Gaussian Process Regression under Inequality Constraints

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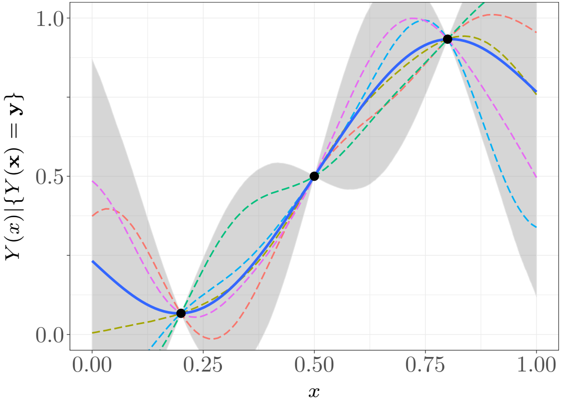
GPs are one of the most famous Bayesian approaches for placing prior distributions over the space of functions (Rasmussen and Williams, 2005).



Mean function
Prediction intervals
⋯ Realizations

- Interpolation conditions

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

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

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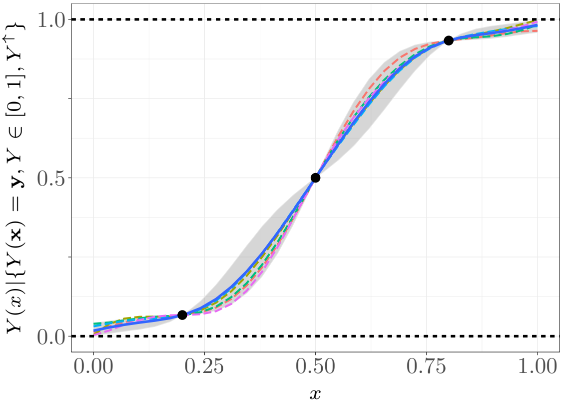


Mean function

Prediction intervals

$\cdots$ Realizations

• Interpolation conditions

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

- - Boundedness condition

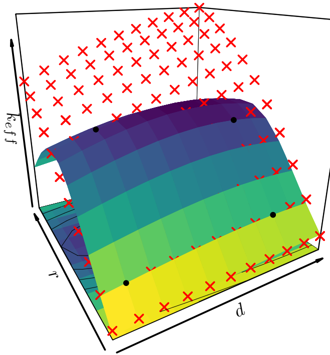
$$Y \in [0, 1]$$

$\uparrow$ Monotonicity condition

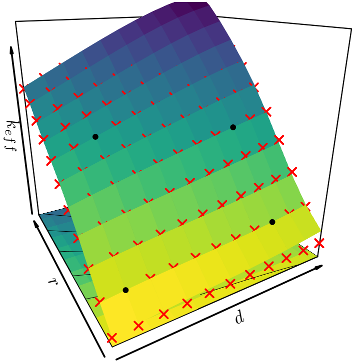
$$Y(x) \leq Y(x'), \quad \forall\, x \leq x'.$$

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

2D models for interpolating the IRSN's dataset using $n = 4$.



(a) Unconstrained GP



(b) GP with positivity & monotonicity

k_{eff}: effective neutron multiplication factor.

● interpolation points ✕ test data

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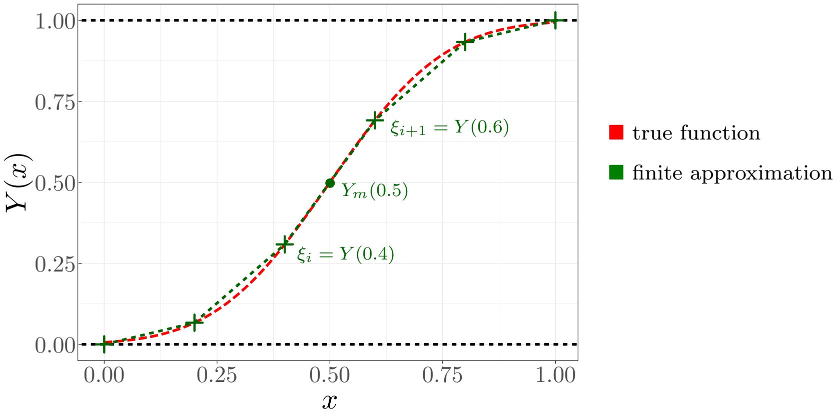
1D finite-dimensional Gaussian approximation

Finite-dimensional representation Y_m: also bounded & monotonic.



