Block-Additive constrained Gaussian processes

July, 2025

Workshop on Gaussian processes and related topics

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· **Transform functional constraints into finite dimensional linear constraints:** Given a family of functions $\mathbf{\Phi} := (\phi_1, \cdots, \phi_m)$ (e.g. hat functions):

$$\underset{\text{Infinite Dimensional}}{\boxed{f \in \mathcal{C}}} \quad \longrightarrow \quad \underset{\text{Finite Dimensional}}{\boxed{\Pi_{\mathbf{\Phi}}(f) = \mathbf{\Phi}^\top \boldsymbol{\alpha} \in \mathcal{C}}} \quad \Longleftrightarrow \quad \underset{\text{Linear Constraints}}{\boxed{\mathbf{\Lambda}\boldsymbol{\alpha} \leqslant \boldsymbol{b}}}$$

Summary on finite dimensional constrained GPs

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Infinite Dimensional — Finite Dimensional — Linear Constraints

· **Solve a Quadratic Programming Problem:** $\mathcal{Y}$ the GP, $\boxed{\widetilde{\mathcal{Y}}_{\mathbf{\Phi}} := \Pi_{\mathbf{\Phi}}(\mathcal{Y})}$ the finite dimensional GP, $(\mathbf{X}, \mathbf{Y})$ the observations, the constrained predictor is $\widehat{f}_{\mathbf{\Phi}}$:

$$\boxed{\mathrm{mod}(\widetilde{\mathcal{Y}}_{\mathbf{\Phi}} \mid \widetilde{\mathcal{Y}}_{\mathbf{\Phi}}(\mathbf{X}) + \boldsymbol{\epsilon} = \mathbf{Y}, \widetilde{\mathcal{Y}}_{\mathbf{\Phi}} \in \mathcal{C})} \Longleftrightarrow \boxed{\arg\min \{\|\boldsymbol{\alpha} - \boldsymbol{\mu}\|^2_{\mathbf{\Gamma}} \mid \mathbf{\Lambda}\boldsymbol{\alpha} \leqslant \boldsymbol{b}\}}$$

Find the Max Of Distribution — Solve the Quadratic Problem

Summary on finite dimensional constrained GPs

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Find the Max Of Distribution — Solve the Quadratic Problem

· **The computational cost depends on the Dimension:** The Quadratic Programming Problem can be solved in $\boxed{\mathcal{O}(M^{3.5})}$ operations where $M = |\boldsymbol{\Phi}|$.

Theorem (From finite to infinite dimension, Bay et al. [2016]))

For a convex set $\mathcal{C}$ if natural assumptions over the families $(\mathbf{\Phi}_m)_{m\in\mathbb{N}}$ are satisfied:

- ***Density***: $\overline{\cup_{m\in\mathbb{N}} \operatorname{span} \mathbf{\Phi}_m} = \mathcal{H}_{\mathcal{Y}}$, *($\mathcal{H}_{\mathcal{Y}}$ is the RKHS associated to the GP $\mathcal{Y}$)*
- ***Stability***: $\Pi_{\mathbf{\Phi}_m}(\mathcal{C}) \subset \mathcal{C}$, $\forall m \in \mathbb{N}$
- ***Existence***: $\exists f \in \mathcal{H}_{\mathcal{Y}}$, *s.t.* $f(\mathbf{X}) = \mathbf{Y}$ *and* $f \in \mathcal{C}$

Then, the following asymptotic result holds:

$$\boxed{\widehat{f}_{\mathbf{\Phi}_m} \underset{m\to\infty}{\longrightarrow} f^\star := \arg\min\{\|f\|_{\mathcal{H}_{\mathcal{Y}}} \mid f(\mathbf{X}) = \mathbf{Y}, f \in \mathcal{C}\}}.$$

Important results and Challenges in High dimension

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- **In practice, we want :**
  - $\mathbf{\Phi}$ for appropriate constraints (Maatouk and Bay [2017], B-splines P. Casteras).
  - To quantify $\left\|f^{\star} - \widehat{f}_{\mathbf{\Phi}_m}\right\|$.
  - Get the "best" ratio $\left\|f^{\star} - \widehat{f}_{\mathbf{\Phi}_m}\right\| / |\mathbf{\Phi}_m|$.

