Metamodeling under Inequality Constraints

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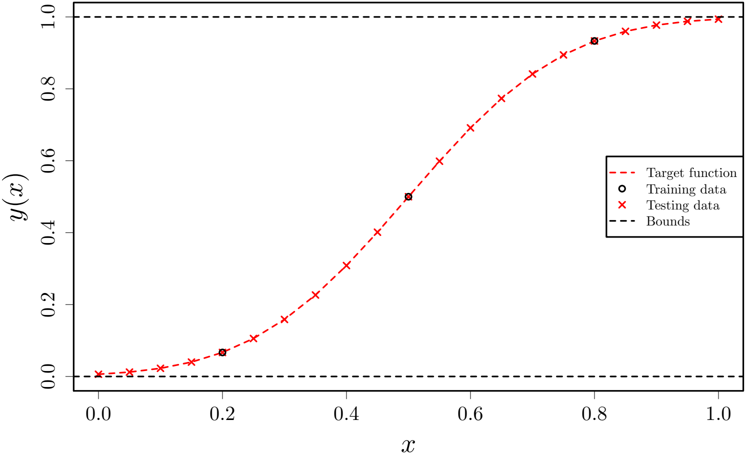
Motivation

Toy example. $y(x) = \frac{1}{2}\left[1 + \operatorname{erf}\left\{\frac{x-0.5}{0.2\sqrt{2}}\right\}\right]$ (Gaussian CDF).



$\Rightarrow$ Data are bounded and monotonic!!

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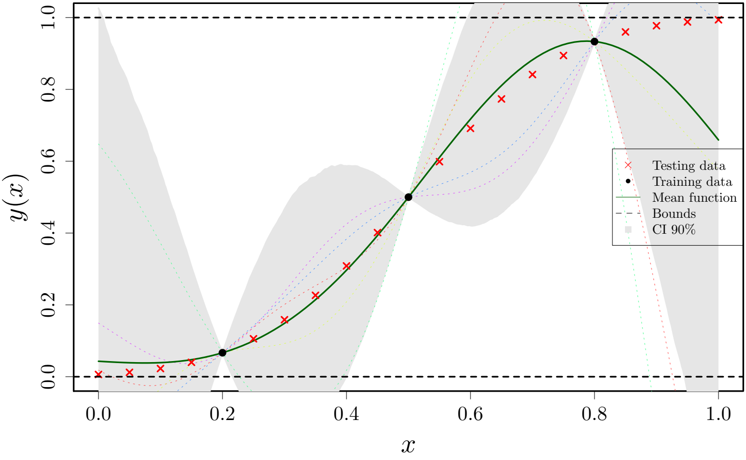

Unconstrained Kriging

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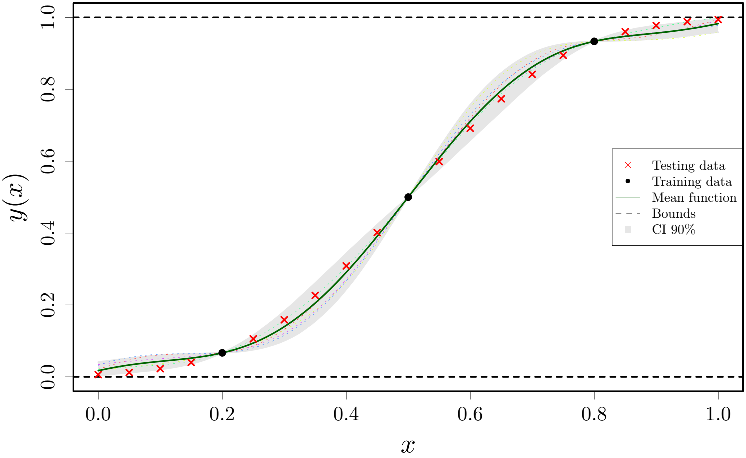