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

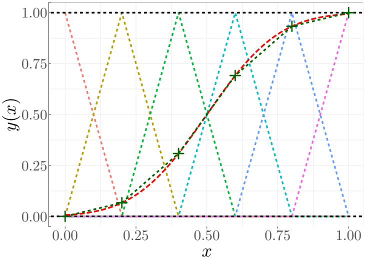
1D finite-dimensional Gaussian approximation

- Let the finite-dimensional Gaussian approximation 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 $i = 1, \cdots, n$; and

- $\boldsymbol{\xi} = [\xi_1, \cdots, \xi_m]^\top \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma}_\theta)$ 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 functions as in (Maatouk and Bay, 2017):



- Since the Gaussianity is preserved for linear operations, we have that

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

where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the mean vector and covariance matrix of the distribution $\boldsymbol{\xi} | \{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}\} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ (Rasmussen and Williams, 2005):

$$\mathbf{K} = \boldsymbol{\Phi}\boldsymbol{\Gamma}\boldsymbol{\Phi}^\top, \quad \boldsymbol{\mu} = \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top\mathbf{K}^{-1}\mathbf{y}, \quad \boldsymbol{\Sigma} = \boldsymbol{\Gamma} - \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top\mathbf{K}^{-1}\boldsymbol{\Phi}\boldsymbol{\Gamma}. \tag{3}$$

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- Then, the posterior distribution follows (López-Lopera et al., 2018)

$$\boldsymbol{\Lambda}\boldsymbol{\xi} | \{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\} \sim \mathcal{TN}(\boldsymbol{\Lambda}\boldsymbol{\mu}, \boldsymbol{\Lambda}\boldsymbol{\Sigma}\boldsymbol{\Lambda}^\top, \boldsymbol{l}, \boldsymbol{u}), \tag{4}$$

✦ The posterior distribution in (4) can be approximated via MC/MCMC (e.g. via Hamiltonian MC–HMC as in Pakman and Paninski, 2014).

- In practice, the posterior mode (MAP solution) can be used as starting point for MCMC algorithms aiming a rapid convergence.
- Let $\boldsymbol{\mu}^*$ be the mode that maximises the pdf $\boldsymbol{\xi}|\{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\}$, i.e.

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

- Then, the MAP estimate of Y_m is given by

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

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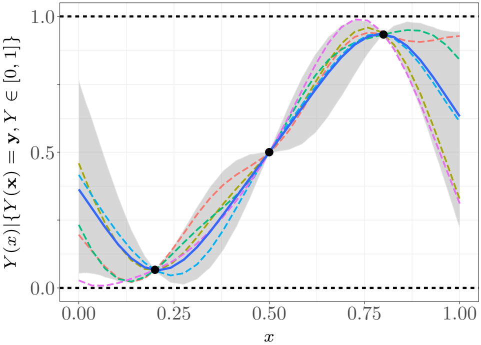
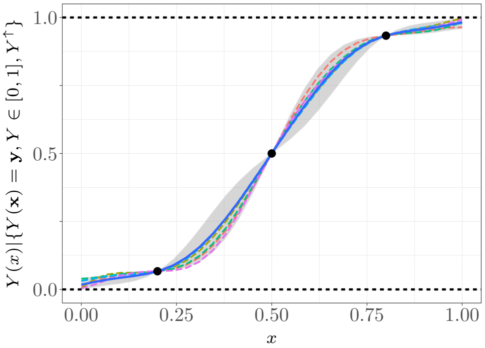
- The benefits of computing $\boldsymbol{\mu}^*$ are:
  - $\boldsymbol{\mu}^*$ can be easily used as a point estimate since its easy calculation,
  - it converges to the spline solution as $m \to \infty$ (Bay et al., 2016).

