Ecole Nationale Supérieure des Mines SAINT-ETIENNE

INSTITUT de MATHEMATIQUES de TOULOUSE

Gaussian process regression models under linear inequality conditions

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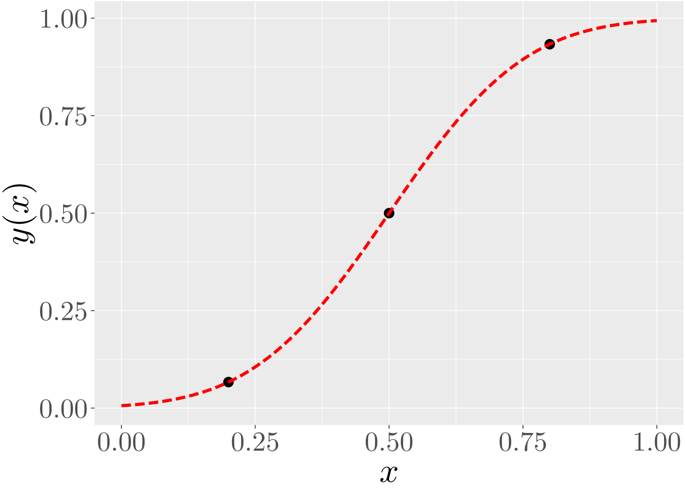
Regression models: a stochastic point of view

Target function: $x \mapsto \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF)



● Interpolation data

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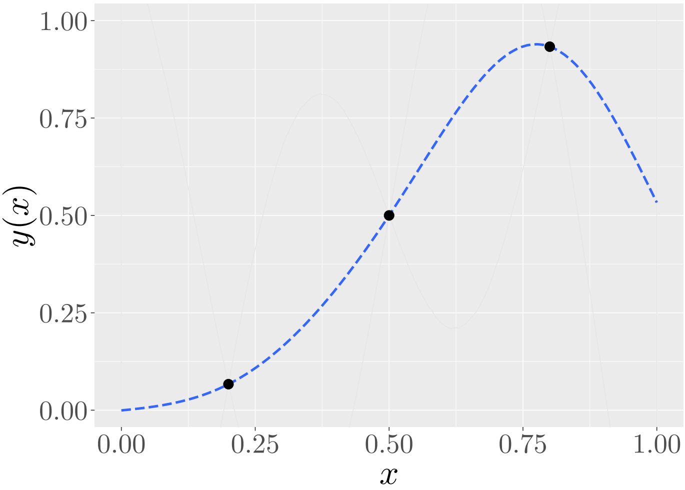

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■ solution 1

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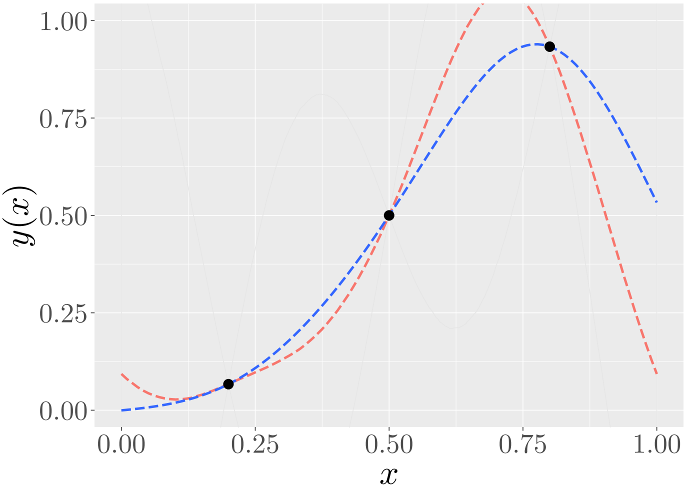

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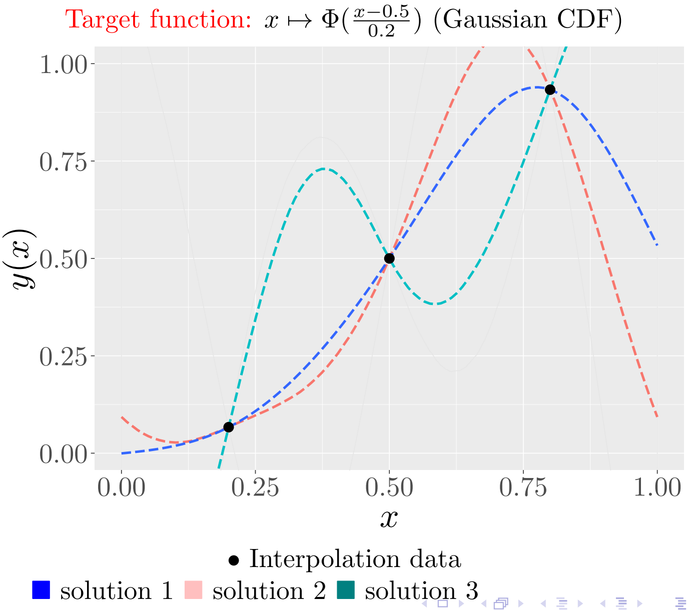
solution 1 solution 2

Regression models: a stochastic point of view



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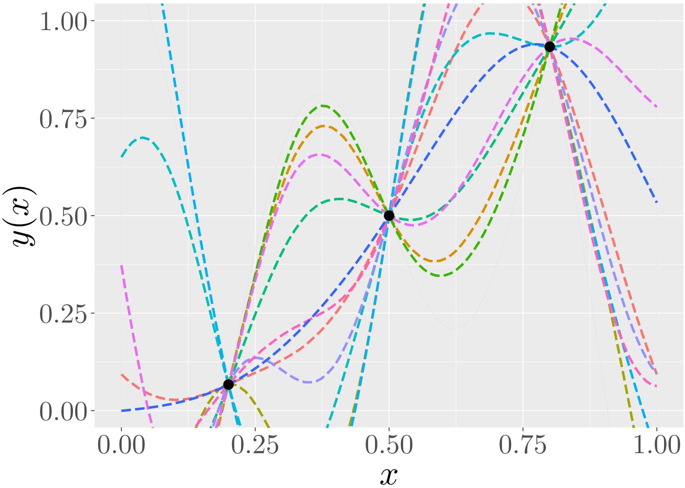
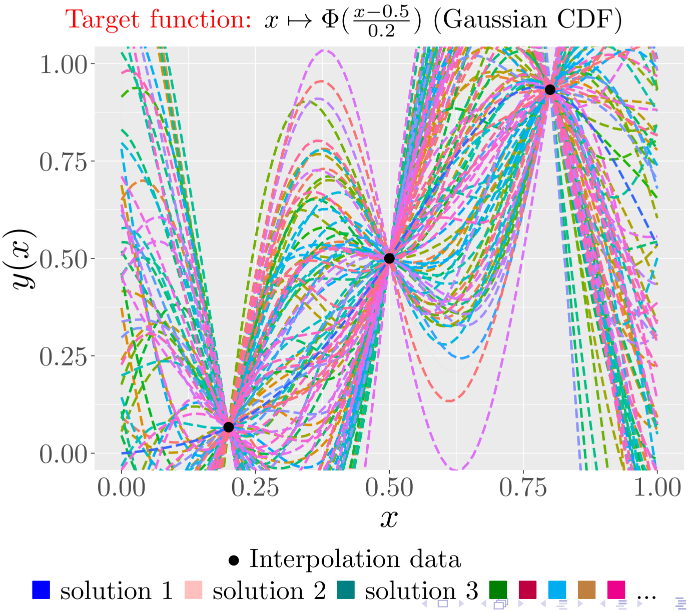


● Interpolation data

solution 1 solution 2 solution 3 ...

Regression models: a stochastic point of view



Gaussian process regression

Gaussian process (GP) (Rasmussen and Williams, 2005)

A GP is a collection of random variables, any finite number of which have a joint Gaussian distribution.

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Notation (Rasmussen and Williams, 2005)

Let Y be a GP. Then, $Y(x)$ is completely defined by its mean function $m(x)$ and covariance function $k(x, x')$

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

with

$$\begin{aligned} m(x) &= \mathbb{E}\left\{Y(x)\right\}, \\ k(x, x') &= \mathbb{E}\left\{[Y(x) - m(x)][Y(x') - m(x')]\right\}. \end{aligned}$$

where the operator $\mathbb{E}\left\{\cdot\right\}$ denotes the expectation of a random variable.