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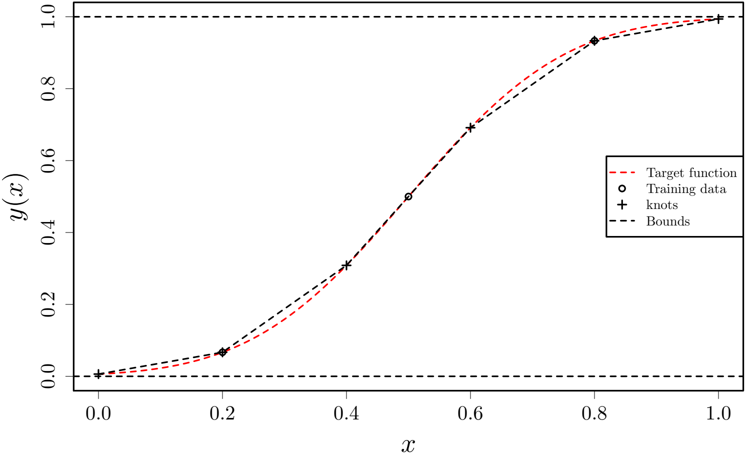
Constrained Kriging: finite-dimensional approximation

Figure: toy example $y(x) = \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF).



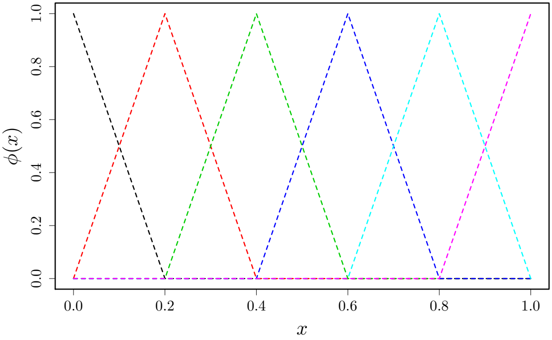
$\Rightarrow$ The finite approx. is also bounded and monotonic!!

Constrained Kriging: Maatouk and Bay (2016)

Let the finite-one-dimensional GP-based 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.



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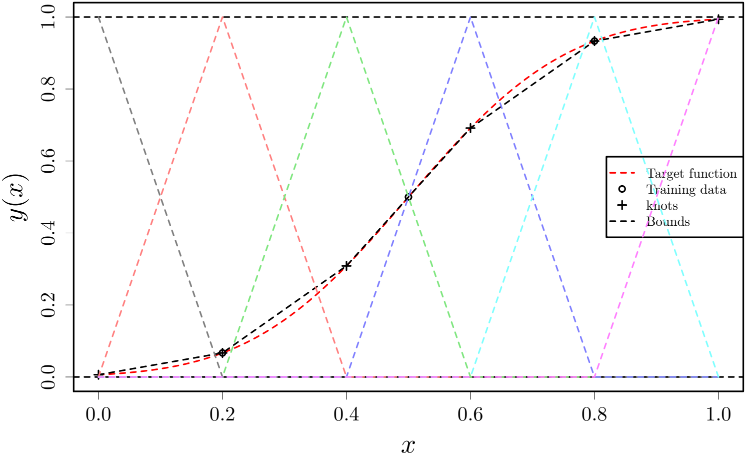

Finite-dimensional approximation.

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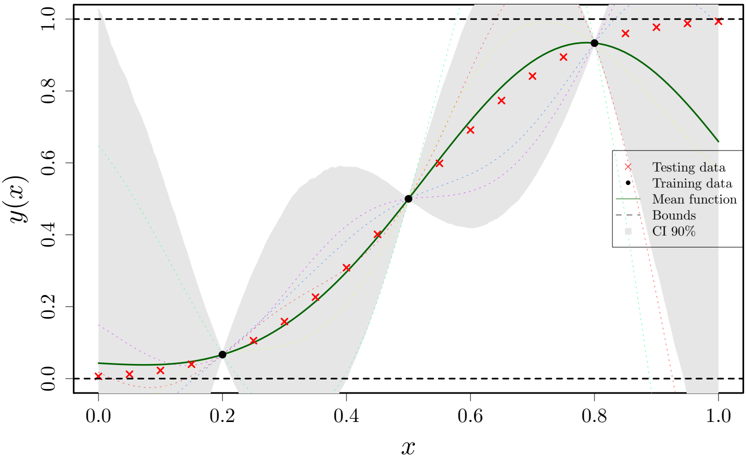

Unconstrained GP.

