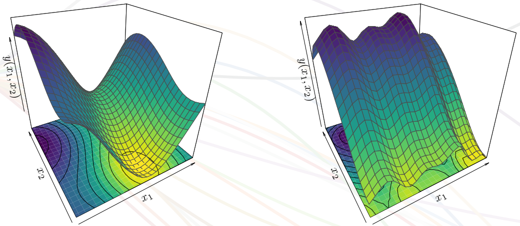
Additive GPs





2D examples of additive GPs.

Additive GPs



2D examples of additive GPs.

- Let Y be the additive process on $\mathbb{R}^d$ given by

$$Y(\boldsymbol{x}) = \sum_{p=1}^{d} Y_p(x_p), \quad \text{with} \quad Y_p \sim \mathcal{GP}(0, k_p). \tag{10}$$

- Assume that $Y_1, \ldots, Y_d$ are independent. Then, $Y \sim \mathcal{GP}(0, k)$ with:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sum_{p=1}^{d} k_p(x_p, x_p{}').$$

Additive GPs under inequality constraints

- Assume that Y exhibits certain constraints along Y_p, then Y_m is

$$Y_p \to Y_{p,m_p}$$

$$Y_m(\boldsymbol{x}) = \sum_{p=1}^{d} Y_{p,m_p}(x_p), \quad \text{s.t.} \quad \begin{cases} Y_m(\boldsymbol{x}_i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}_\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{11}$$

with $\boldsymbol{x}_i \in [0,1]^d$, $y_i \in \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}\left(0, \tau^2\right)$ for $i = 1, \ldots, n$.

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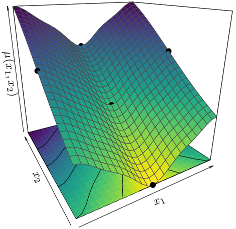
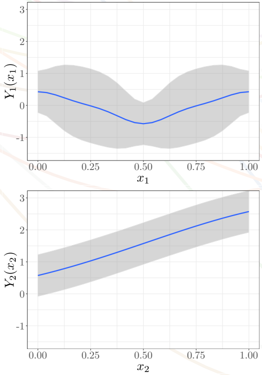
2D toy example:

$$Y(x_1, x_2) = \underbrace{4(x_1 - 0.5)^2}_{Y_1(x_1)} + \underbrace{2x_2}_{Y_2(x_2)}$$

Predictive mean without constraints





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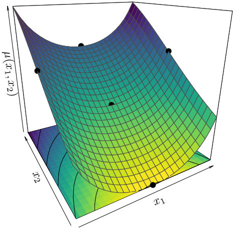
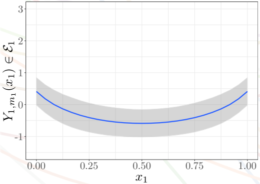
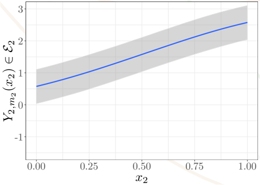


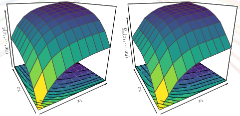




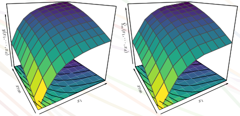
Numerical illustration in hundreds of dimensions

- Consider the (monotonic) target function:

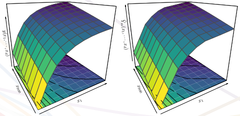
$$y(\boldsymbol{x}) = \sum_{p=1}^{d} \arctan\left(5\left[1 - \frac{p}{d}\right] x_p\right), \quad \text{with} \quad \boldsymbol{x} \in [0,1]^d.$$



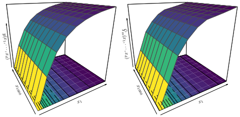
$y_1(x_1) + y_2(x_2)$



$y_1(x_1) + y_{700}(x_{700})$



$y_1(x_1) + y_{900}(x_{900})$



$y_1(x_1) + y_{1000}(x_{1000})$

	CPU Time [s]					
d	10	50	100	200	500	**1000**
Prediction	0.1	0.3	1.4	10.5	165.9	1364.5
Sampling	0.2	1.1	2.9	2.7	5.3	10.8

CPU times for sampling 10^3 trajectories via HMC.