Gaussian process regression

GP regression model (Rasmussen and Williams, 2005)

Let Y be a zero-mean GP with covariance function k. Let $\{x_i, y_i\}$ for all $i = 1, \cdots, n$ be a set of observations. Then, the joint distribution of the vector of observations $\mathbf{y}$, and the vector of predictions $\mathbf{y}^*$ is Gaussian

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{y}^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{K}(\mathbf{x}, \mathbf{x}) & \mathbf{K}(\mathbf{x}, \mathbf{x}^*) \\ \mathbf{K}(\mathbf{x}^*, \mathbf{x}) & \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*) \end{bmatrix} \right), \tag{2}$$

and the conditional distribution $\mathbf{y}^*|\mathbf{y}$ is also Gaussian

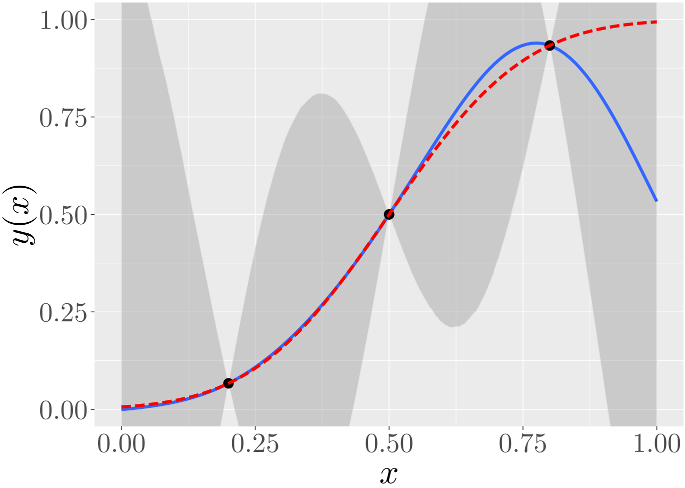
$$\mathbf{y}^*|\mathbf{y} \sim \mathcal{N}\left(\mathbf{m}_{\mathbf{y}^*|\mathbf{y}}, \mathbf{K}_{\mathbf{y}^*|\mathbf{y}} \right), \tag{3}$$

where

$$\begin{aligned} \mathbf{m}_{\mathbf{y}^*|\mathbf{y}} &= \mathbf{K}(\mathbf{x}^*, \mathbf{x})\mathbf{K}(\mathbf{x}, \mathbf{x})^{-1}\mathbf{y}, \\ \mathbf{K}_{\mathbf{y}^*|\mathbf{y}} &= \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*) - \mathbf{K}(\mathbf{x}^*, \mathbf{x})\mathbf{K}(\mathbf{x}, \mathbf{x})^{-1}\mathbf{K}(\mathbf{x}, \mathbf{x}^*). \end{aligned}$$

Gaussian process regression

Target function: $x \mapsto \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF)



$$\mathbf{m}_{\mathbf{y}^*|\mathbf{y}} = \mathbf{K}(\mathbf{x}^*, \mathbf{x})\mathbf{K}(\mathbf{x}, \mathbf{x})^{-1}\mathbf{y}$$

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Gaussian process regression

The GP model performed pretty well although only three training points were considered. But, how can the results be improved?

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Possible answers:

1. Adding more training points... but they are not always available.
2. Encoding extra information in the model about the target function.
3. Playing with the kernel function k.

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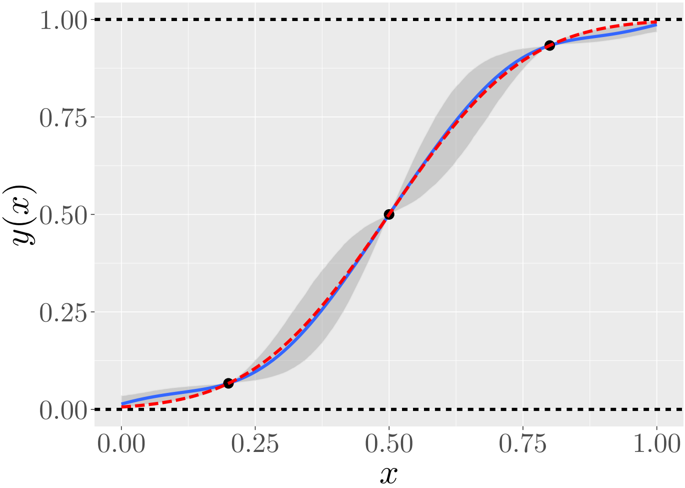
What about if we encode a priori both monotonicity and boundedness trends from the Gaussian CDF into the GP model...

Gaussian process regression

Target function: $x \mapsto \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF)



$\mathbf{m}_{\mathbf{y}^*|\mathbf{y}} = \mathbf{K}(\mathbf{x}^*, \mathbf{x})\mathbf{K}(\mathbf{x}, \mathbf{x})^{-1}\mathbf{y}$?

$\mathbf{K}_{\mathbf{y}^*|\mathbf{y}} = \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*) - \mathbf{K}(\mathbf{x}^*, \mathbf{x})\mathbf{K}(\mathbf{x}, \mathbf{x})^{-1}\mathbf{K}(\mathbf{x}, \mathbf{x}^*)$?

Gaussian process regression

Advantages of using GP models

1. GP models place prior distributions over function spaces.
2. Prior assumptions (e.g. smoothness, stationarity, sparsity) can be encoded in covariance functions.
3. They can be also used in classification task.
4. They have been used in a great variety of real-world problems:
    - Computer science,
    - Physics,
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Gaussian process regression

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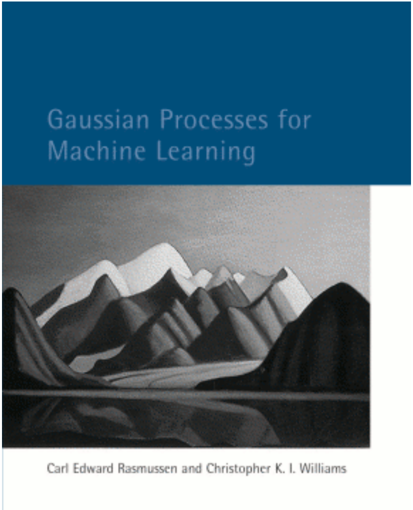
Disadvantages

1. They are purely data-driven approaches.
2. Curse of dimensionality: $\mathcal{O}(n^3)$.

Rasmussen and Williams (2005)



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

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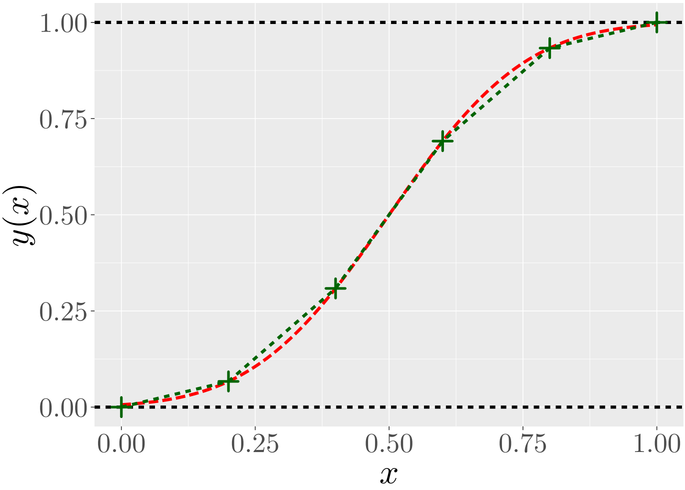
Finite-dimensional Gaussian approximation

Target function: $x \mapsto \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF)



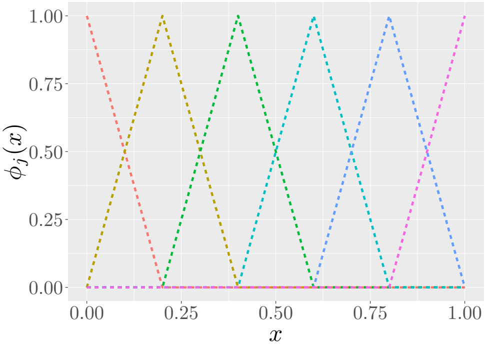
$\Rightarrow$ The finite approx. is also bounded and monotonic!!

Finite-dimensional Gaussian approximation

Let the finite-dimensional GP approximation be defined as

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x), \quad \text{s.t.} \quad Y_m(x_i) = y_i \quad \text{(interpolation conditions)}$$

where $\boldsymbol{\xi} = [\xi_1, \cdots, \xi_m]^\top \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma})$, with covariance matrix $\mathbf{\Gamma} = (k(t_i, t_j))1 \leq i, j \leq m$, and $\phi_j : [0, 1] \to \mathbb{R}$ are hat functions.