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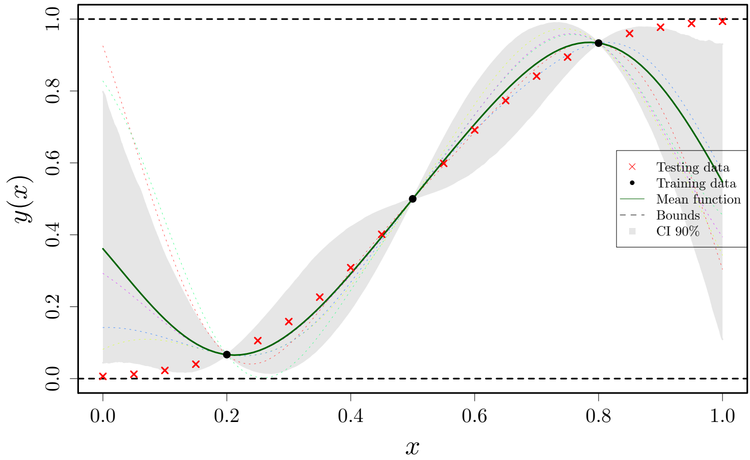
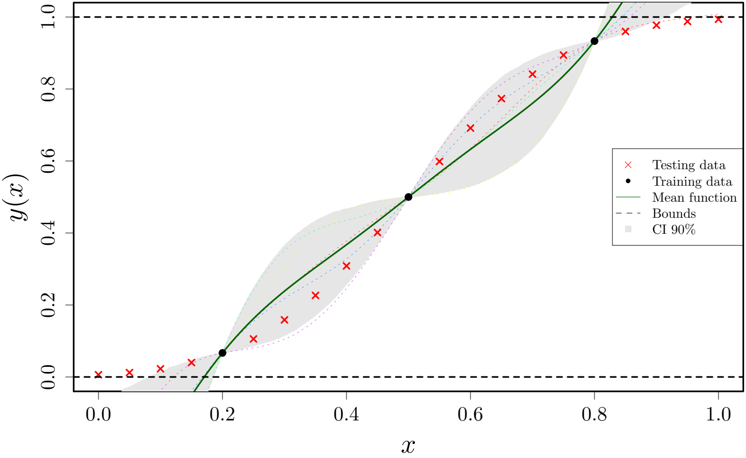


Constrained GP with boundedness constraint.

Constrained Kriging: finite-dimensional approximation

Figure: toy example $y(x) = \Phi(\frac{x-0.5}{0.2})$ (Gaussian CDF).



Constrained GP with monotonicity constraint.

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Old contributions (Nice, 2017)

1. First, since $Y_m \in \mathcal{E} \Leftrightarrow \boldsymbol{\xi} \in \mathcal{C}$, and assuming that $\mathcal{C}$ is composed by a set of q linear inequalities of the form

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

the posterior distribution is given by a truncated multinormal

$$\boldsymbol{\Lambda}\boldsymbol{\xi} | \{\boldsymbol{\Phi}\boldsymbol{\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda}\boldsymbol{\xi} \leq \boldsymbol{u}\} \sim \mathcal{TN}\left(\boldsymbol{\Lambda}\boldsymbol{\mu},\ \boldsymbol{\Lambda}\boldsymbol{\Sigma}\boldsymbol{\Lambda}^\top,\ \boldsymbol{l},\ \boldsymbol{u}\right), \qquad (1)$$

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

$$\boldsymbol{\mu} = \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top [\boldsymbol{\Phi}\boldsymbol{\Gamma}\boldsymbol{\Phi}^\top]^{-1}\mathbf{y}, \quad \text{and} \quad \boldsymbol{\Sigma} = \boldsymbol{\Gamma} - \boldsymbol{\Gamma}\boldsymbol{\Phi}^\top [\boldsymbol{\Phi}\boldsymbol{\Gamma}\boldsymbol{\Phi}^\top]^{-1}\boldsymbol{\Phi}\boldsymbol{\Gamma}. \qquad (2)$$

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$\Rightarrow$ The distribution of Equation (1) can be approximated using MCMC.