Examples of an additive GP under monotonicity constraints in 10^3 dimensions. Each panel shows: the true (left) and predictive (right) mean profiles.

Main contributions

1. The improvement of the **applicability of GPs under constraints**: ✓
   - applicable up to 5D without further assumptions.
2. The **scalability** of constrained GPs **to high dimensions**: ✓
   - i.e. involving hundreds of input variables under additive assumptions.
3. Parameter estimation under inequality constraints.

Table of Contents

Maximum likelihood estimator (MLE)

- The covariance parameters $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ can be estimated via ML (Stein, 1999):

$$\widehat{\boldsymbol{\theta}}_n = \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{argmax}\ \mathcal{L}_n(\boldsymbol{\theta}),$$

where $\mathcal{L}_n(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_n)$ is the unconstrained log-likelihood:

$$\mathcal{L}_n(\boldsymbol{\theta}) = -\frac{1}{2}\log(\det(\mathbf{R}_{\boldsymbol{\theta}})) - \frac{1}{2}\mathbf{Y}_n^\top \mathbf{R}_{\boldsymbol{\theta}}^{-1}\mathbf{Y}_n - \frac{n}{2}\log 2\pi, \tag{12}$$

with $\mathbf{R}_{\boldsymbol{\theta}} = (k_{\boldsymbol{\theta}}(x_i, x_j))_{1 \leq i,j \leq n}$.

✗ **Note that the MLE $\widehat{\boldsymbol{\theta}}_n$ does not take into account the inequality conditions.**

Constrained maximum likelihood estimator (cMLE)

- Consider a convex set with linear inequality constraints $\mathcal{E}$.
- Let $\mathcal{L}_{n,c}(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_n | Y \in \mathcal{E})$ be the constrained log-likelihood:

$$\begin{aligned}\mathcal{L}_{n,c}(\boldsymbol{\theta}) &= \log \frac{p_{\boldsymbol{\theta}}(\mathbf{Y}_n) p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n)}{p_{\boldsymbol{\theta}}(Y \in \mathcal{E})} \\ &= \mathcal{L}_n(\boldsymbol{\theta}) + \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n) - \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E}).\end{aligned} \tag{13}$$

- Then, the cMLE is given by

$$\widehat{\boldsymbol{\theta}}_{n,c} = \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{argmax}\ \mathcal{L}_{n,c}(\boldsymbol{\theta}).$$

✓ **The cMLE $\widehat{\boldsymbol{\theta}}_{n,c}$ accounts for the inequality constraints.**

✗ **Both $p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n)$ and $p_{\boldsymbol{\theta}}(Y \in \mathcal{E})$ are approximated via MC.**

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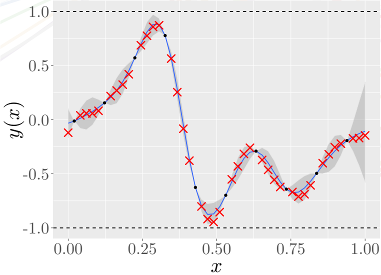
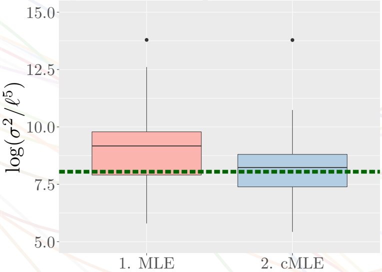
Numerical illustration

Assessment of the MLE and cMLE for $\mathbf{10^2}$ **realisations** drawn from a constrained GP $Y \in [-1, 1]$ with Matérn 5/2 kernel and true parameters $\boldsymbol{\theta}_0 = (\sigma^2 = 1, \ell = 0.2)$.