· **The MaxMod algorithm - A sequential procedure.** Iteratively increase the bases $\boldsymbol{\Phi}_m$ to get the "best" ration between $\left\| f^\star - \widehat{f}_{\boldsymbol{\Phi}_m} \right\| / |\boldsymbol{\Phi}_m|$:

$\boxed{\boldsymbol{\Phi}_{m-1} \to \boldsymbol{\Phi}_m}$ choose $\boldsymbol{\Phi}_m$ (among possible bases) maximizing a criterion:

$$\mathcal{K}(\boldsymbol{\Phi}_m) := \left\| \widehat{f}_{\boldsymbol{\Phi}_m} - \widehat{f}_{\boldsymbol{\Phi}_{m-1}} \right\|_{L^2} / (|\boldsymbol{\Phi}_m| - |\boldsymbol{\Phi}_{m-1}|).$$

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· **The (block)-additive assumption in high dimension.** Suppose the target function $y : [0,1]^D \to \mathbb{R}$ is block-additive:

$$\boxed{y(\mathbf{x}) = y_1(\mathbf{x}_{\mathcal{B}_1}) + \cdots + y_B(\mathbf{x}_{\mathcal{B}_B})},$$

$\mathcal{B}_j$ are disjoints sets of $\{1, \cdots, D\}$, $\mathbf{x}_{\mathcal{B}_j} = (x_i)_{i \in \mathcal{B}_j}$.

The partition $\mathcal{P} : \{\mathcal{B}_1, \cdots, \mathcal{B}_B\}$ is unknown.

· **Interpretation of the assumption.** It corresponds to the fact that only few variables interact with each others.

(Block-)Additive Gaussian Processes

Work done and to be done

Solved Problems. López-Lopera et al. [2022], Deronzier et al. [2025]

- Construct finite dimensional (block-)additive GPs framework.
- Use the block-additive structure to reduce the computational cost of the predictor: Woodbury inversion lemma.
- Deal with non linear constraint issue in the boundedness case.
- New MaxMod algorithm designed to find a block-additive structure.
- Implementation of a package for block-additive constrained Gaussian processes **LineqGPR** López-Lopera and Deronzier [2022].

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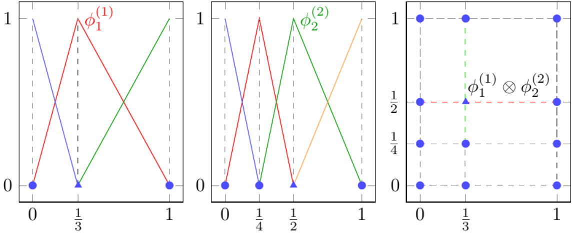
Unsolved Problems.

- Theoretical guarantees of the convergence of the estimator with MaxMod.
- Theoretical guarantees to reconstruct the block structure with MaxMod.
- Implementation of the optimization algorithm for the boundedness case.

Block-additive structure advantages in high dimension



2-dimensional tensorized hat basis family:

$$\Phi^{(1)} \otimes \Phi^{(2)} = \{\phi_{i_1}^{(1)} \otimes \phi_{i_2}^{(2)}\}_{\substack{0 \leqslant i_1 \leqslant m_1, \\ 0 \leqslant i_2 \leqslant m_2}}$$

$$\phi_{i_1}^{(1)} \otimes \phi_{i_2}^{(2)}(x_1, x_2) = \phi_{i_1}^{(1)}(x_1)\phi_{i_2}^{(2)}(x_2)$$

· **Recall on the block-additive model.** For a D dimensional tensorized hat basis family, the size of the basis is:

$$\boxed{\left|\bigotimes_{i=1}^{D} \Phi^{(i)}\right| = \prod_{i=1}^{D} \left|\Phi^{(i)}\right|}$$, which grows exponentially with D.