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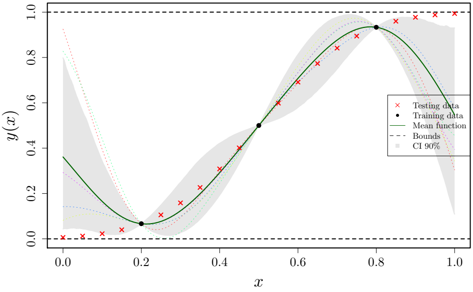
$\Rightarrow$ The distribution of Equation (1) can be approximated using MCMC.

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

Old contributions (Nice, 2017)

Boundedness constraint: $y(x) = \Phi(\frac{x-0.5}{0.2})$.



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

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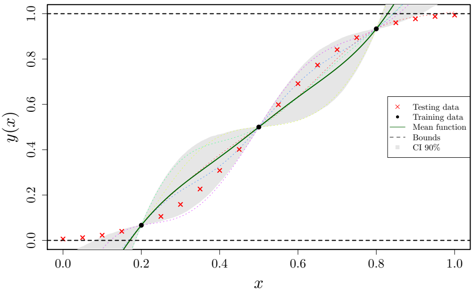
Monotonicity constraint: $y(x) = \Phi(\frac{x-0.5}{0.2})$.



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

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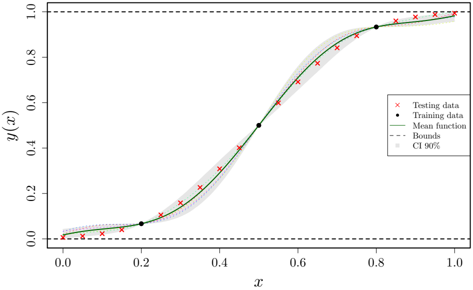
Boundedness and monotonicity constraints: $y(x) = \Phi(\frac{x-0.5}{0.2})$.



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

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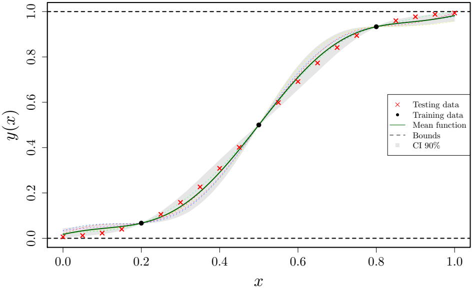

or simply,

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

Old contributions (Nice, 2017)

2. Second, the truncated multinormal $\boldsymbol{\Lambda\xi}|\{\boldsymbol{\Phi\xi} = \mathbf{y}, \boldsymbol{l} \leq \boldsymbol{\Lambda\xi} \leq \boldsymbol{u}\}$ can be sampled efficiently via Hamiltonian Monte-Carlo (HMC) (Pakman and Paninski, 2014).

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$\Rightarrow$ Denoting $\boldsymbol{\eta} = \boldsymbol{\Lambda\xi}$ with $\boldsymbol{\Lambda}$ injective, notice that the samples of $\boldsymbol{\xi}$ can be obtained using the samples of $\boldsymbol{\eta}$ by solving the linear system.

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3. Third, a constrained likelihood was suggested empirically

$$\begin{aligned}
\mathcal{L}_{\mathcal{C},m}(\boldsymbol{\theta}) &= \log p_{\boldsymbol{\theta}}(\mathbf{Y}_m | \boldsymbol{\xi} \in \mathcal{C}) \\
&= \log \frac{p_{\boldsymbol{\theta}}(\mathbf{Y}_m) P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C} | \boldsymbol{\Phi\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\xi} = \mathbf{Y}_m) - \log P_{\boldsymbol{\theta}}(\boldsymbol{\xi} \in \mathcal{C}).
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$\Rightarrow$ unconstrained log-likelihood.

$\Rightarrow$ truncated multinormals to be estimated!!