1D example with boundedness constraints via HMC



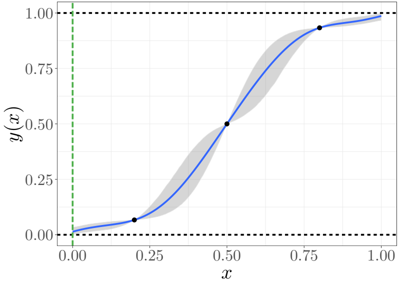
$$\underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}}_{\boldsymbol{l}} \leq \underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\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

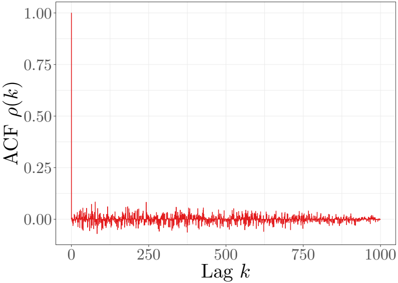
1D example with boundedness & monotonicity constraints via HMC



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

GP under boundedness & monotonicity constraints ($m = 100,\ N = 10^3$)





MC/MCMC Method	CPU Time $[s]$	Effective sampling rate $[s^{-1}]$
(Maatouk and Bay, 2016)	-	-
(Botev, 2017)	73.7	0.012
Gibbs – (Taylor and Benjamini, 2017)	29.0	0.006
HMC – (Pakman and Paninski, 2014)	**12.6**	**0.061**

1D finite-dimensional Gaussian approximation with noisy data

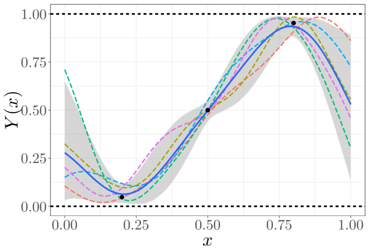
- Noise effects can also be considered (López-Lopera et al., 2019):

$$Y_m(x_i) + \varepsilon_i = y_i \tag{7}$$

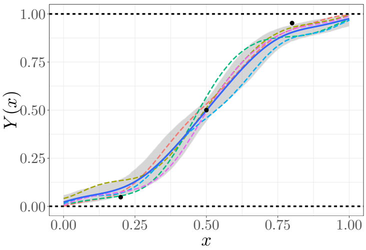
where $x_i \in [0, 1]$, $y_i \in \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}(0, \tau^2)$ with noise variance τ^2.

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

boundedness



boundedness & monotonicity



✦ Adding ε_i leads to more flexible GP models and less restrictive sample spaces improving the performance of MC/MCMC algorithms (López-Lopera et al., 2019).

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- The finite representation Y_m can be scaled to $d \geq 2$ by **tensorisation**:

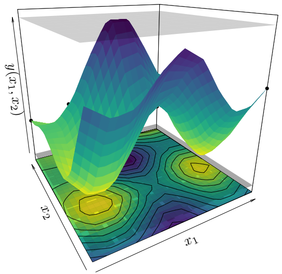
$$Y_m(\mathbf{x}) = \sum_{j_1,\cdots,j_d=1}^{m_1,\cdots,m_d} \left[\prod_{k=1,\cdots,d} \phi_{j_k}^k(x_k) \right] \xi_{j_1,\cdots,j_d}, \text{ s.t. } \begin{cases} Y_m(\mathbf{x}_i) = y_i, \\ \boldsymbol{\xi} \in \mathcal{C}, \end{cases} \tag{8}$$

where $\mathbf{x}_i \in [0,1]^d$, $y_i \in \mathbb{R}$ for $i = 1, \cdots, n$; and

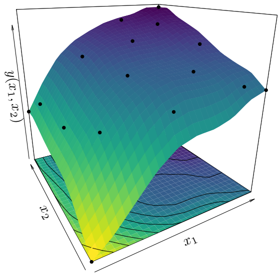
- $\xi_{j_1,\cdots,j_d} := [\xi_{1,\cdots,1}, \ \cdots, \ \xi_{m_1,\cdots,m_d}]^\top \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma}_\theta)$ with covariance $\boldsymbol{\Gamma}_\theta$,
- $\mathcal{C}$ is a convex set of $\mathbb{R}^{m_1 \times \cdots \times m_d}$ composed by a set of linear inequalities,
- $\phi_{j_i}^i : [0,1] \mapsto \mathbb{R}$ are hat basis functions.

Extension to high dimensions: 2D examples

2D Examples under boundedness constr.



2D Examples under monotonicity constr.