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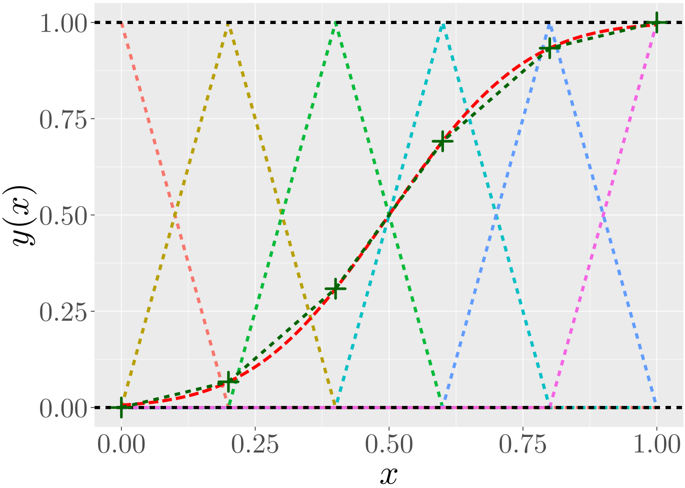

Finite-dimensional representation.

Finite-dimensional Gaussian approximation

Since $\boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma})$, then $\mathbf{Y}_m = [Y_m(x_1), \cdots, Y_m(x_n)]^\top = \boldsymbol{\Phi}\boldsymbol{\xi}$, is also Gaussian

$$\mathbf{Y}_m \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{\Phi}\boldsymbol{\Gamma}\boldsymbol{\Phi}^\top\right), \tag{4}$$

where $\boldsymbol{\Phi}$ is an $n \times m$ matrix defined by $\boldsymbol{\Phi}_{i,j} = \phi_j(x_i)$. Furthermore, the posterior distribution $\boldsymbol{\xi}|\{\mathbf{Y}_m = \mathbf{y}\}$ follows

$$\boldsymbol{\xi}|\{\mathbf{Y}_m = \mathbf{y}\} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \tag{5}$$

with

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

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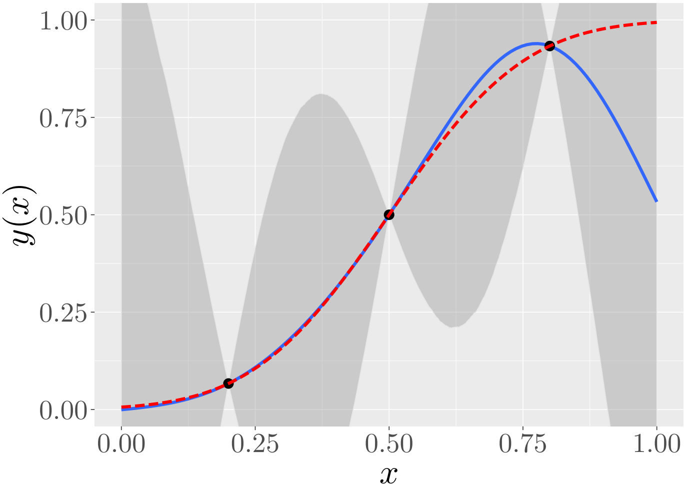

Finite-dimensional Gaussian approximation with $m = 100$.

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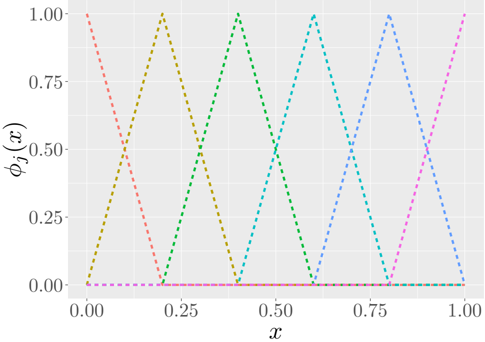
Constrained finite-dimensional Gaussian approximation

Let the finite-dimensional GP approximation be defined as

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x), \quad \text{s.t.} \quad \begin{cases} Y_m(x_i) = y_i & \text{(interpolation conditions)}, \\ Y_m \in \mathcal{E} & \text{(inequality conditions)}, \end{cases}$$

where $\boldsymbol{\xi} = [\xi_1, \cdots, \xi_m]^\top \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma})$, and $\phi_j : [0, 1] \to \mathbb{R}$ are hat functions (Maatouk and Bay, 2017).



Constrained finite-dimensional Gaussian approximation

First, since $Y_m \in \mathcal{E} \Leftrightarrow \boldsymbol{\xi} \in \mathcal{C}$, we consider $\mathcal{C}$ is composed by a set of q linear inequalities of the form

$$\mathcal{C} = \left\{ \mathbf{c} \in \mathbb{R}^m;\ \forall\, j = 1, \ldots, m, \forall\, k = 1, \ldots, q, \lambda_{k,j} \in \mathbb{R} \ :\ \ell_k \leq \sum_{j=1}^{m} \lambda_{k,j} c_j \leq u_k \right\}.$$

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Therefore, we have $\boldsymbol{\Lambda\xi} | \{\boldsymbol{\Phi\xi} = \mathbf{y}\} \sim \mathcal{N}\left(\boldsymbol{\Lambda\mu}, \boldsymbol{\Lambda\Sigma\Lambda}^\top\right)$, and the posterior follows a truncated multinormal (López-Lopera et al., 2017)

$$\boldsymbol{\Lambda\xi} | \{\boldsymbol{\Phi\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda\xi} \leq \boldsymbol{u}\} \sim \mathcal{TN}\left(\boldsymbol{\Lambda\mu},\ \boldsymbol{\Lambda\Sigma\Lambda}^\top,\ \boldsymbol{l},\ \boldsymbol{u}\right), \tag{6}$$

where $\boldsymbol{\Lambda} = (\lambda_{k,j})_{1\leq k\leq q, 1\leq j\leq m}$, $\boldsymbol{l} = (\ell_k)_{1\leq k\leq q}$, $\boldsymbol{u} = (u_k)_{1\leq k\leq q}$, and

$$\boldsymbol{\mu} = \boldsymbol{\Gamma\Phi}^\top[\boldsymbol{\Phi\Gamma\Phi}^\top]^{-1}\mathbf{y}, \quad \text{and} \quad \boldsymbol{\Sigma} = \boldsymbol{\Gamma} - \boldsymbol{\Gamma\Phi}^\top[\boldsymbol{\Phi\Gamma\Phi}^\top]^{-1}\boldsymbol{\Phi\Gamma}. \tag{7}$$

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$\Rightarrow$ The distribution of Equation (6) can be approximated using MCMC.

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$$\boldsymbol{\Lambda}\boldsymbol{\xi} | \{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\} \sim \mathcal{TN}\left(\boldsymbol{\Lambda}\boldsymbol{\mu},\ \boldsymbol{\Lambda}\boldsymbol{\Sigma}\boldsymbol{\Lambda}^\top,\ \boldsymbol{l},\ \boldsymbol{u}\right), \tag{6}$$

where $\boldsymbol{\Lambda} = (\lambda_{k,j})_{1 \leq k \leq q, 1 \leq j \leq m}$, $\boldsymbol{l} = (\ell_k)_{1 \leq k \leq q}$, $\boldsymbol{u} = (u_k)_{1 \leq k \leq q}$, and

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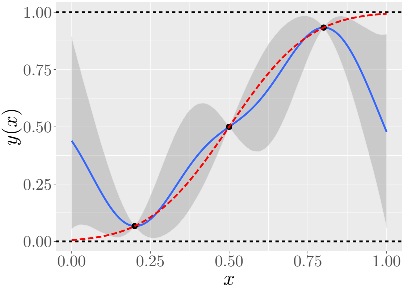
$\Rightarrow$ The distribution of Equation (6) can be approximated using MCMC.

$\Rightarrow$ What about $\boldsymbol{\Lambda}$, $\boldsymbol{l}$, $\boldsymbol{u}$?