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\end{aligned}$$

$\Rightarrow$ unconstrained log-likelihood.
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4. Finally, the full framework was assessed under different inequality constraints in synthetic examples.

Old contributions (Nice, 2017)

In this sense, we proposed at (Nice, 2017):

- to implement a gradient-based method to estimate automatically the covariance parameters of the model;
- to investigate theoretical properties of the proposed constrained likelihood;
- to evaluate the proposed approach with real-world datasets;
- to build an R package;
- and to extend this approach when the input space is multi-dimensional, i.e. $\mathbf{x} \in [0\ 1]^d$.

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- to investigate theoretical properties of the proposed constrained likelihood; ✓
- to evaluate the proposed approach with real-world datasets; ✓
- to build an R package; ✓
- and to extend this approach when the input space is multi-dimensional, i.e. $\mathbf{x} \in [0\ 1]^d$. **2D ✓ More than 2D ✗**

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Maximum likelihood (ML): asymptotic properties.

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)

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

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Finite-dimensional approximation for 2D input spaces

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

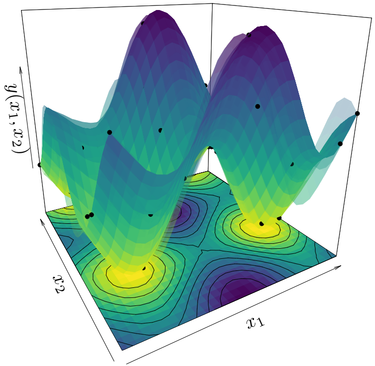
$$Y_{m_1,m_2}(x_1,x_2) := \sum_{j_1=1}^{m_1}\sum_{j_2=1}^{m_2} \xi_{j_2,j_1}\phi^1_{j_1}(x_1)\phi^2_{j_2}(x_2), \text{ s.t. } \begin{cases} Y_{m_1,m_2}\left(x_1^i, x_2^i\right) = y_i, \\ \xi_{j_2,j_1} \in \mathcal{C}, \end{cases}$$

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 $\boldsymbol{\Gamma}$.

Finite-dimensional approximation for 2D input spaces

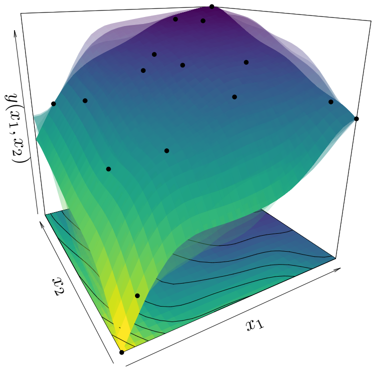
Boundedness in 2D.



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

Finite-dimensional approximation for 2D input spaces

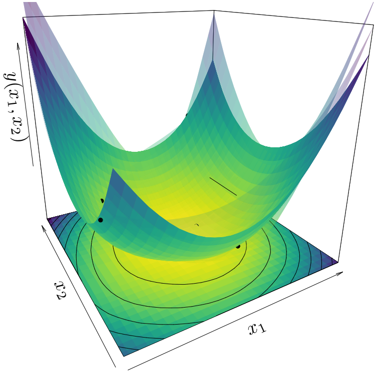
Monotonicity in 2D.



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

Finite-dimensional approximation for 2D input spaces

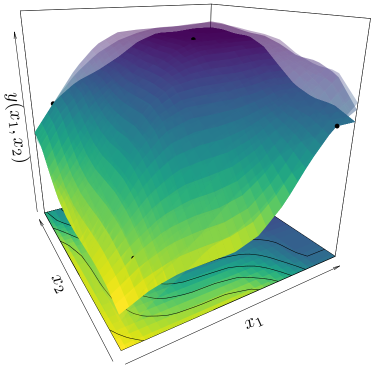
Convexity in 2D (a weak version).



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

Finite-dimensional approximation for 2D input spaces

Boundedness and monotonicity in 2D.