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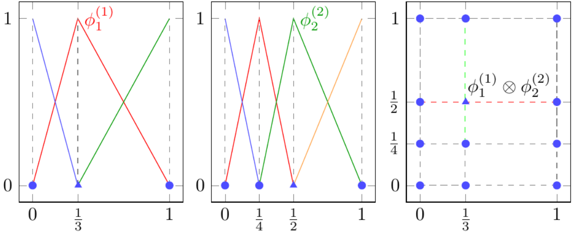

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· **The block-additive assumption:**

- $\boxed{y(\mathbf{x}) = y_1(\mathbf{x}_{\mathcal{B}_1}) + \cdots + y_B(\mathbf{x}_{\mathcal{B}_B})}$, we need to find the basis
- $\boxed{\mathbf{\Phi}(\mathbf{x}) = \mathbf{\Phi}_1(\mathbf{x}_{\mathcal{B}_1}) + \cdots + \mathbf{\Phi}_B(\mathbf{x}_{\mathcal{B}_B})}$, with $\mathbf{\Phi}_j := \bigotimes_{i \in \mathcal{B}_j} \Phi^{(i)}$.

· **hopes:** $\boxed{\sum_{j=1}^{B} \prod_{i \in \mathcal{B}_j} \left|\Phi^{(i)}\right|} \ll \prod_{i=1}^{D} \left|\Phi^{(i)}\right|$

Let set $X = [0,1]^D$, $\mathcal{P} = \{\mathcal{B}_1, \cdots, \mathcal{B}_B\}$, the functional constraint $\mathcal{C}$ and the one dimensional basis $\Phi^{(1)}, \cdots, \Phi^{(D)}$

· **Infinite dimensional baGP.** $\mathcal{Y}_1, \cdots, \mathcal{Y}_B$ independent GPs, $\mathcal{Y}_j$ is defined on $[0,1]^{|\mathcal{B}_j|}$. We define the block-additive GP (baGP):

$$\boxed{\mathcal{Y}(\mathbf{x}) = \mathcal{Y}_1(\mathbf{x}_{\mathcal{B}_1}) + \cdots + \mathcal{Y}_B(\mathbf{x}_{\mathcal{B}_B})}.$$

The block-additive framework

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· **Finite dimensional baGP.** Consider 1 dim family bases $\Phi^{(1)}, \cdots, \Phi^{(D)}$, and the multidimensional block bases $\mathbf{\Phi}_1, \cdots \mathbf{\Phi}_B$, where $\mathbf{\Phi}_j = \otimes_{i \in \mathcal{B}_j} \Phi^{(i)}$

$$\boxed{\widetilde{\mathcal{Y}}_{\mathbf{\Phi}}(\mathbf{x}) = \Pi_{\mathbf{\Phi}_1}(\mathcal{Y}_1)(\mathbf{x}_{\mathcal{B}_1}) + \cdots + \Pi_{\mathbf{\Phi}_B}(\mathcal{Y}_B)(\mathbf{x}_{\mathcal{B}_B})}.$$

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· **Deal with the functional constraints.** Calling $\boldsymbol{\Phi} = \cup_j \Phi_j$ find a way to solve

$$\boxed{\mathrm{mod}(\widetilde{\mathcal{Y}}_{\boldsymbol{\Phi}} \mid \widetilde{\mathcal{Y}}_{\boldsymbol{\Phi}}(\mathbf{X}) + \boldsymbol{\epsilon} = \mathbf{Y}, \widetilde{\mathcal{Y}}_{\boldsymbol{\Phi}} \in \mathcal{C})} \iff \boxed{\arg\min \{\|\boldsymbol{\alpha} - \boldsymbol{\mu}\|^2_{\boldsymbol{\Gamma}} \mid \boldsymbol{\alpha} \in \mathcal{C}'\}}$$

Find the Max Of Distribution — Solve the Quadratic Problem

The MaxMod algorithm

For given observations of $\mathbf{X}, \mathbf{Y}$ of $y = y_1 \oplus \cdots \oplus y_B$ we want to find:

- The blocks $\boxed{\mathcal{P} = \{\mathcal{B}_1, \cdots, \mathcal{B}_B\}}$, together with
- The 1-dim families $\boxed{\Phi^{(1)}, \cdots, \Phi^{(D)}}$, s.t. $\boxed{y_j \underset{\sim}{\in} \mathbf{\Phi}_j = \bigotimes_{i \in \mathcal{B}_j} \Phi^{(i)}}$ for $j = 1, \cdots, B$.