Constrained finite-dimensional Gaussian approximation

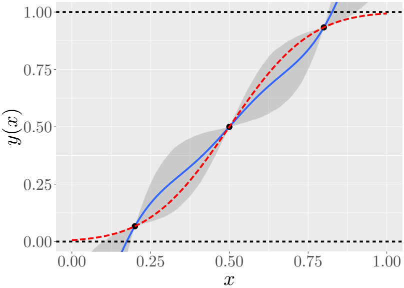
Defining boundedness constraints



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

Constrained finite-dimensional Gaussian approximation

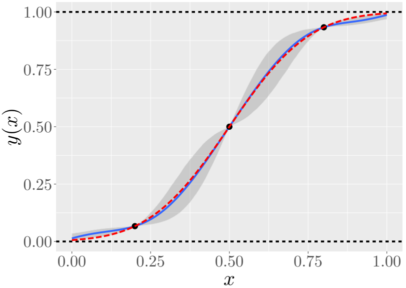
Defining monotonicity constraints



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

Constrained finite-dimensional Gaussian approximation

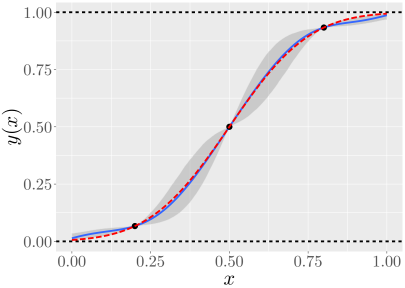
Defining boundedness and monotonicity constraints



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

Constrained finite-dimensional Gaussian approximation

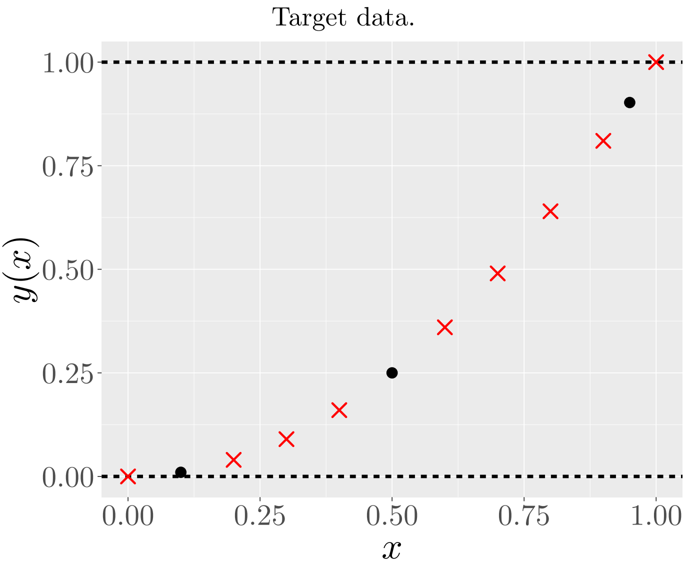
Defining boundedness and monotonicity constraints



or simply,

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

Toy example 1: $x \mapsto x^2$



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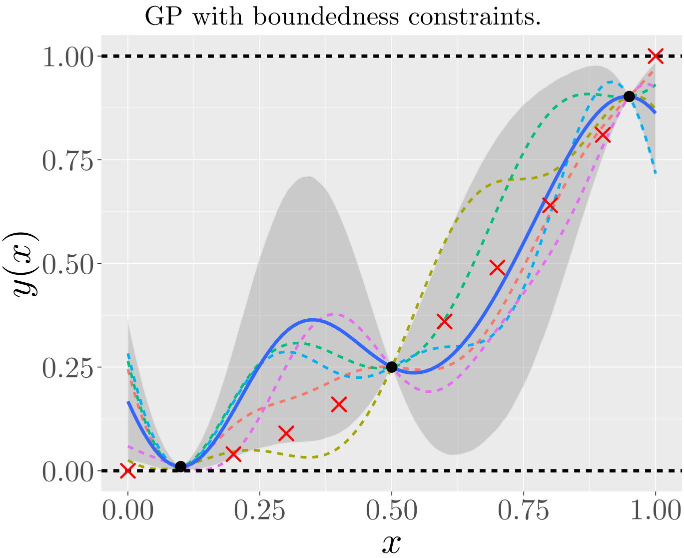

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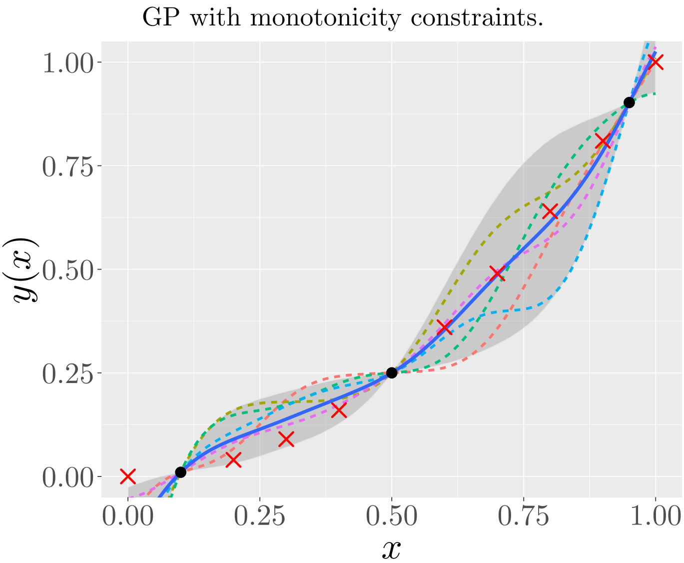
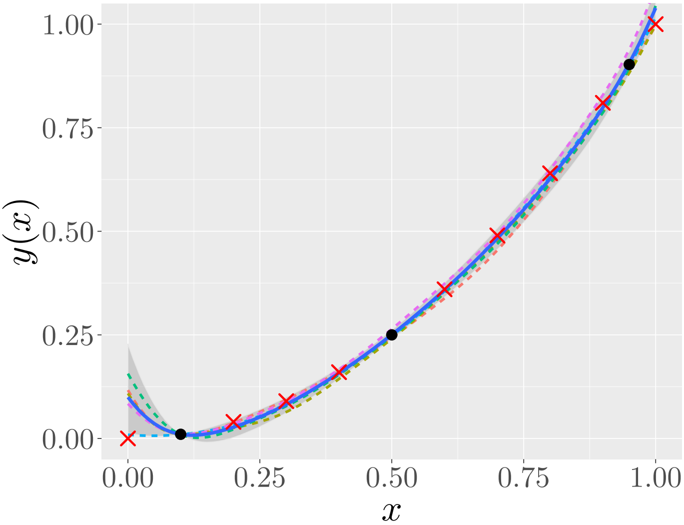


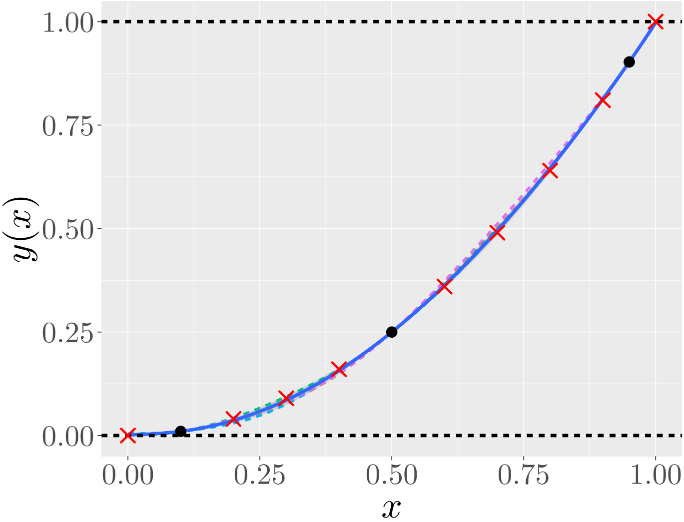
Toy example 1: $x \mapsto x^2$

GP with convexity constraints.

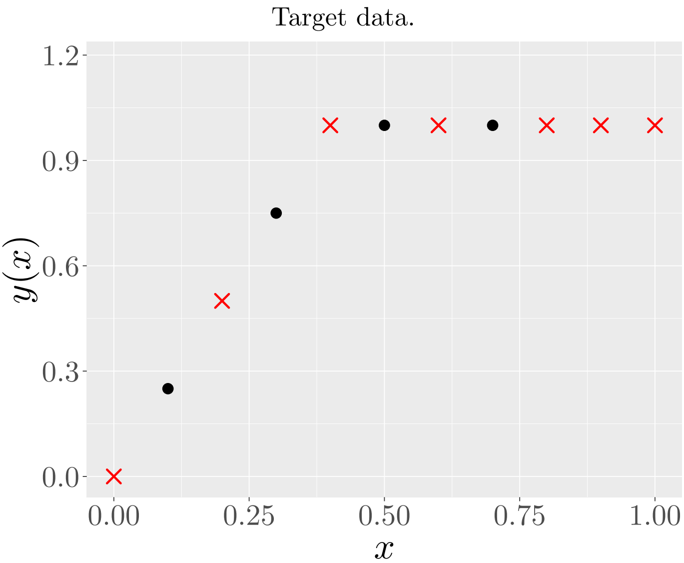


Toy example 1: $x \mapsto x^2$

GP with boundedness+monotonicity+convexity constraints.