(b) Consistently estimable ratio $\log(\sigma^2/\ell^5)$

Notation

- Let $\mathcal{E}_\kappa$ be one of the following convex set of functions (mild conditions)

$$\mathcal{E}_\kappa = \begin{cases} f \;:\; \mathbb{X} \to \mathbb{R}, f \text{ is } C^0 \text{ and } \forall \boldsymbol{x} \in \mathbb{X},\; \ell \leq f(\boldsymbol{x}) \leq u & \text{if } \kappa = 0, \\ f \;:\; \mathbb{X} \to \mathbb{R}, f \text{ is } C^1 \text{ and } \forall \boldsymbol{x} \in \mathbb{X},\; \forall i = 1, \cdots, d,\; \frac{\partial}{\partial x_i} f(\boldsymbol{x}) \geq 0 & \text{if } \kappa = 1, \\ f \;:\; \mathbb{X} \to \mathbb{R}, f \text{ is } C^2 \text{ and } \forall \boldsymbol{x} \in \mathbb{X},\; \frac{\partial^2}{\partial \boldsymbol{x}^2} f(\boldsymbol{x}) \text{ is a p.s.d. matrix} & \text{if } \kappa = 2. \end{cases}$$

- Denote: $\boldsymbol{\theta}_0$ (true covariance parameters), $\widehat{\boldsymbol{\theta}}_n$ (MLE), $\widehat{\boldsymbol{\theta}}_{n,c}$ (cMLE).

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Proposition (Consistency of the MLE and cMLE, López-Lopera et al. (2018))

Assume $\forall \varepsilon > 0$ and $\forall M < \infty$, ***(Consistency of the unconditional ML)***

$$P(\sup_{\|\boldsymbol{\theta}-\boldsymbol{\theta}_0\| \geq \varepsilon} (\mathcal{L}_n(\boldsymbol{\theta}) - \mathcal{L}_n(\boldsymbol{\theta}_0)) \geq -M) \xrightarrow[n \to +\infty]{} 0.$$

Then, ***(Consistency of the conditional cML)***

$$P(\sup_{\|\boldsymbol{\theta}-\boldsymbol{\theta}_0\| \geq \varepsilon} (\mathcal{L}_{n,c}(\boldsymbol{\theta}) - \mathcal{L}_{n,c}(\boldsymbol{\theta}_0)) \geq -M \mid Y \in \mathcal{E}_\kappa) \xrightarrow[n \to +\infty]{} 0.$$

Consequently, both the MLE and cMLE are consistent estimators:

$$\widehat{\boldsymbol{\theta}}_n \in \operatorname{argmax}_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \ \mathcal{L}_n(\boldsymbol{\theta}) \xrightarrow[n \to +\infty]{P} \boldsymbol{\theta}_0, \quad \widehat{\boldsymbol{\theta}}_{n,c} \in \operatorname{argmax}_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \ \mathcal{L}_{n,c}(\boldsymbol{\theta}) \xrightarrow[n \to +\infty]{P | Y \in \mathcal{E}_\kappa} \boldsymbol{\theta}_0.$$

Notation

- For instance, we focus on estimating a single variance parameter σ_0^2, i.e.

$$k_{\sigma_0^2}(x, x') = \sigma_0^2 \; k_1(x, x'),$$

with fixed known correlation function k_1.

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Theorem (Asymptotic normality of the MLE and cMLE, Bachoc et al. (2019))

- *Assume mild conditions. Then, the MLE $\widehat{\sigma}_n^2$ of σ_0^2 conditioned on $\{Y \in \mathcal{E}_\kappa\}$ is asymptotically Gaussian distributed. More precisely, for $\kappa = 0, 1, 2$,*

$$\sqrt{n}\left(\widehat{\sigma}_n^2 - \sigma_0^2\right) \xrightarrow[n \to +\infty]{\mathcal{L} | Y \in \mathcal{E}_\kappa} \mathcal{N}(0, 2\sigma_0^4).$$

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- *Furthermore, the cMLE $\widehat{\sigma}_{n,c}^2$ of σ_0^2 conditioned on $\{Y \in \mathcal{E}_\kappa\}$ is also asymptotically Gaussian distributed:*