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MaxMod: A greedy procedure

· **Initialization:** $\mathcal{P} = \{1, 2, \cdots, D\}$, $0 = \Phi^{(1)} = \cdots = \Phi^{(D)}$, and $\mathbf{\Phi} = \Phi^{(1)} + \cdots + \Phi^{(D)}$.

· **Iterative Step :** Given $\boxed{\mathcal{P} = \{\mathcal{B}_1, \cdots, \mathcal{B}_k\}}$ and $\boxed{\mathbf{\Phi} = \bigotimes_{i \in \mathcal{B}_1} \Phi^{(i)} + \cdots + \bigotimes_{i \in \mathcal{B}_k} \Phi^{(i)}}$, propose a new basis $\mathbf{\Phi}^\star$:

- **Activate/Refine.** Add a function in $\Phi^{(i)}$: $\boxed{\Phi^{(i)} \to \Phi^{\star(i)} = \Phi^{(i)} \cup \phi^\star}$ and don't change $\mathcal{P} = \{\mathcal{B}_1, \cdots, \mathcal{B}_k\}$.
- **Merge.** Merge two blocks $\mathcal{B}_a$ and $\mathcal{B}_b \in \mathcal{P}$: $\boxed{\mathcal{P} \to \mathcal{P}^\star := \mathcal{P} \backslash \{\mathcal{B}_a, \mathcal{B}_b\} \cup \{\mathcal{B}_a \cup \mathcal{B}_b\}}$ and don't change the $\Phi^{(i)}$.

Construction of the criteria to choose the new basis

· **Two criteria.** Among the choices for the new bases $\mathbf{\Phi}^\star$ (**activate/refine, merge**), we choose $\mathbf{\Phi}^\star$ maximizing a criterion constructed from :

- The **$\mathbf{L^2}$-Modification (L2Mod)** between our two predictors $\widehat{f}_{\mathbf{\Phi}}$ and $\widehat{f}_{\mathbf{\Phi}^\star}$:

$$\mathsf{L2Mod}(\mathbf{\Phi}^\star) = \left\| \widehat{f}_{\mathbf{\Phi}^\star} - \widehat{f}_{\mathbf{\Phi}} \right\|_{L^2}^2, \tag{1}$$

- and the **Squared Error (SE)** criterion:

$$\mathsf{SE}(\mathbf{\Phi}^\star) = \left\| \widehat{f}_{\mathbf{\Phi}^\star}(\mathbf{X}) - \mathbf{Y} \right\|^2. \tag{2}$$

· **Final criterion for the block-additive MaxMod.** The criterion to choose the new basis is then:

$$\mathcal{K}(\mathbf{\Phi}^\star) = \frac{1}{(|\mathbf{\Phi}^\star| - |\mathbf{\Phi}|)^\alpha} \frac{\mathsf{L2Mod}(\mathbf{\Phi}^\star)}{\mathsf{SE}(\mathbf{\Phi}^\star)^\gamma}, \tag{3}$$

$\alpha = 1.4$, $\gamma = 0.5$ has been chosen empirically.

Numerical Results

Application of constrained baGPs in High dimension

We provide a toy function **Increasing per dimension** to test the efficiency of finite dimensional constrained GPs, for some D even number:

$$y(\mathbf{x}) = \sum_{j=1}^{D/2} \arctan\left(5\left[1 - \frac{j}{D+1}\right](x_{2j-1} + 2x_{2j})\right).$$

Results (mean $\pm$ one standard deviation over ten replicates) with $n = 3D$, $n_{knots} = 18D$.
For $i \in \{1, \cdots, D\}$ we take $s^{(i)} = (0, 0.2, 0.4, 0.6, 0.8, 1)$ and
$\mathcal{P} = \{\{1,2\}, \cdots, \{D-1, D\}\}_{1 \leqslant i \leqslant D/2}$.