Toy example 2: sequential constraints



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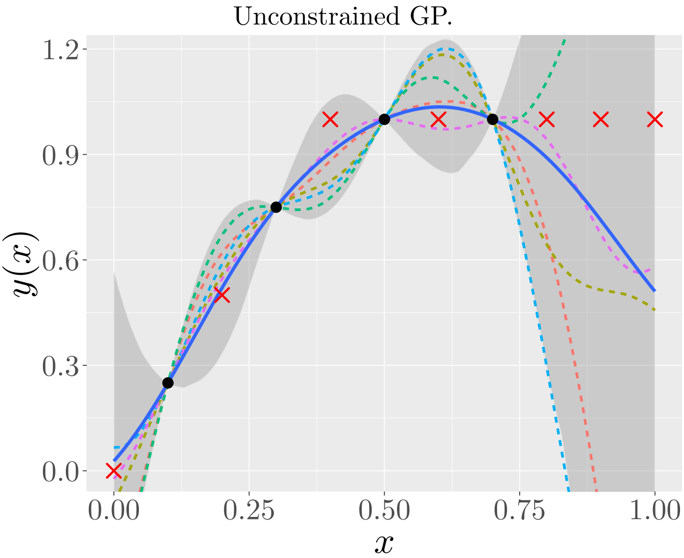
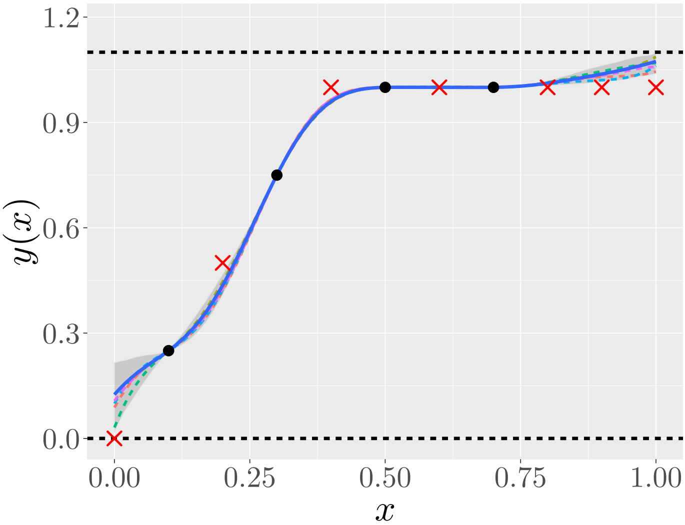


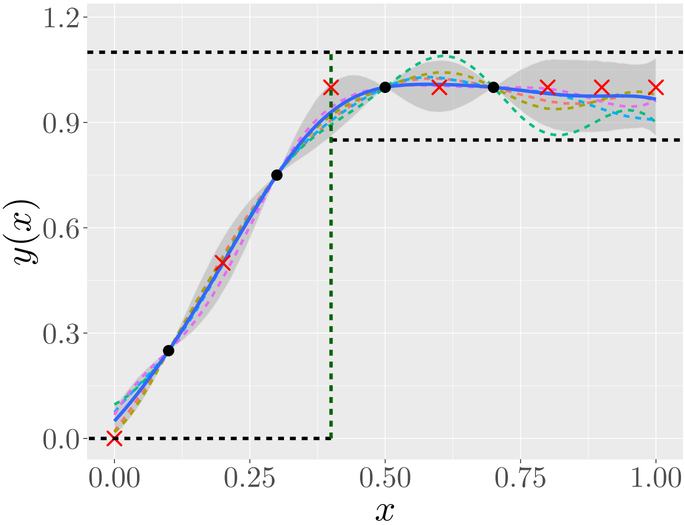
Toy example 2: sequential constraints

GP with boundedness+monotonicity constraints.



Toy example 2: sequential constraints

GP with sequential constraints.



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Extension for 2D input spaces

The approximation can be extended to two dimensional input spaces by tensorisation:

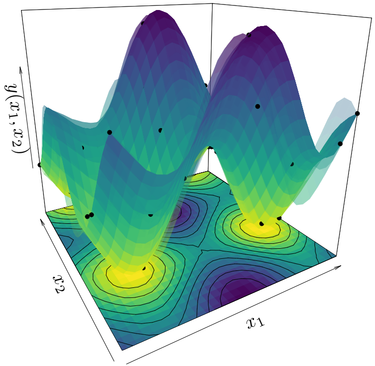
$$Y_{m_1,m_2}(x_1,x_2) := \sum_{j_1=1}^{m_1}\sum_{j_2=1}^{m_2} \xi_{j_2,j_1}\phi^1_{j_1}(x_1)\phi^2_{j_2}(x_2), \text{ s.t. } \begin{cases} Y_{m_1,m_2}\left(x_1^i, x_2^i\right) = y_i, \\ \xi_{j_2,j_1} \in \mathcal{C}, \end{cases}$$

where $\xi_{j_2,j_1} = Y(t_{j_1}, t_{j_2})$ and $(x_1^1, x_2^1), \cdots, (x_1^n, x_2^n)$ constitute a DoE, and $\phi^1_{j_1}, \phi^2_{j_2} : [0,1] \to \mathbb{R}$ are hat functions.

$\Rightarrow$ We can also assume that $\boldsymbol{\xi} = \left[\xi_{1,1}, \cdots, \xi_{1,m1}, \cdots, \xi_{m2,1}, \cdots \xi_{m2,m1}\right]^\top$ is a zero-mean Gaussian vector with covariance matrix $\boldsymbol{\Gamma}$.

Extension for 2D input spaces

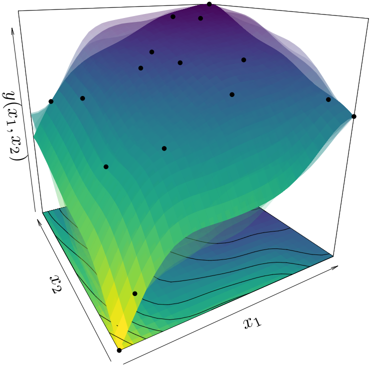
Boundedness in 2D.



Examples of 2D Gaussian models with different types of constraints.

Extension for 2D input spaces

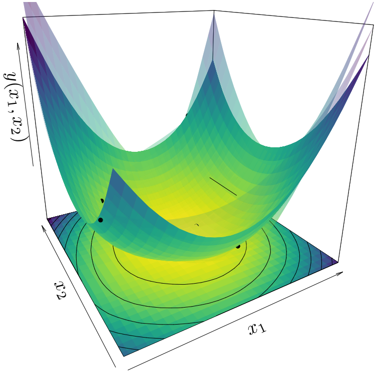
Monotonicity in 2D.



Examples of 2D Gaussian models with different types of constraints.

Extension for 2D input spaces

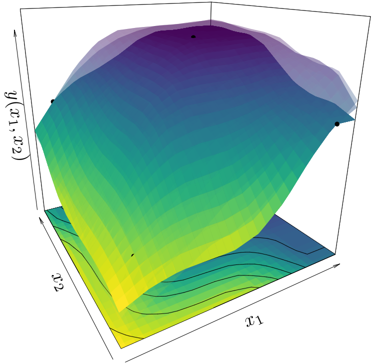
Convexity in 2D (a weak version).



Examples of 2D Gaussian models with different types of constraints.

Extension for 2D input spaces

Boundedness and monotonicity in 2D.



Examples of 2D Gaussian models with different types of constraints.

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Maximum likelihood estimation (MLE)

Maximum likelihood (ML) estimation

Consider that the zero-mean GP Y has covariance function $k_{\boldsymbol{\theta}^*}$ for an unknown $\boldsymbol{\theta}^* \in \boldsymbol{\Theta}$. Let $\mathcal{L}_m(\boldsymbol{\theta})$ be the log likelihood of $\boldsymbol{\theta}$

$$\mathcal{L}_m(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m) = -\frac{1}{2}\log(\det(\mathbf{K}_{\boldsymbol{\theta}})) - \frac{1}{2}\mathbf{Y}_m^\top \mathbf{K}_{\boldsymbol{\theta}}^{-1}\mathbf{Y}_m - \frac{n}{2}\log 2\pi, \tag{8}$$

with $\mathbf{K}_{\boldsymbol{\theta}} = \boldsymbol{\Phi}\boldsymbol{\Gamma}_{\boldsymbol{\theta}}\boldsymbol{\Phi}^\top$ and $\boldsymbol{\Gamma}_{\boldsymbol{\theta}} = (k_{\boldsymbol{\theta}}(t_i, t_j))_{1 \leq i,j \leq m}$. Then, $\boldsymbol{\theta}^*$ can be estimated by maximising Equation (8) w.r.t. $\boldsymbol{\theta} \in \boldsymbol{\Theta}$

$$\widehat{\boldsymbol{\theta}}_{\mathrm{MLE}} = \arg\max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \ \mathcal{L}_m(\boldsymbol{\theta}). \tag{9}$$

Maximum likelihood estimation (MLE)

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$\Rightarrow$ Equation (9) does not take into account the constraints $\boldsymbol{\xi} \in \mathcal{C}$.

