`lineqGPR`: an R package for Gaussian process modelling with inequality constraints

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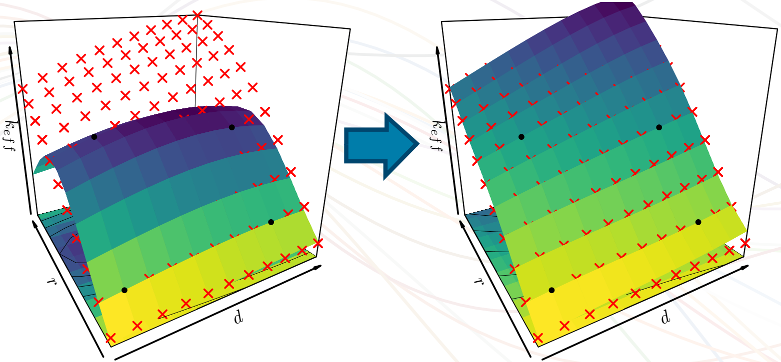
2D models for interpolating the IRSN's dataset (López-Lopera et al., 2018).

k_{eff}: effective neutron multiplication factor



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

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

Other applications

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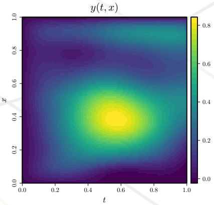

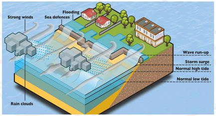

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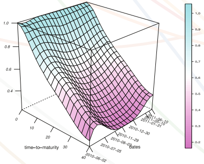
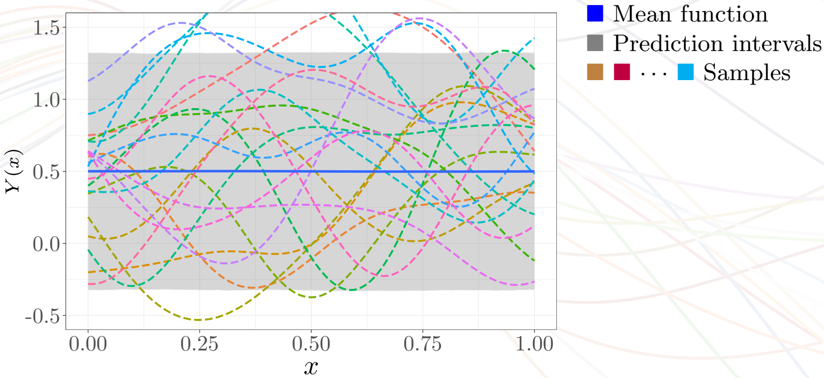


Cousin et al. (2016)

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



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

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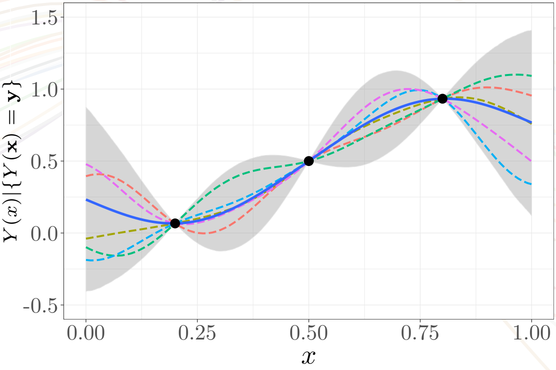
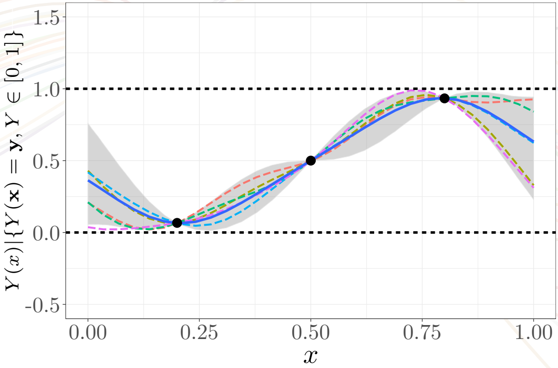