● interpolation points ■ predictive mean ■ bounds

MC/MCMC Method	2D boundedness example CPU Time [s]	2D boundedness example Eff. sampling rate [s^{-1}]	2D monotonicity example CPU Time [s]	2D monotonicity example Eff. sampling rate [s^{-1}]
(Maatouk and Bay, 2016)	-	-	-	-
(Botev, 2017)	0.9	1.009	1488.3	0.001
(Taylor and Benjamini, 2017)	9.7	0.088	-	-
(Pakman and Paninski, 2014)	**0.6**	**1.493**	**8.6**	**0.093**

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

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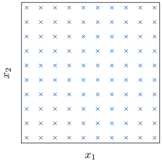
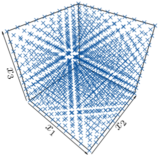
Curse of dimensionality

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



$m = m_1 \times m_2 = 10^2$



$m = m_1 \times m_2 \times m_3 = 10^3$

Extension to high dimensions

Curse of dimensionality

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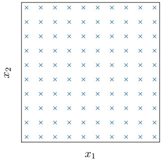
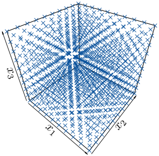
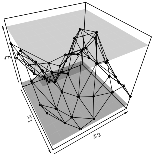


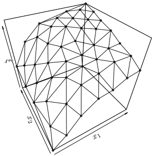


$m = m_1 \times m_2 = 10^2$ $\qquad$ $m = m_1 \times m_2 \times m_3 = 10^3$

However, this downside can be partially mitigated in different ways...

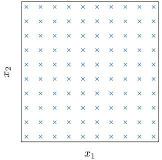
- Using a smarter construction of rectangular grids of the knots.
- Assuming further assumptions for complexity simplification.
  - e.g. inactive dimensions, additive conditions.
- Using other types of designs for the knots: e.g. Delaunay tessellation.

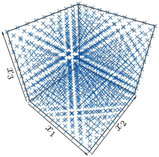




Curse of dimensionality

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





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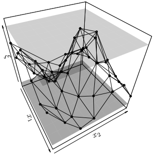
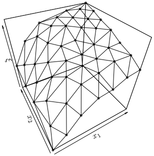
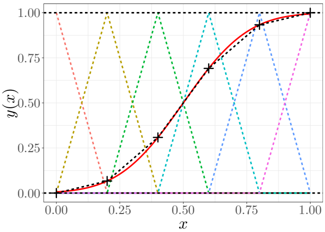
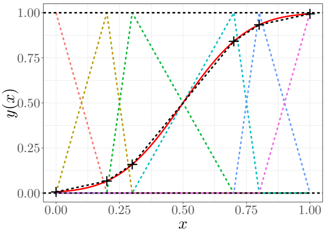




- Using a "smarter" construction of rectangular grids of the knots:



Standard hat basis functions.

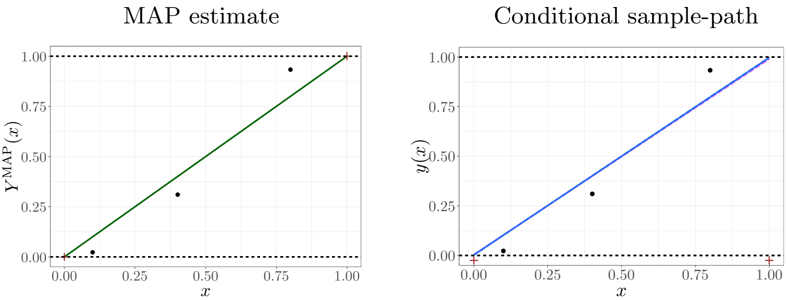


Asymmetric hat basis functions.

✦ This allows refining the grid in places requiring more quality of resolution.

- The "optimal" addition of knots can be achieved by maximising the MAP total-variation (MAP-TV) criterion,

$$t_*^{\mathrm{opt}} = \operatorname{argmax}_{t_*} \int_0^1 [Y_{m_i+1}^{\mathrm{MAP}}(x) - Y_{m_i}^{\mathrm{MAP}}(x)]^2 dx. \tag{9}$$

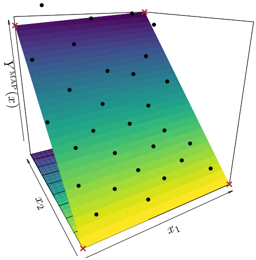


● training points + knots ■ MAP estimate
■ predictive mean ■ 90% confidence intervals