Constrained maximum likelihood estimation (CMLE)

Constrained maximum likelihood (CML) estimation

Let $p_{\boldsymbol{\theta}}(\mathbf{Y}_m|\boldsymbol{\xi} \in \mathcal{C})$ be the conditional pdf of $\mathbf{Y}_m$ given $\boldsymbol{\xi} \in \mathcal{C}$, when Y has covariance function $k_{\boldsymbol{\theta}}$. By using Bayes' theorem, the constrained log likelihood $\mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m|\boldsymbol{\xi} \in \mathcal{C})$ is

$$\begin{aligned}\mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}) &= \log \frac{p_{\boldsymbol{\theta}}(\mathbf{Y}_m) P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C}|\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{Y}_m)}{P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C})} \\ &= \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m) + \log P_{\boldsymbol{\theta}}(\boldsymbol{\xi}\in\mathcal{C}|\boldsymbol{\Phi}\boldsymbol{\xi}=\mathbf{Y}_m) - \log P_{\boldsymbol{\theta}}(\boldsymbol{\xi}\in\mathcal{C}),\end{aligned} \tag{10}$$

Then, the constrained CML estimator is given by

$$\widehat{\boldsymbol{\theta}}_{\text{CMLE}} = \arg\max_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}). \tag{11}$$

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Let $p_{\boldsymbol{\theta}}(\mathbf{Y}_m | \boldsymbol{\xi} \in \mathcal{C})$ be the conditional pdf of $\mathbf{Y}_m$ given $\boldsymbol{\xi} \in \mathcal{C}$, when Y has covariance function $k_{\boldsymbol{\theta}}$. By using Bayes' theorem, the constrained log likelihood $\mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m | \boldsymbol{\xi} \in \mathcal{C})$ is

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- Unconstrained log likelihood.
- Gaussian orthant probabilities (Botev, 2017; Genz, 1992).

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Asymptotic analysis

Let $\mathcal{E}_\kappa$ be one of the following convex set of functions

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

which corresponds to boundedness, monotonicity, and convexity constraints. We will focus on the GP Y and the observation vector

$$\mathbf{Y}_n = \left[Y(x_1), \cdots, Y(x_n) \right]^\top.$$

Maximum likelihood (ML)

Proposition 1: asymptotic consistency of ML

Let Y be a centred GP on $\mathbb{X} \subset \mathbb{R}^d$ with covariance k satisfying Condition A.1 from (López-Lopera et al., 2017). Let $\mathbf{Y}_n = \left[\, Y(x_1), \cdots, Y(x_n) \,\right]^\top$. Let

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

with $\mathbf{R}_{\boldsymbol{\theta}} = (k_{\boldsymbol{\theta}}(x_i, x_j))_{1 \leq i,j \leq n}$. Let $\widehat{\boldsymbol{\theta}} \in \arg\max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \mathcal{L}_n(\boldsymbol{\theta})$. Assume $\forall \varepsilon > 0$,

$$P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon) \xrightarrow[n \to \infty]{} 0. \quad \text{(Consistency of the unconditional ML)}$$

Let $\kappa \in \{0, 1, 2\}$. Let $\mathcal{E}_\kappa$. Then, we have $P(Y \in \mathcal{E}_\kappa) > 0$ from Lemmas A.3, A.4 and A.5 of (López-Lopera et al., 2017), and thus

$$P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon \mid Y \in \mathcal{E}_\kappa) \xrightarrow[n \to \infty]{} 0. \quad \text{(Consistency of the conditional ML)}$$

Maximum likelihood (ML)

Proof 1: asymptotic consistency of ML

We have

$$P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon |\ Y \in \mathcal{E}_\kappa) = \frac{P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon,\ Y \in \mathcal{E}_\kappa)}{P(Y \in \mathcal{E}_\kappa)} \leq \frac{P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon)}{P(Y \in \mathcal{E}_\kappa)}.$$

Since $P(Y \in \mathcal{E}_\kappa) > 0$ is fixed, and $P(\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\| \geq \varepsilon) \xrightarrow[n \to \infty]{} 0$, the result follows.

Constrained maximum likelihood (CML)

Proposition 2: asymptotic consistency of CML

We use the same notations and assumptions as in Proposition 1. Let $P_{\boldsymbol{\theta}}$ be the distribution of Y with covariance function $k_{\boldsymbol{\theta}}$. Let

$$\mathcal{L}_{\mathcal{C},n}(\boldsymbol{\theta}) = \mathcal{L}_n(\boldsymbol{\theta}) + \log P_{\boldsymbol{\theta}}(Y \in \mathcal{E}_\kappa | \mathbf{Y}_n) - \log P_{\boldsymbol{\theta}}(Y \in \mathcal{E}_\kappa). \quad \text{(Constrained ML)}$$

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

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

Then, (Consistency of the conditional CML)

$$P\left(\sup_{\|\boldsymbol{\theta}-\boldsymbol{\theta}^*\| \geq \varepsilon} (\mathcal{L}_{\mathcal{C},n}(\boldsymbol{\theta}) - \mathcal{L}_{\mathcal{C},n}(\boldsymbol{\theta}^*)) \geq -M \;\middle|\; Y \in \mathcal{E}_\kappa \right) \xrightarrow[n\to\infty]{} 0.$$

Consequently (Consistency of ML and CML estimators)

$$\operatorname{argmax}_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \; \mathcal{L}_n(\boldsymbol{\theta}) \xrightarrow[n\to\infty]{P} \boldsymbol{\theta}^*, \quad \text{and} \quad \operatorname{argmax}_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \; \mathcal{L}_{\mathcal{C},n}(\boldsymbol{\theta}) \xrightarrow[n\to\infty]{P|Y\in\mathcal{E}_\kappa} \boldsymbol{\theta}^*.$$

Constrained maximum likelihood (CML)

Proof 2: asymptotic consistency of CML

We have from Lemmas A.1 and A.2 from (López-Lopera et al., 2017) that $\forall \varepsilon > 0$

$$P(\log(P_{\boldsymbol{\theta}^*}(Y \in \mathcal{E}_\kappa \mid \mathbf{Y}_n)) \geq \log(1-\varepsilon) \mid Y \in \mathcal{E}_\kappa) \xrightarrow[n\to\infty]{} 1.$$

Hence $\forall \delta > 0$

$$P\left(\sup_{\|\boldsymbol{\theta}-\boldsymbol{\theta}^*\| \geq \varepsilon} \log(P_{\boldsymbol{\theta}}(Y \in \mathcal{E}_\kappa \mid \mathbf{Y}_n)) - \log(P_{\boldsymbol{\theta}^*}(Y \in \mathcal{E}_\kappa \mid \mathbf{Y}_n)) \geq \delta \,\middle|\, Y \in \mathcal{E}_\kappa \right) \xrightarrow[n\to\infty]{} 0.$$

Also, from Lemma A.6, there exists $\Delta > 0$ so that we have

$$\inf_{\|\boldsymbol{\theta}-\boldsymbol{\theta}^*\| \geq \varepsilon} P_{\boldsymbol{\theta}}(Y \in \mathcal{E}_\kappa) \geq \Delta > 0,$$

so that

$$\sup_{\|\boldsymbol{\theta}-\boldsymbol{\theta}^*\| \geq \varepsilon} -\log(P_{\boldsymbol{\theta}}(Y \in \mathcal{E}_\kappa)) + \log(P_{\boldsymbol{\theta}^*}(Y \in \mathcal{E}_\kappa)) \leq -\log(\Delta) < \infty.$$

Hence, the proposition follows.