- Mean function
- Prediction intervals
- ··· Samples
- Interpolation conditions

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

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

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



Mean function

Prediction intervals

$\cdots$ Samples

● Interpolation conditions

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

- - Boundedness condition

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

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

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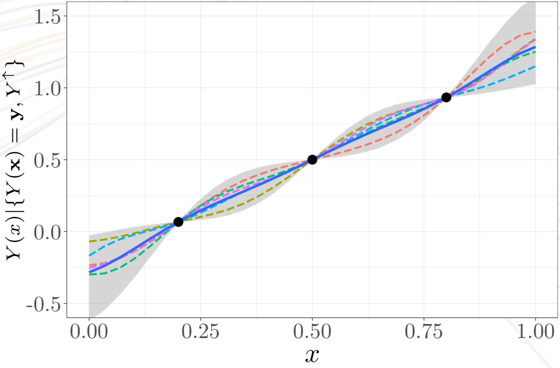

$Y|\{Y(\mathbf{x}) = \mathbf{y}, Y^{\uparrow}\} \sim$?

- Mean function
- Prediction intervals
- ⋯ Samples

● Interpolation conditions

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↑ Monotonicity condition

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

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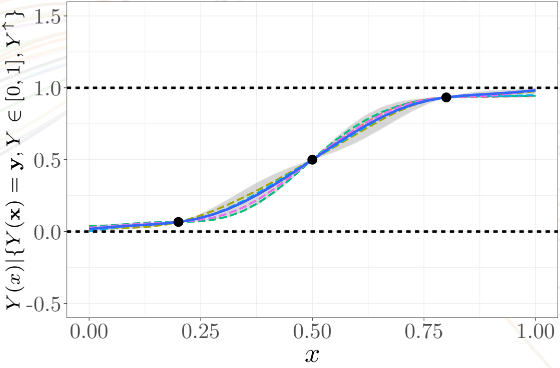

$Y | \{Y(\mathbf{x}) = \mathbf{y}, Y \in [0,1], Y^{\uparrow}\} \sim$ **?**

- Mean function
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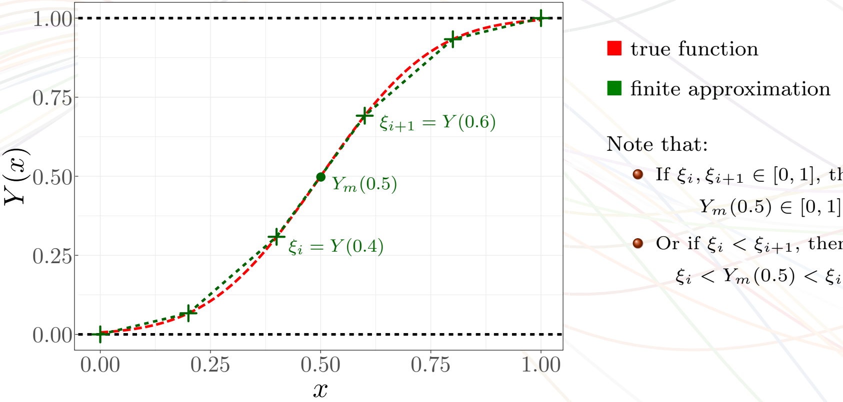
The main contributions in `lineqGPR` are threefold:

1. The improvement of the **applicability of GPs under constraints**.
2. The **scalability** of constrained GPs **to high dimensions**:
   - i.e. involving hundreds of input variables under additivity conditions.
3. **Parameter estimation under inequality constraints**.

1D finite-dimensional Gaussian approximation

Finite-dimensional representation Y_m: also bounded & monotonic.



Note that:

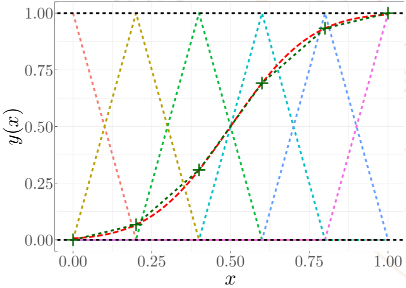
- If $\xi_i, \xi_{i+1} \in [0, 1]$, then $Y_m(0.5) \in [0, 1]$.
- Or if $\xi_i < \xi_{i+1}$, then $\xi_i < Y_m(0.5) < \xi_{i+1}$.