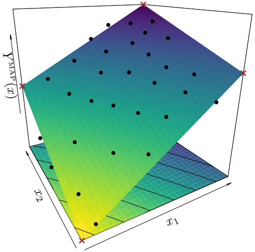
- For the multidimensional case ($d \geq 2$), the MAP-TV criterion is given by,

$$t_*^{\text{opt}} = \operatorname{argmax}_{t_*} \int_{\mathbf{x}\in[0,1]^d} \left[Y_{m_{i+1}}^{\text{MAP}}(\mathbf{x}) - Y_{m_i}^{\text{MAP}}(\mathbf{x})\right]^2 d\mathbf{x}. \tag{10}$$

Toy 1 – MAP estimate
$y(x_1, x_2) = x_2^2$



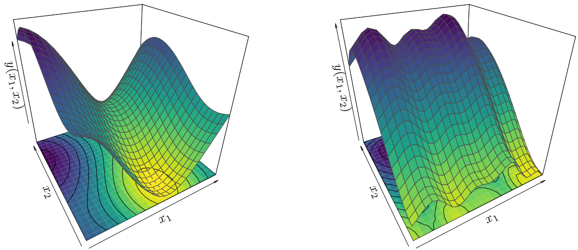
Toy 2 – MAP estimate
$y(x_1, x_2) = \arctan(5x_1) + \arctan(x_2)$



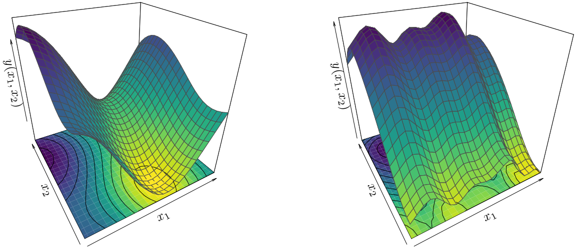
• training points + knots ■ MAP estimate

✦ This construction has been tested up to 5D applications!

Variation II: additive GPs under inequality constraints



2D examples of additive GPs $Y(x_1, x_2) = Y_1(x_1) + Y_2(x_2)$.



2D examples of additive GPs $Y(x_1, x_2) = Y_1(x_1) + Y_2(x_2)$.

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

$$Y(x_1, \cdots, x_d) = \sum_{\kappa=1}^{d} Y_\kappa(x_\kappa), \tag{11}$$

where the Y_κ's are centred GPs on $\mathbb{R}$ with covariances k_κ's.

- Assuming that $Y_1, \cdots, Y_d$ are independent, then Y is also a centred GP with covariance function given by (Durrande et al., 2012)

$$k(x_1, \cdots, x_d; x_1', \cdots, x_d') = \sum_{\kappa=1}^{d} k_\kappa(x_\kappa, x_\kappa').$$

- Assume that Y exhibits certain inequalities along each Y_κ, then Y_m is

$$Y_m(x_1, \cdots, x_d) = \sum_{\kappa=1}^{d} Y_\kappa^{m_\kappa}(x_\kappa), \ \text{s.t.} \ \begin{cases} Y_m(x_1^i, \cdots, x_d^i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}^\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{12}$$

where $(x_1^i, \cdots, x_d^i) \in [0,1]^d$, $y_i \in \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}\left(0, \tau^2\right)$ for $i = 1, \cdots, n$.

- Assume that Y exhibits certain inequalities along each Y_κ, then Y_m is

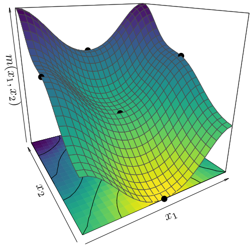
$$Y_m(x_1, \cdots, x_d) = \sum_{\kappa=1}^{d} Y_\kappa^{m_\kappa}(x_\kappa), \text{ s.t. } \begin{cases} Y_m(x_1^i, \cdots, x_d^i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}^\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{12}$$

where $(x_1^i, \cdots, x_d^i) \in [0,1]^d$, $y_i \in \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}\left(0, \tau^2\right)$ for $i = 1, \cdots, n$.