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

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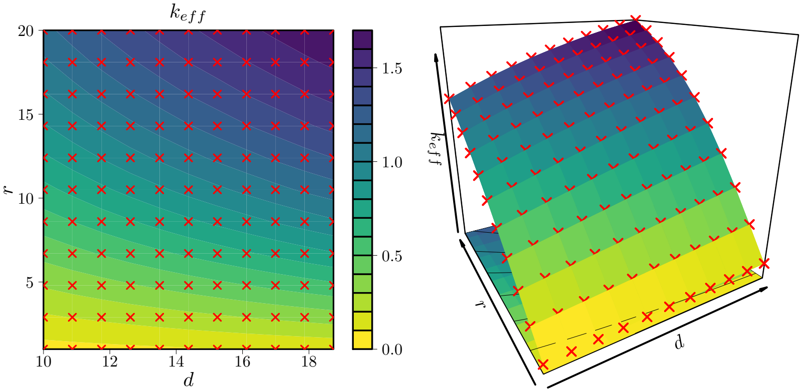
2D example (IRSN)



Nuclear criticality safety assessments: IRSN's dataset.

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

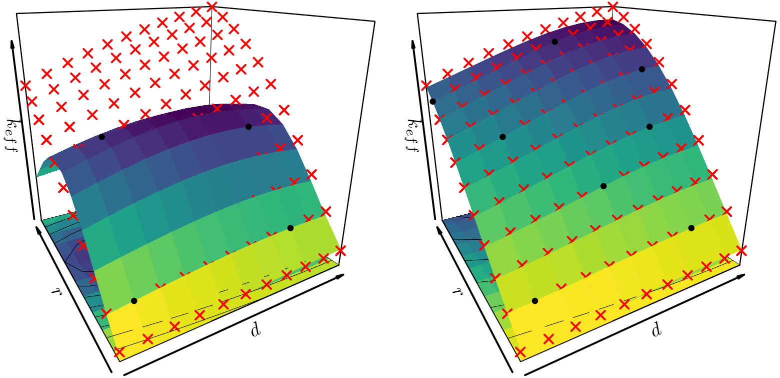
2D example (IRSN)

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

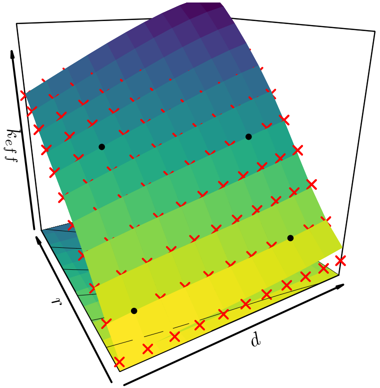


(a) (b)

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

2D example (IRSN)

Constrained model + MLE

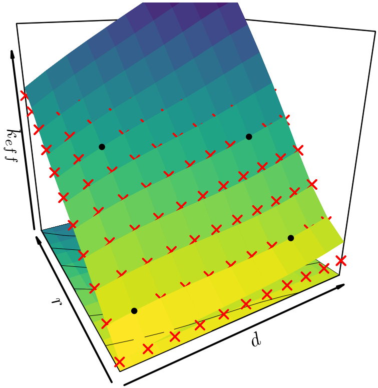


(c) (d)

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:

$$Q^2 = 1 - \frac{\sum_{i=1}^{n_t} (\widehat{z}_i - z_i)^2}{\sum_{i=1}^{n_t} (\overline{z} - z_i)^2}, \tag{3}$$

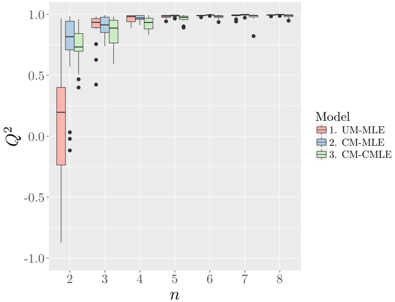
where $\overline{z}$ is the mean of the test data. $\Rightarrow Q^2 \to 1$ ✓