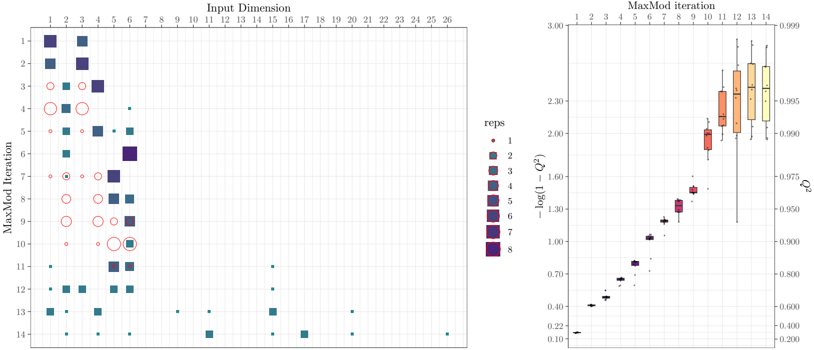
	CPU Time [s]	Q^2 [%]	
D	bacGP mode	baGP mean	bacGP mode
10	0.27 ± 0.01	78.9 ± 9.0	$\mathbf{89.5 \pm 4.5}$
20	0.50 ± 0.05	82.5 ± 4.7	$\mathbf{92.0 \pm 1.0}$
40	1.09 ± 0.06	86.1 ± 1.8	$\mathbf{91.3 \pm 1.2}$
80	3.17 ± 0.15	86.1 ± 1.3	$\mathbf{92.0 \pm 1.0}$
120	6.47 ± 0.35	87.4 ± 1.1	$\mathbf{89.9 \pm 0.8}$

Application of MaxMod

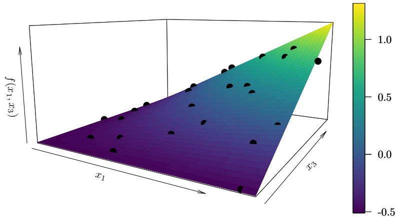
We considere the block-additive function

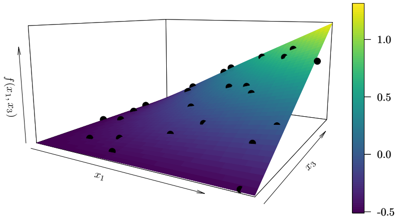
$$y(\mathbf{x}) = 2x_1x_3 + \sin(x_2x_4) + \arctan(3x_5 + 5x_6).$$

The function y is considered as a function of 26 dimensions with 6 actives ones. The panels show: (right) the choices made by the MaxMod and (left) the boxplot of the Q^2 criterion per iteration of the algorithm with 10 differents replicates of design of experiment. The number of obervation is $n = 7D_o$ with $D_o = 6$.



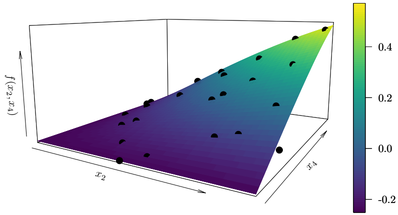
Plot of the centered functions:
$f_1 : (x_1, x_3) \mapsto 2x_1x_3$ (left) and the constructed predictor $\widehat{f_1}$ (right)