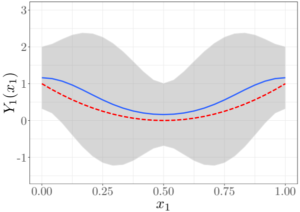
2D toy: $Y(x_1, x_2) = \underbrace{4(x_1 - 0.5)^2}_{Y_1(x_1)} + \underbrace{2x_2}_{Y_2(x_2)}$

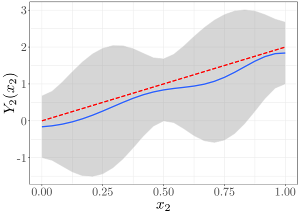
Predictive mean without constraints

$$m(x_1, x_2) = m_1(x_1) + m_2(x_2)$$



$(\sigma_1^2, \ell_1) = (\sigma_2^2, \ell_2) = (1, 0.2)$





- Assume that Y exhibits certain inequalities along each Y_κ, then Y_m is

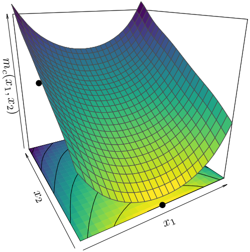
$$Y_m(x_1, \cdots, x_d) = \sum_{\kappa=1}^{d} Y_\kappa^{m_\kappa}(x_\kappa), \text{ s.t. } \begin{cases} Y_m(x_1^i, \cdots, x_d^i) + \varepsilon_i = y_i, \\ \boldsymbol{\xi}^\kappa \in \mathcal{C}_\kappa, \end{cases} \tag{12}$$

where $(x_1^i, \cdots, x_d^i) \in [0,1]^d$, $y_i \in \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}\left(0, \tau^2\right)$ for $i = 1, \cdots, n$.

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

Predictive mean with constraints

$m_c(x_1, x_2) = m_{c,1}(x_1) + m_{c,2}(x_2)$



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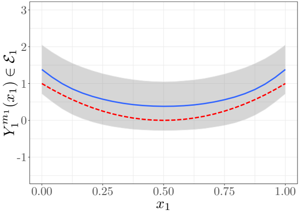
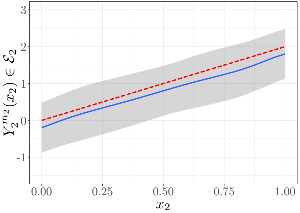
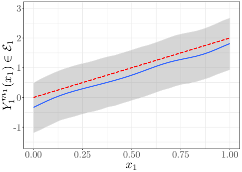


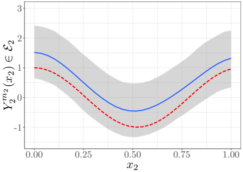


5D Toy example:

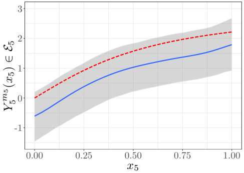
$$Y(x_1, \cdots, x_5) = \underbrace{2x_1}_{Y_1(x_1)} + \underbrace{\cos(6x_2)}_{Y_2(x_2)} + \underbrace{2x_3^2}_{Y_3(x_3)} + \underbrace{4(x_4 - 0.5)^2}_{Y_4(x_4)} + \underbrace{2\arctan(2x_5)}_{Y_5(x_5)}$$



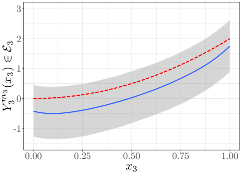
(a) Monotonicity



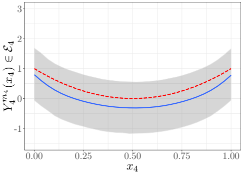
(b) No constraints



(e) Monotonicity



(c) Convexity



(d) Convexity

- We used 25 points from a maximin LHS.
- For κ=1,$\cdots$,5, we fixed $(\sigma_\kappa^2, \ell_\kappa) = (1, 0.2)$.

✦ Higher dimensions can be considered since HMC is performed in 1D!

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- The GP covariance parameters $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ can be estimated via maximum likelihood (Stein, 1999).
  - Consider the observation vector

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

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

$$\mathcal{L}_n(\boldsymbol{\theta}) = -\frac{1}{2}\log(\det(\mathbf{R}_{\boldsymbol{\theta}})) - \frac{1}{2}\mathbf{Y}_n^\top \mathbf{R}_{\boldsymbol{\theta}}^{-1}\mathbf{Y}_n - \frac{n}{2}\log 2\pi, \tag{13}$$

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

- Then, the MLE is given by

$$\widehat{\boldsymbol{\theta}}_n \in \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{argmax}\ \mathcal{L}_n(\boldsymbol{\theta}). \tag{14}$$

✗ Notice that the MLE does not take into account the inequality conditions.