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

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

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

where $x_i \in [0, 1]$, $y_i \in \mathbb{R}$ for $i = 1, \ldots, n$; and
  - $\boldsymbol{\xi} = [\xi_1, \ldots, \xi_m]^\top \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma}_\theta)$ 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*:

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

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

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

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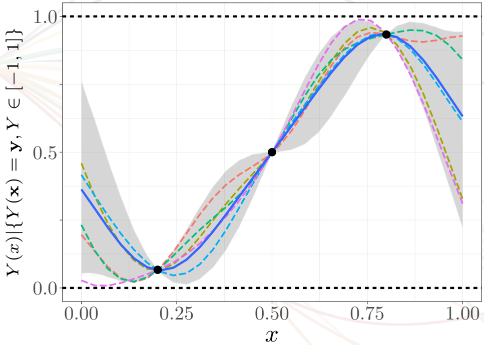
- Then, *quantifying uncertainty* on $Y_m(x) = \sum_{j=1}^m \xi_j \phi_j(x)$ relies on simulating the **truncated Gaussian vector** $\boldsymbol{\xi}$:

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

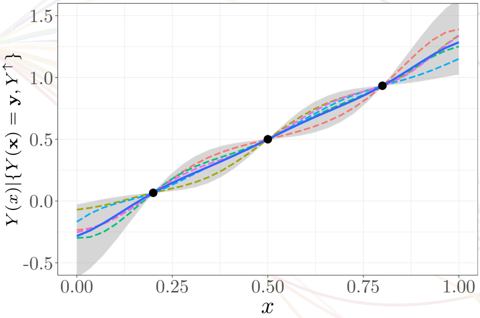
(3) is computed via *Monte Carlo* (MC) or *Markov Chain MC* (MCMC):
- **e.g. *Hamiltonian MC* (HMC) (Pakman and Paninski, 2014).**

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



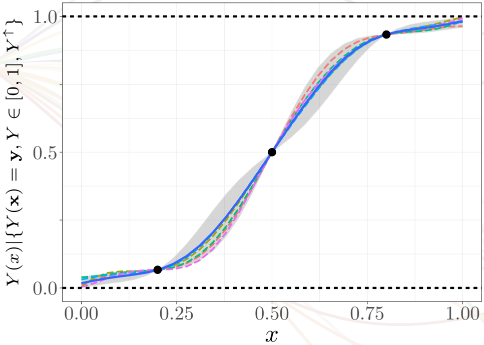
$$\underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\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

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



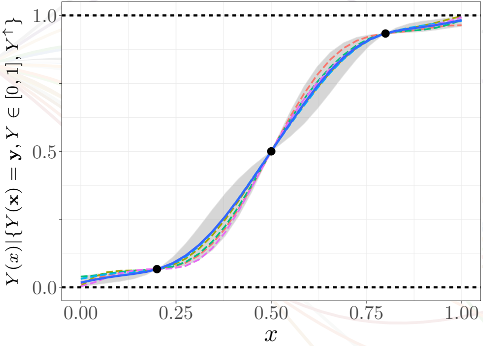
$$\underbrace{\begin{bmatrix}0\\0\\0\\\vdots\\0\\0\end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0\\ 0 & -1 & 1 & \cdots & 0 & 0\\ 0 & 0 & -1 & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & 1 & 0\\ 0 & 0 & 0 & \cdots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

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



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

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



or simply,

$$\underbrace{\begin{bmatrix} \boldsymbol{l}_b \\ \boldsymbol{l}_m \end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} \boldsymbol{\Lambda}_b \\ \boldsymbol{\Lambda}_m \end{bmatrix}}_{\boldsymbol{\Lambda}} \boldsymbol{\xi} \leq \underbrace{\begin{bmatrix} \boldsymbol{u}_b \\ \boldsymbol{u}_m \end{bmatrix}}_{\boldsymbol{u}}.$$

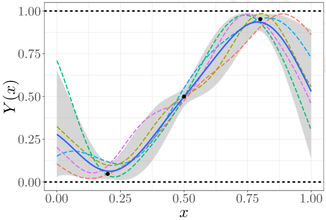
Considering noisy observations

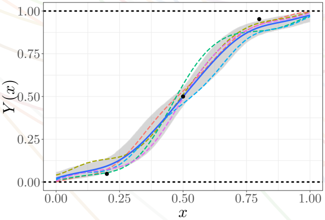
$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x), \text{ s.t. } \begin{cases} Y_m(x_i) + \varepsilon_i = y_i & \text{(interpolation conditions)}, \\ \boldsymbol{l} \leq \boldsymbol{\Lambda\xi} \leq \boldsymbol{u} & \text{(linear inequality conditions)}, \end{cases} \quad (4)$$

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

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

boundedness | **boundedness** & **monotonicity**





Adding ε leads to more flexible GP models and less restrictive sample spaces for MC/MCMC algorithms (López-Lopera et al., 2019).