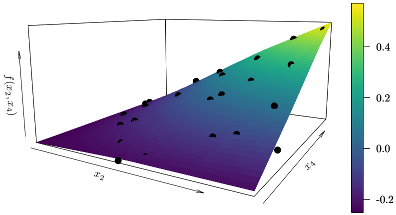




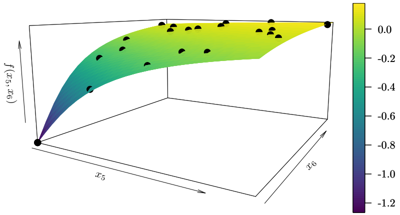
Reconstruction of the block functions

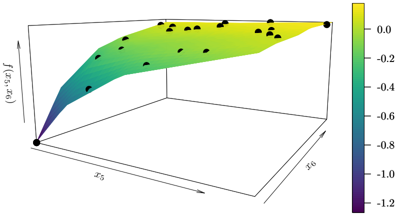
Plot of the centered functions:
$f_2 : (x_2, x_4) \mapsto \sin(x_2 x_4)$ (left) and the constructed predictor $\widehat{f_2}$ (right)





Plot of the centered functions:
$f_3 : (x_5, x_6) \mapsto \mathrm{arctan}(3x_5 + 5x_6)$ (left) and the constructed predictor $\widehat{f_3}$(right)





The boundedness constraint in the block-additive case

· **Boundedness** For a subpartition $\mathcal{P} = \{\mathcal{B}_1, \cdots, \mathcal{B}_B\}$ and fixed families of bases, $\boxed{f(\mathbf{x}) = \mathbf{\Phi}_1(\mathbf{x}_{\mathcal{B}_1})^\top \boldsymbol{\alpha}_1 + \cdots + \mathbf{\Phi}_B(\mathbf{x}_{\mathcal{B}_B})^\top \boldsymbol{\alpha}_B}$, We have the following equivalence for the boundedness constraint:

$$\underset{f \in \mathcal{C}}{\boxed{f \leqslant u}} \quad \Longleftrightarrow \quad \underset{\boldsymbol{\alpha} \in \mathcal{C}'}{\boxed{\textstyle\sum_{j=1}^{B} \max \boldsymbol{\alpha}_j \leqslant u}}$$

The constraint is **non linear**.

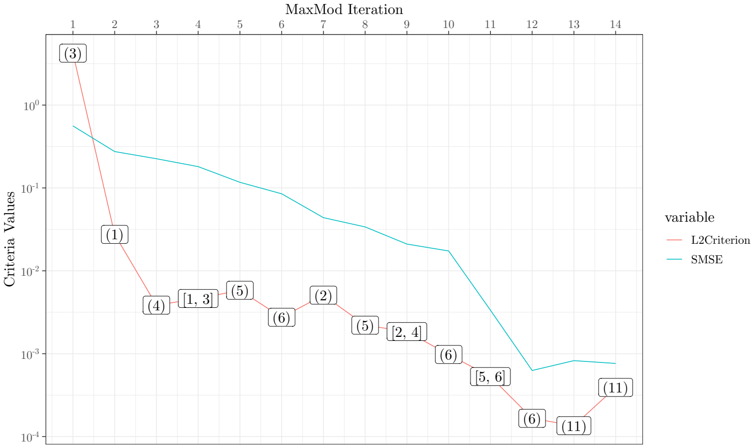
· **Reformulation of the problem.** We then need to solve:

$$\boxed{\arg\min \{\|\boldsymbol{\alpha} - \boldsymbol{\mu}\|_{\mathbf{\Gamma}}^2 \mid \boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \cdots, \boldsymbol{\alpha}_B), \textstyle\sum_{j=1}^{B} \max \boldsymbol{\alpha}_j \leqslant u\}},$$

· **Proposed solution:** Projected gradient descent, hence find an efficient way to project on $\mathcal{C}'$.

Iterations of MaxMod

Evolution over iterations of L2Mod $:= \left\| \widehat{f}_{\mathbf{\Phi}^\star} - \widehat{f}_{\mathbf{\Phi}} \right\|_{L^2}$ (red curve) and SMSE $:= \left\| \widehat{f}_{\mathbf{\Phi}^\star}(\mathbf{X}) - \mathbf{Y} \right\| / \widehat{\mathrm{VAR}}(\mathbf{Y})^{1/2}$ (blue curve). "(i)" indicates the activation or the refinement of the variable i, while "$[i_1, \dots, i_k]$" indicates the creation of a block composed of variables $i_1, \dots, i_k$.



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