- We studied a constrained likelihood in (López-Lopera et al., 2018).
  - 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:

$$\begin{aligned} \mathcal{L}_{n,c}(\boldsymbol{\theta}) &= \log \frac{p_{\boldsymbol{\theta}}(\mathbf{Y}_n) p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n)}{p_{\boldsymbol{\theta}}(Y \in \mathcal{E})} \\ &= \mathcal{L}_n(\boldsymbol{\theta}) + \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n) - \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E}). \end{aligned} \tag{15}$$

- Then, the cMLE is given by

$$\widehat{\boldsymbol{\theta}}_{n,c} \in \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{argmax}\ \mathcal{L}_{n,c}(\boldsymbol{\theta}). \tag{16}$$

✓ Note that the cMLE accounts for the inequality constraints.

- The terms $p_{\boldsymbol{\theta}}(Y \in \mathcal{E} | \mathbf{Y}_n)$ and $p_{\boldsymbol{\theta}}(Y \in \mathcal{E})$ have to be approximated via MC.

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Consistency of the MLE & cMLE

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

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

corresponding to boundedness, monotonicity, and convexity constraints.

- We consider $\boldsymbol{\theta}_0$ as the true unknown covariance parameters.

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

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Proposition (Asymptotic consistency of cMLE, López-Lopera et al. (2018))

Assume mild conditions (López-Lopera et al., 2018). Assume $\forall \varepsilon > 0$ and $\forall M < \infty$, (Consistency of the unconditional ML)

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

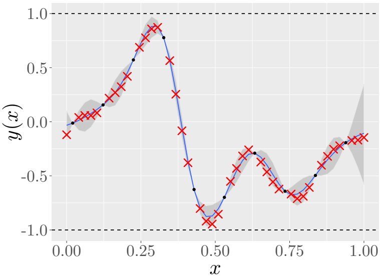
Then, (Consistency of the conditional cML)

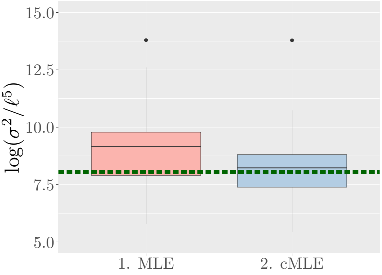
$$P\left(\sup_{\|\boldsymbol{\theta} - \boldsymbol{\theta}_0\| \geq \varepsilon} (\mathcal{L}_{n,c}(\boldsymbol{\theta}) - \mathcal{L}_{n,c}(\boldsymbol{\theta}_0)) \geq -M \;\middle|\; Y \in \mathcal{E}_\kappa \right) \xrightarrow[n \to +\infty]{} 0.$$

Consequently, both MLE and cMLE are consistent estimators

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

Assessment of the MLE and cMLE for **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 $\log(\sigma^2/\ell^5)$

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

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

with known correlation function k_1 and true variance parameter σ_0^2.

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Theorem (Asymptotic normality of MLE, Bachoc et al. (2018))

Assume mild conditions (Bachoc et al., 2018). 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 $\kappa = 0, 1, 2$,

$$\sqrt{n}\left(\widehat{\sigma}_n^2 - \sigma_0^2\right) \xrightarrow[n \to +\infty]{\mathcal{L}|Y \in \mathcal{E}_\kappa} \mathcal{N}(0, 2\sigma_0^4). \quad (17)$$

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Theorem (Asymptotic normality of cMLE, Bachoc et al. (2018))

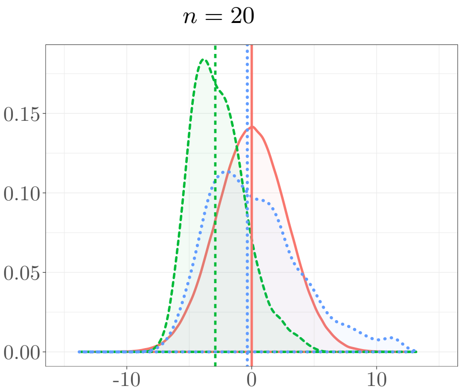
The cMLE $\widehat{\sigma}_{n,c}^2$ of σ_0^2 conditioned on $\{Y \in \mathcal{E}_\kappa\}$ is also asymptotically Gaussian distributed. More precisely, for $\kappa = 0, 1, 2$,

$$\sqrt{n}\left(\widehat{\sigma}_{n,c}^2 - \sigma_0^2\right) \xrightarrow[n \to +\infty]{\mathcal{L}|Y \in \mathcal{E}_\kappa} \mathcal{N}(0, 2\sigma_0^4). \tag{18}$$

✦ These results can be extended for the Matérn models (Bachoc et al., 2018).