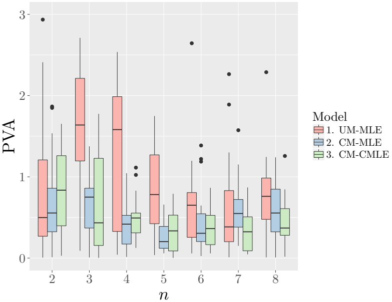
Predictive variance adequation (PVA) criterion:

$$\mathrm{PVA} = \left| \log \left(\frac{1}{n_t} \sum_{i=1}^{n_t} \frac{(\widehat{z}_i - z_i)^2}{\widehat{\sigma}_i^2} \right) \right|, \tag{4}$$

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

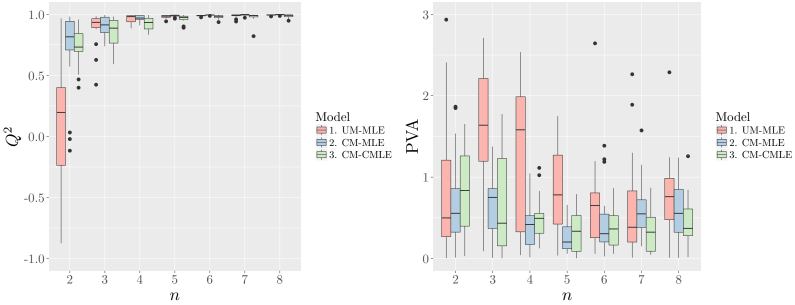
2D example (IRSN)





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

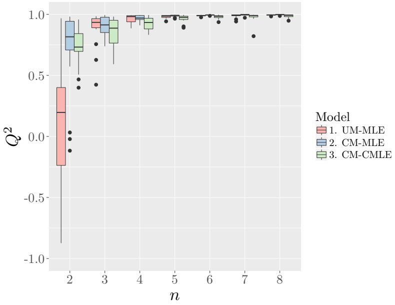
2D example (IRSN)

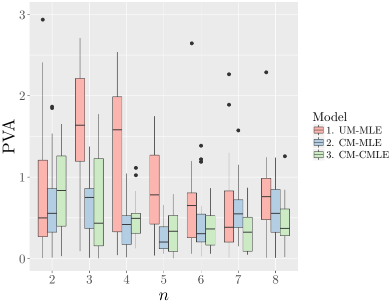


Assessment of the models for interpolating the IRSN's dataset using different number of training points n and using twenty different Latin hypercube designs.

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

2D example (IRSN)

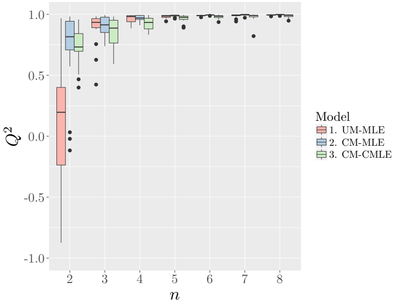


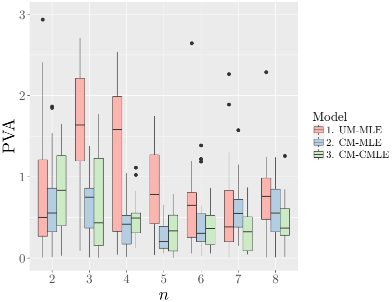


Assessment of the models for interpolating the IRSN's dataset using different number of training points n and using twenty different Latin hypercube designs.

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

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.

$\Rightarrow$ 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 (second round!!).

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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. (Bon courage!!)

Conclusions and Future Works

Future works

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

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

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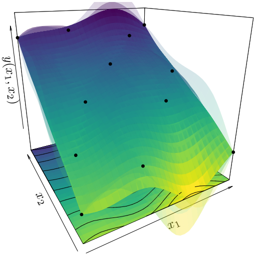
- To work in the full framework for higher dimensions...



For example, in multidimensional problems with specific constrained dimensions.

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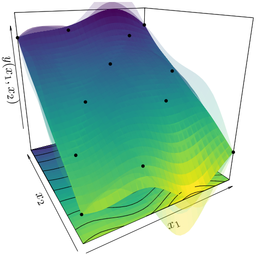

For example, in multidimensional problems with specific constrained dimensions.

- To study more asymptotic properties of the proposed framework.

Acknowledgement

We thank Yann Richet (IRSN) for providing the nuclear criticality safety data.

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