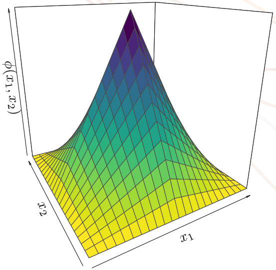
Finite-dimensional approximation in d dimensions

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

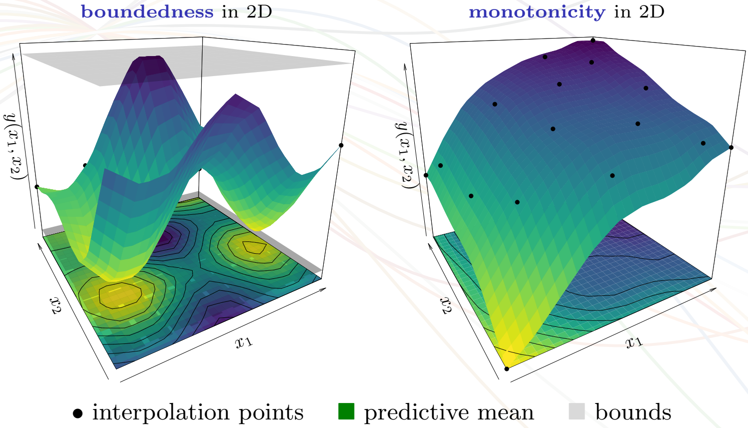
$$Y_m(\boldsymbol{x}) = \sum_{j_1,\ldots,j_d=1}^{m_1,\ldots,m_d} \left[\prod_{p=1,\ldots,d} \phi_{j_p}^{(p)}(x_p) \right] \xi_{j_1,\cdots,j_d}, \text{ s.t. } \begin{cases} Y_m(\boldsymbol{x}_i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi} \in \mathcal{C}, \end{cases} \quad (5)$$

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

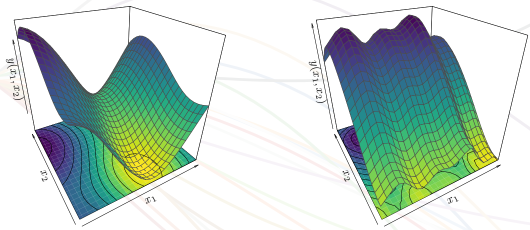
- $\boldsymbol{\xi} = [\xi_{1,\ldots,1}, \ldots, \xi_{m_1,\ldots,m_d}]^\top \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}_\theta)$,
- $\mathcal{C}$ is a convex set of linear inequality constraints, and
- $\phi_{j_i}^{(i)} : [0,1] \mapsto \mathbb{R}$ are hat basis functions.



2D numerical illustration



Additive GPs



2D examples of additive GPs.

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

$$Y(\boldsymbol{x}) = \sum_{p=1}^{d} Y_p(x_p), \quad \text{with} \quad Y_p \sim \mathcal{GP}(0, k_p). \tag{6}$$

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

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

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

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

$$Y_m(\boldsymbol{x}) = \sum_{p=1}^{d} Y_{p,m_p}(x_p), \quad \text{s.t.} \quad \begin{cases} Y_m(\boldsymbol{x}_i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}_\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{7}$$

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 $i = 1, \ldots, n$.

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

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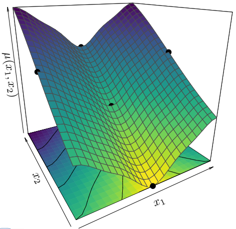
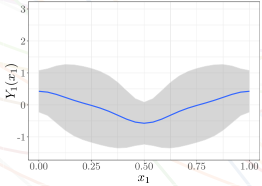
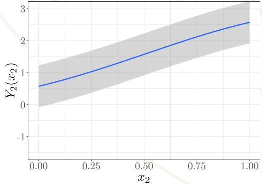
2D toy example:

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

Predictive mean without constraints







Additive GPs under inequality constraints

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

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

$$Y_m(\boldsymbol{x}) = \sum_{p=1}^{d} Y_{p,m_p}(x_p), \quad \text{s.t.} \quad \begin{cases} Y_m(\boldsymbol{x}_i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}_\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{7}$$

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 $i = 1, \ldots, n$.