Asymptotic normality of the MLE and cMLE: numerical illustration.

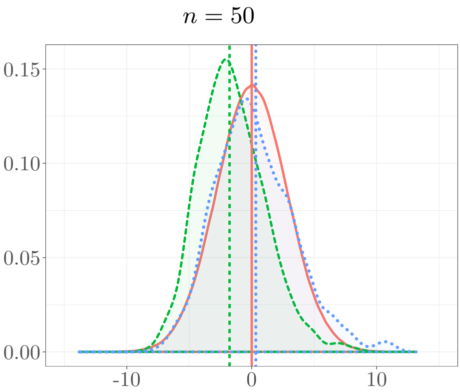
Assessment of the MLE and cMLE normality for **10^3 trajectories** drawn from a constrained. GP $Y \in [0, 1]$ with Matérn 5/2 kernel and parameters $\boldsymbol{\theta}_0 = (\sigma_0^2 = 0.2, \ell = 0.2)$.



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

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

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 $\boldsymbol{\theta}_0 = (\sigma_0^2 = 0.2, \ell = 0.2)$.



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✦ **cMLE** converges faster to the limit Gaussian distribution.

Asymptotic normality of the MLE and cMLE: numerical illustration.

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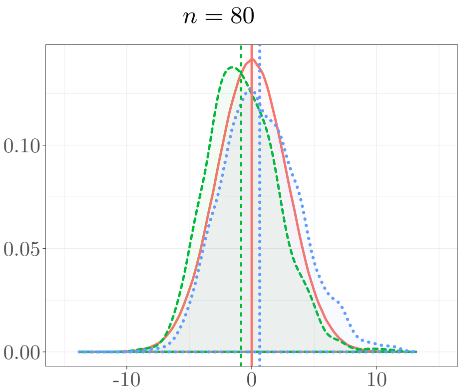

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✦ For large values of n , **MLE** and **cMLE** provide similar performances.

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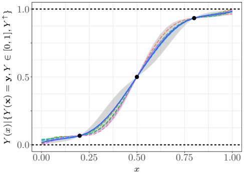
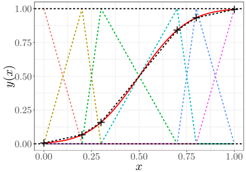
Conclusions

- We further investigated (Maatouk and Bay, 2017) to account for sets of linear inequality constraints.



- We explored the use of MCMC (i.e. HMC) for the posterior approximation.

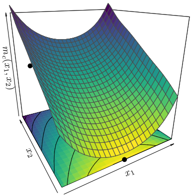


- We proposed variations of the model in high dimensions:
  - Noisy data,
  - “Optimal” rectangular designs,
  - Additive functions.

- We studied a constrained likelihood analysing their consistency and asymptotic normality.

$$\mathcal{L}_{n,c}(\boldsymbol{\theta}) = \mathcal{L}_n(\boldsymbol{\theta}) + \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E}|\mathbf{Y}_n) - \log p_{\boldsymbol{\theta}}(Y \in \mathcal{E}).$$

  - **cMLE** is suggested for small number of obs n.
  - **MLE** can also be used when n is large.



Papers, technical reports & R packages

- ✦ A.F. López-Lopera, F. Bachoc, N. Durrande, and O. Roustant (2018). *Finite-dimensional Gaussian approximation with linear inequality constraints.* SIAM/ASA Journal on Uncertainty Quantification, 6(3): 1224–1255.
- – A.F. López-Lopera, F. Bachoc, N. Durrande, and O. Roustant (+2019). *Approximating Gaussian process emulators with linear inequality constraints and noisy observations via MC and MCMC.* (submitted).
- – F. Bachoc, A. Lagnoux, and A.F. López-Lopera (+2018). *Maximum likelihood estimation for Gaussian processes under inequality constraints* (submitted).
- ✦ A.F. López-Lopera. *LineqGPR: Gaussian process regression models with linear inequality constraints*, 2018. CRAN.

Working papers

- A.F. López-Lopera, F. Bachoc, N. Durrande, and O. Roustant (2019+). *Additive Gaussian processes under linear inequality constraints.*
- — (2019+). *Optimal grid construction for finite-dimensional Gaussian approximations under inequality constraints.*
- — (2019+). *Finite element methods for Gaussian processes under inequality constraints.*

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