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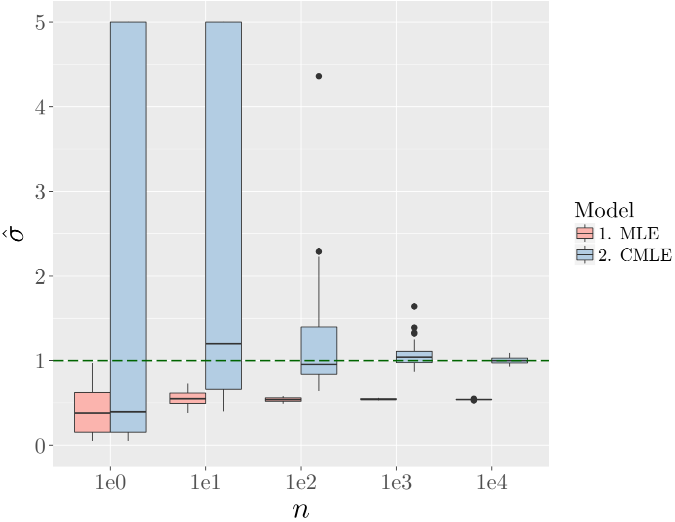
Results: univariate truncated normal

We estimate $(\sigma^*)^2 = 1$ using different nb of observations.

- We simulate from the truncated normal $Y_i \sim \mathcal{TN}\left(0, (\sigma^*)^2, -1, 1\right)$ for $i = 1, \cdots n$.
- We estimate $\hat{\sigma}$ via MLE and CMLE.
- We repeat the experiment 100 times.

Results: univariate truncated normal

Estimating $\hat{\sigma}$ given different nb of samples.



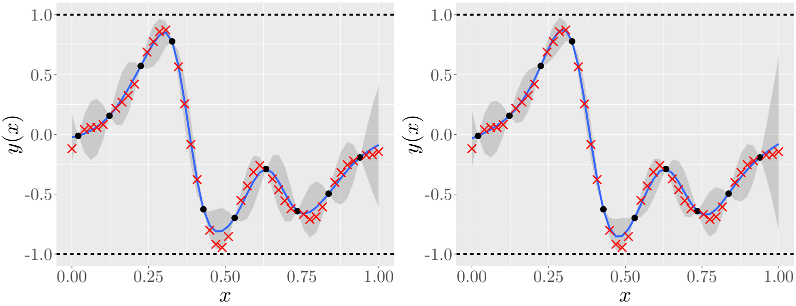
Results: simulation study

We estimate $\boldsymbol{\theta}^* = (\sigma^2 = 1, \theta = 0.2)$ using different realizations.

- We simulate from a zero-mean constrained GP Y using a Matérn 5/2 covariance function such that $Y \in [-1, 1]$.
- Nb of realizations: 100.
- We estimate $\hat{\boldsymbol{\theta}}$ via MLE and CMLE.
- We evaluate the consistently estimable ratio $\rho = \sigma^2/\theta^5$.

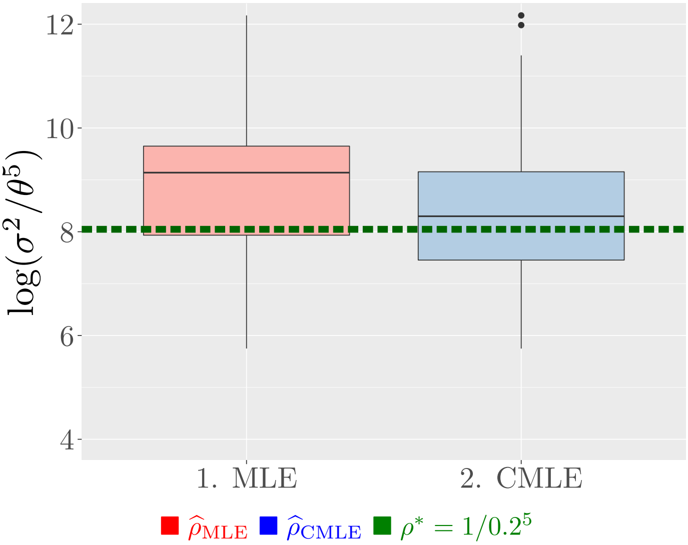
Results: simulation study

Prediction results using (left) MLE and (right) CMLE.



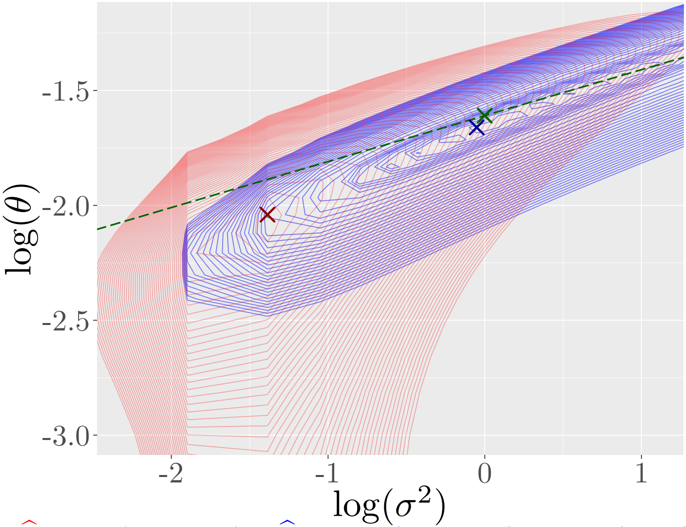
Results: simulation study

Estimation results obtained for each realization.



Results: simulation study

Estimation results obtained using all the realizations.



$\times\widehat{\boldsymbol{\theta}}_{\mathrm{MLE}} = (0.25, 0.13)$ $\times\widehat{\boldsymbol{\theta}}_{\mathrm{CMLE}} = (0.95, 0.19)$ $\times\boldsymbol{\theta}^* = (1, 0.2)$

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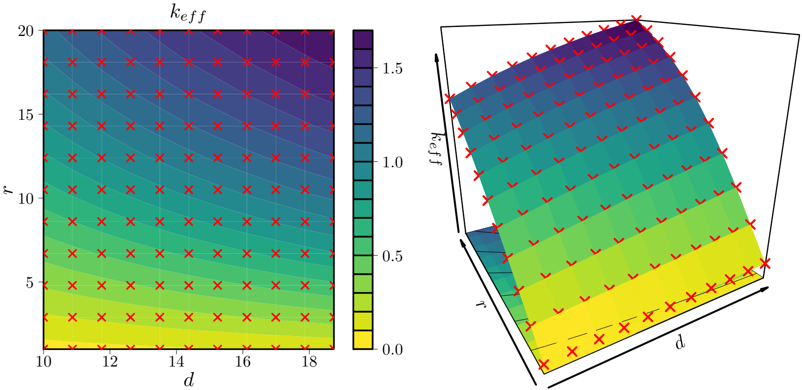
2D example (IRSN)



Nuclear criticality safety assessments: IRSN's dataset.

$\Rightarrow$ k_{eff} is positive and non-decreasing.

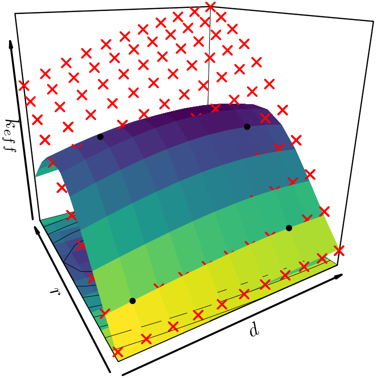
2D example (IRSN)

Procedure:

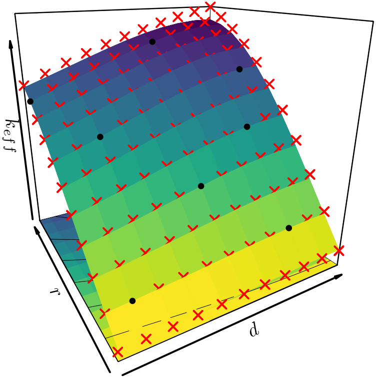
1. We used a Latin hypercube design (LHD) with different number of training points n.
2. We trained unconstrained and constrained models using either MLE or CMLE.
3. For the constrained models, we imposed both positivity and monotonicity constraints.
4. We evaluated their performances over the test points (i.e. $121 - n$).

2D example (IRSN)

Unconstrained model + MLE



(a)

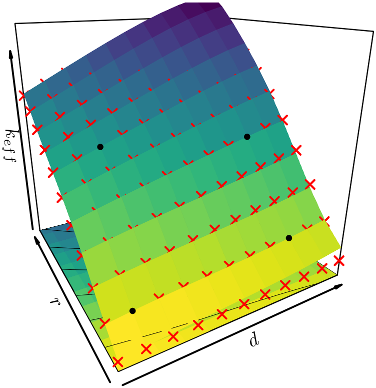


(b)

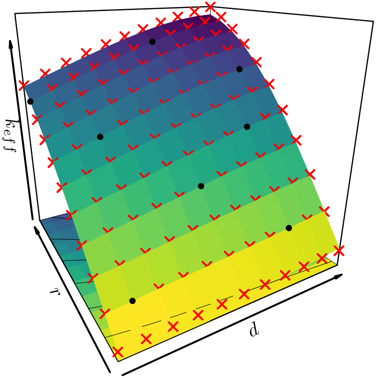
2D Gaussian models for interpolating the IRSN's dataset.