2D toy example:

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

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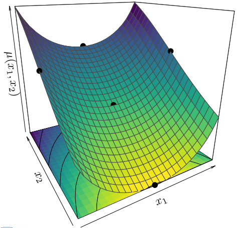

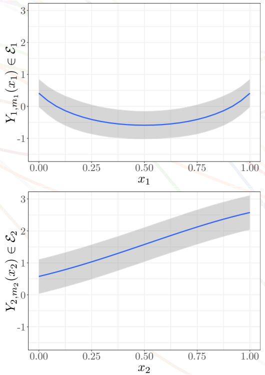

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- `lineqGPR` is an R package for GP modelling under inequality constraints.
- It is based on multiple contributions:
  - L-L, A.F., Bachoc, F., Durrande, N., and Roustant, O. (2018). Finite-dimensional Gaussian approximation with linear inequality 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*.
  - 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 *MCQMC*.

The main functionalities of `lineqGPR` are implemented as S3 methods.

Method Name	Description
create	Creation of GP models under inequality constraints.
lineqGPOptim	Parameter estimation under inequality constraints.
predict	Prediction of the objective function at new points.
simulate	Simulation of GP models under inequality constraints.
plot, ggplot	Plot for GP models.

Example

```
## ----------------------------------------------------------------- ##
## Gaussian process regression modelling under boundedness constraints ##
## ----------------------------------------------------------------- ##
library(lineqGPR)
library(ggplot2)

#### generating synthetic data ####
sigfun <- function(x) return(1/(1+exp(-7*(x-0.5))))
x <- seq(0, 1, 0.001); y <- sigfun(x)
DoE <- splitDoE(x, y, DoE.idx = c(201, 501, 801))

#### GP with active boundedness constraints ####
# creating the "lineqGP" model
model <- create(class = "lineqGP",
                x = DoE$xdesign, y = DoE$ydesign,
                constrType = "boundedness")
model$localParam$m <- 100 # nb of knots
model$bounds <- c(0,1) # defining the bounds

# sampling from the model
sim.model <- simulate(model, nsim = 1e4, seed = 1, xtest = DoE$xtest)
plot(sim.model, bounds = model$bounds, xlab = "x", ylab = "y(x)")
lines(x, y, lty = 2)
```

Note: see more example in the Jupyter Notebooks.

Bachoc, F., Lagnoux, A., and López-Lopera, A. F. (2019). Maximum likelihood estimation for Gaussian processes under inequality constraints. *Electronic J. of Statistics*, 13(2):2921–2969.

Cousin, A., Maatouk, H., and Rullière, D. (2016). Kriging of financial term-structures. *European Journal of Operational Research*, 255(2):631–648.

Durrande, N., Ginsbourger, D., and Roustant, O. (2012). Additive covariance kernels for high-dimensional Gaussian process modeling. *Annales de la Faculté de Sciences de Toulouse*, 21(3):481–499.

Lawrence, N. D., Sanguinetti, G., and Rattray, M. (2007). Modelling transcriptional regulation using Gaussian processes. In *Neural Information Processing Systems*, pages 785–792.

López-Lopera, A. F. (2018). lineqGPR: Gaussian process regression models with linear inequality constraints. `https://cran.r-project.org/web/packages/lineqGPR/index.html`.

López-Lopera, A. F., Bachoc, F., Durrande, N., and Roustant, O. (2018). Finite-dimensional Gaussian approximation with linear inequality constraints. *SIAM/ASA Journal on Uncertainty Quantification*, 6(3):1224–1255.

López-Lopera, A. F., Bachoc, F., Durrande, N., and Roustant, O. (2019). Approximating Gaussian process emulators with linear inequality constraints and noisy observations via MC and MCMC. *To appear in Proceedings in Monte Carlo and Quasi-Monte Carlo Methods*.

López-Lopera, A. F., John, S., and Durrande, N. (2019). Gaussian process modulated Cox processes under linear inequality constraints. In *AISTATS*, pages 1997–2006.

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