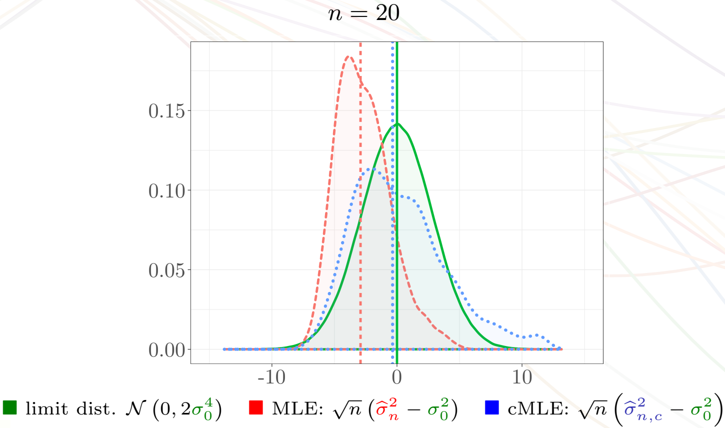
$$\sqrt{n}\left(\widehat{\sigma}_{n,c}^2 - \sigma_0^2\right) \xrightarrow[n\to+\infty]{\mathcal{L}|Y\in\mathcal{E}_\kappa} \mathcal{N}(0, 2\sigma_0^4).$$

The results can be extended for Matérn models (Bachoc et al., 2019).

Numerical illustration

Assessment of the MLE and cMLE normality for 10^3 **trajectories** drawn from a constrained GP $Y \in [0, 1]$ with Matérn 5/2 kernel and parameters $\boldsymbol{\theta}_0 = (\sigma_0^2 = 0.2, \ell = 0.2)$.

For small values of n, cMLE seems to be more accurate.



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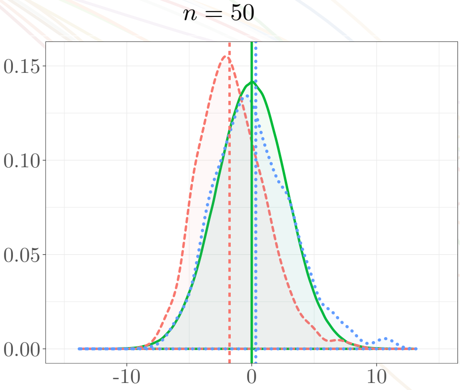
cMLE converges faster to the limit Gaussian distribution.



limit dist. $\mathcal{N}(0, 2\sigma_0^4)$ MLE: $\sqrt{n}\left(\widehat{\sigma}_n^2 - \sigma_0^2\right)$ cMLE: $\sqrt{n}\left(\widehat{\sigma}_{n,c}^2 - \sigma_0^2\right)$

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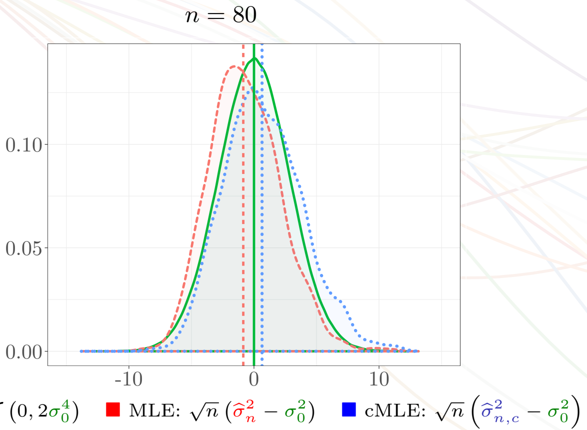
For large values of n, MLE and cMLE provide similar performances.



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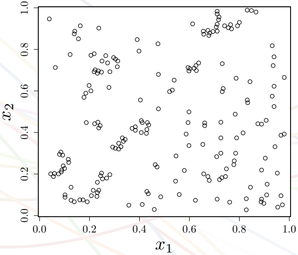
   - i.e. involving hundreds of input variables under additive assumptions.
3. **Parameter estimation under inequality constraints**: ✓
   - the use of **cMLE** is suggested for small amount of data.

Point Poisson process

- **Random countable subset** where *point patterns occur independently*.