2D example (IRSN)

Constrained model + MLE



(c)

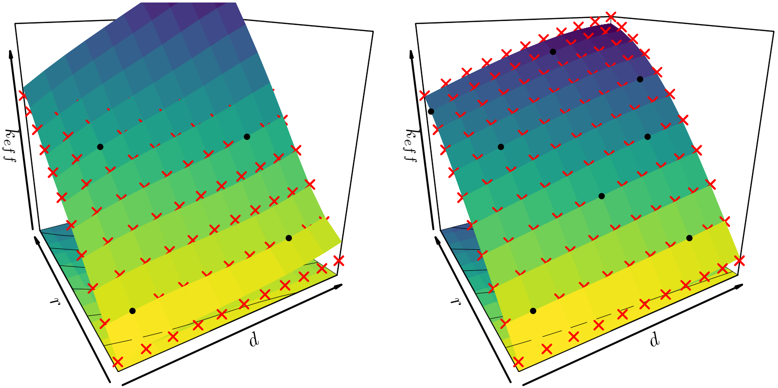


(d)

2D Gaussian models for interpolating the IRSN's dataset.

2D example (IRSN)

Constrained model + CMLE



(e) (f)

2D Gaussian models for interpolating the IRSN's dataset.

2D example (IRSN)

Now, we repeat the procedure for 20 random LHDs, and we compute the Q^2 and predictive variance adequation (PVA) criteria...

2D example (IRSN)

Let n_t be the number of test points, $z_1, \cdots, z_{n_t}$ and $\widehat{z}_1, \cdots, \widehat{z}_{n_t}$ the sets of test and predicted observations (respectively), then...

Q^2 criterion:

$$Q^2 = 1 - \frac{\sum_{i=1}^{n_t} (\widehat{z}_i - z_i)^2}{\sum_{i=1}^{n_t} (\overline{z} - z_i)^2}, \tag{12}$$

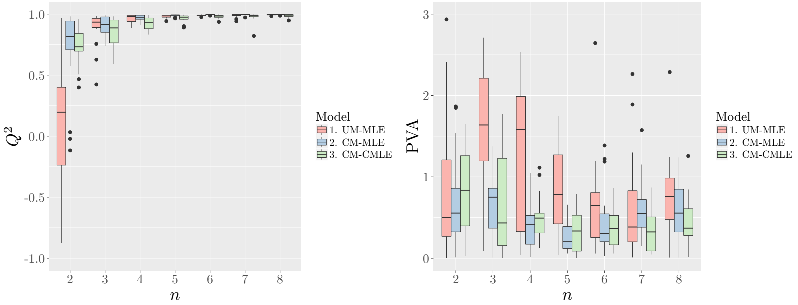
where $\overline{z}$ is the mean of the test data. $\Rightarrow Q^2 \to 1$ ✓

Predictive variance adequation (PVA) criterion:

$$\mathrm{PVA} = \left| \log \left(\frac{1}{n_t} \sum_{i=1}^{n_t} \frac{(\widehat{z}_i - z_i)^2}{\widehat{\sigma}_i^2} \right) \right|, \tag{13}$$

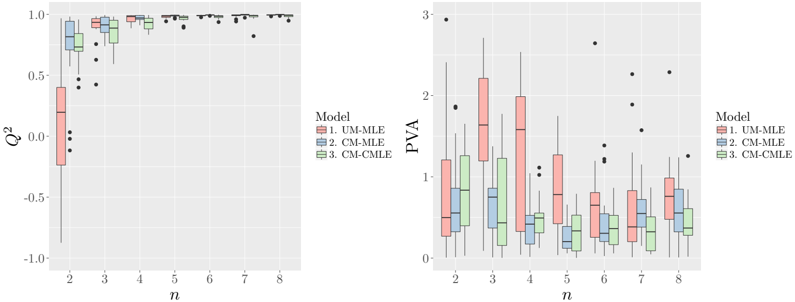
where $\widehat{\sigma}_i^2$ are the predictive variances. $\Rightarrow \mathrm{PVA} \to 0$ ✓

2D example (IRSN)



Assessment of the models for interpolating the IRSN's dataset using different number of training points n and using twenty different Latin hypercube designs.

2D example (IRSN)



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$\Rightarrow$ Unconstrained model was often outperformed by constrained ones.

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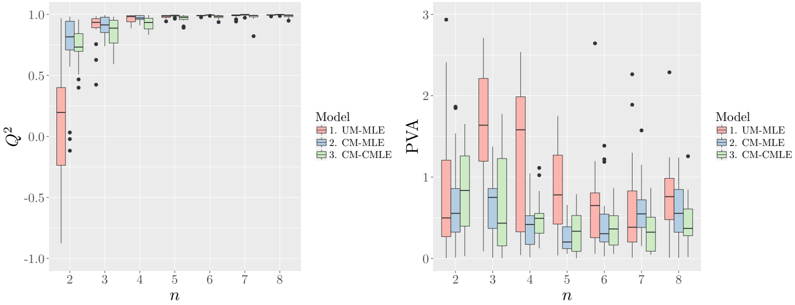

Assessment of the models for interpolating the IRSN's dataset using different number of training points n and using twenty different Latin hypercube designs.

$\Rightarrow$ Unconstrained model was often outperformed by constrained ones.
$\Rightarrow$ MLE achieves a good tradeoff between prediction accuracy and computational cost.

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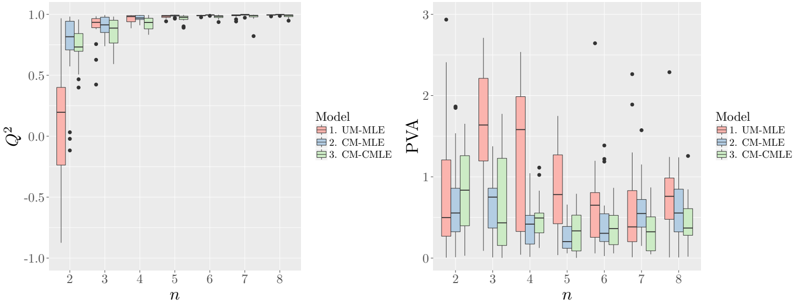

Assessment of the models for interpolating the IRSN's dataset using different number of training points n and using twenty different Latin hypercube designs.

$\Rightarrow$ Unconstrained model was often outperformed by constrained ones.
$\Rightarrow$ MLE achieves a good tradeoff between prediction accuracy and computational cost.
$\Rightarrow$ CMLE is unstable due to numerical approximations.

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Conclusions and Future Works

Conclusions

- We further investigated the approach proposed in (Maatouk and Bay, 2017): now it works for any linear set of inequality constraints in 1D or 2D.
- We proved the consistency of the constrained likelihood for covariance parameter estimation.
- We implemented the R codes: `lineqGP` package.

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✦ Working paper:

López-Lopera, A.F., Bachoc, F., Durrande, N., and Roustant, O. (2017). Finite-dimensional Gaussian approximation with linear inequality constraints. ArXiv e-prints.

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Conclusions and Future Works

Future works

- To find an efficient and more reliable estimator of orthant multinormal distributions

$$\mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m) + \log P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C} | \boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{Y}_m) - \log P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C}).$$

Conclusions and Future Works

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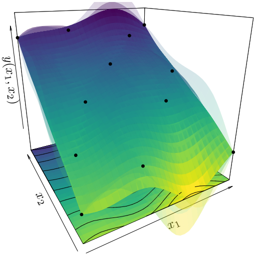
- To work in the full framework for higher dimensions...



For example, in multidimensional problems with specific constrained dimensions.

Conclusions and Future Works

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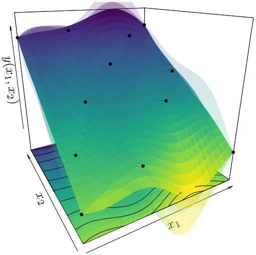

For example, in multidimensional problems with specific constrained dimensions.

- To study more asymptotic properties of the proposed framework.

Acknowledgement

We thank Yann Richet (IRSN) for providing the nuclear criticality safety data. This work is funded by the chair of applied mathematics OQUAIDO (Optimisation et QUAntification d'Incertitude pour les Données Onéreuses).

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