Applications

- Geology (Møller and Waagepetersen, 2004).
- Astronomy (Baddeley et al., 2015).
- Lifetime of items or failure rates (Cha and Finkelstein, 2018).

- Unconditional likelihood under an **inhomogeneous Poisson process**:

$$f_{(N,\mathbf{X}_1,\cdots,\mathbf{X}_n)}(n,\boldsymbol{x}_1,\cdots,\boldsymbol{x}_n) = \exp\left(-\int_{\boldsymbol{x}\in\mathcal{D}} \lambda(\boldsymbol{x})d\boldsymbol{x}\right)\prod_{i=1}^{n}\frac{\lambda(\boldsymbol{x}_i)}{n!}, \qquad (14)$$

with

- $N \in \mathbb{N}$ a r.v. denoting the number of *point patterns*,
- $\mathbf{X}_1,\cdots,\mathbf{X}_n$ a set of n i.i.d. random vectors on $\mathcal{D}$, and
- $\lambda : \mathcal{D} \to [0,\infty]$ the (positive) intensity function.

- In real applications, λ is *unknown and must to be inferred.*

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- In real applications, λ is *unknown and must to be inferred.*

Cox process (Cox, 1955)

- Cox processes considers λ as a positive stochastic process:

$$\Lambda = \{\Lambda(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}.$$

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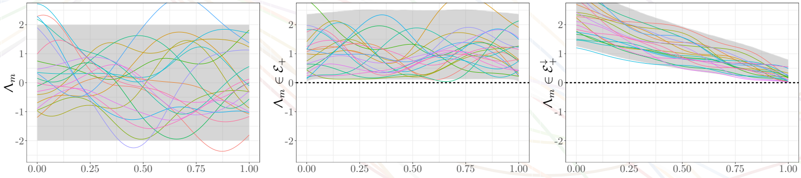
GP-modulated Cox processes under inequality constraints

- Consider the finite-dimensional GP prior (López-Lopera et al., 2019):

$$\Lambda_m \in \mathcal{E},$$

with $\mathcal{E}$ a convex set composed by a set of linear inequalities.



unconstrained GP prior | positive GP prior | monotone GP prior

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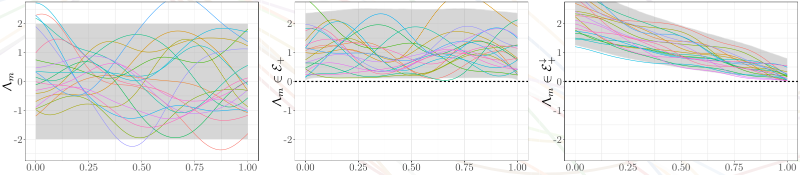
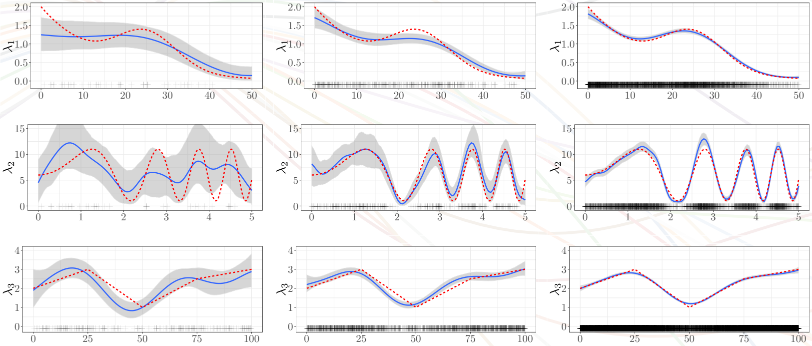


unconstrained GP prior | positive GP prior | monotone GP prior

Benefits:

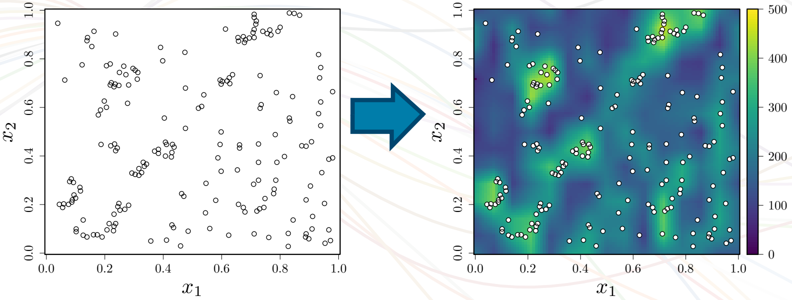
- **Tractable computations of the likelihood**.
- **Cox process inference via MCMC**:
  - *Metropolis-Hastings algorithm* with truncated Gaussian proposals.
- Applications to **other point processes**:
  - e.g. *Renewal processes* with monotone priors (Cha and Finkelstein, 2018).

Inference results for the examples in (Adams et al., 2009).



true intensity λ inferred intensity λ_m 90% confidence intervals

Location of redwood trees (dataset from Ripley, 1977).

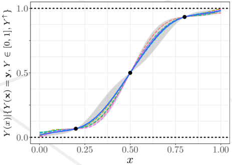


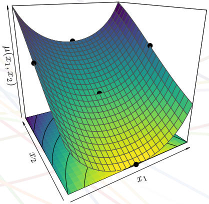
○ location of trees ■ inferred intensity λ

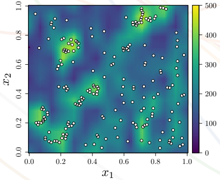
Competitive inference compared to approaches from the literature (e.g. log GPs, Møller et al., 2001).

In summary...

- We further investigated (Maatouk and Bay, 2017) to account for **linear inequality constraints**.
- We explored the use of the **HMC** for the *posterior approximation*.
- We proposed **variations of the GP model**:
  - *Noisy observations*,
  - *Free-knot (rectangular) designs* of knots,
  - *Additive (or block-additive)* functions.
- We studied a **constrained likelihood** analysing some *asymptotic properties*.
- We adapted the constrained GP framework to **modelling Poisson processes**.







Conclusions

- This thesis was dedicated to study **stochastic models based on GPs under inequality constraints**.
- Accounting for those constraints led to **more realistic uncertainty quantifications**, e.g.:
  - *Risk assessment in nuclear safety.*
  - *Coastal flooding modelling.*
  - *Spatial location of trees.*
  - ...
- Inference under constraints yielded **more accurate parameter estimation** for small (or moderate) amount of data.

Future work

- The **extension to high dimensions** is still challenging:
  - Alternative constructions can be explored (e.g. *Delaunay triangulations*).
- Existing methods for **approximating the orthant probabilities** of the cMLE are *time-consuming* and *unstable*.
- Coupling the proposed framework to other types of **GP-modulated processes** under inequality constraints: e.g. *Renewal processes*.

Publications in international journals

- L-L, A.F., Bachoc, F., Durrande, N., and Roustant, O. (2018). Finite-dimensional Gaussian approximation with linear inequality constraints. In ***SIAM/ASA Journal on Uncertainty Quantification***.
- Bachoc, F., Lagnoux, A., and L-L, A.F. (2019). Maximum likelihood estimation for Gaussian processes under inequality constraints. In ***Electronic Journal of Statistics***.

Proceedings in international conferences

- L-L, A.F., John, S., and Durrande, N. (2019). Gaussian process modulated Cox processes under linear inequality constraints. In *International Conference on Artificial Intelligence and Statistics (**AISTATS**)*.
- L-L, A.F., Bachoc, F., Durrande, N., Rohmer, J., Idier, D., and Roustant, O (2019). Approximating Gaussian process emulators with linear inequality constraints and noisy observations via MC and MCMC. In *International Conference in Monte Carlo & Quasi-Monte Carlo Methods (**MCQMC**)*.

R packages

- L-L, A.F. (2019). lineqGPR: Gaussian process regression models with inequality constraints. **CRAN R package**.


Lancement de la Chaire
en Mathématiques Appliquées
Oquaido : Optimisation et Quantification
d'Incertitudes pour les Données Onéreuses

Thanks!

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