Patched Gaussian Processes

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■ GAUSSIAN PROCESS

Gaussian Process : Random surface $W(s)$ over a domain $\mathcal{D}$ such that :
$$\forall \{s_1, \ldots, s_n\} \in \mathcal{D}^n, W := (W(s_1), \ldots, W(s_n)) \sim \mathcal{N}(\mu, C).$$

- **Mean function :** $\mu(s) := \mathbb{E}[W(s)] \longrightarrow \mu := [\mu(s_1), \ldots, \mu(s_N)]^T$
- **Covariance function :** $C(s, s') := \mathbb{C}\mathrm{ov}[W(s), W(s')] \longrightarrow C := [C(s_i, s_j)]_{1 \leqslant i,j \leqslant N}.$

Law of W :

$$p(W) = \frac{1}{\sqrt{(2\pi)^d \det(C)}} \exp\left(-\frac{1}{2}(W - \mu)^T C^{-1}(W - \mu)\right).$$

■ KRIGING

Observations : $\mathcal{D} = \{(x_i, y_i) \mid i \in \{1, \ldots, N\}\}$.

Locations $\boldsymbol{x} := [x_1, \ldots, x_N]^T \longrightarrow$ **Responses** $\boldsymbol{y} := [y_1, \ldots, y_N]^T$.

Kriging : Stochastic predictions based on these observations.

- **Reponses** y seen as realizations of a **gaussian process** f with noise :

$$y_i = f(x_i) + \varepsilon_i, \text{ where } \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2).$$

- **Prediction** $f_* := f(x^*)$ at new location $x^* \longrightarrow$ **Joint law of** (f_*, y):

$$p(f_*, y) \sim \mathcal{N}\left(0, \begin{bmatrix} c_{**} & c_{*x} \\ c_{x*} & \sigma^2 I + C_{xx} \end{bmatrix}\right).$$

where $c_{**} = C(x^*, x^*), c_{x*} = [C(x_1, x^*), \ldots, C(x_N, x^*)]^T, C_{xx} = [C(x_i, x_j)]_{1 \leqslant i, j \leqslant N}$.

■ KRIGING

Predictive distribution :

$$p(f_* \mid y) \sim \mathcal{N}(\underbrace{c_{x*}^T(\sigma^2 I + C_{xx})^{-1}y}_{\text{predictive mean}}, \underbrace{c_{**} - c_{x*}^T(\sigma^2 I + C_{xx})^{-1}c_{x*}}_{\text{predictive variance}})$$

- **Predicted value :** $f(x^*) \approx c_{x*}^T(\sigma^2 I + C_{xx})^{-1}y$.

- **Uncertainty :** $c_{**} - c_{x*}^T(\sigma^2 I + C_{xx})^{-1}c_{x*}$.

■ BAYESIAN APPROACH

Hierarchical model :

$$y_i = X(x_i) \cdot \beta + f_\theta(x_i) + \varepsilon_i.$$

- **Regression term $X(x_i) \cdot \beta$:** Captures effects of known explanatory variables X.

- **Spatial effect $f_\theta(x_i)$:** Realization of a gaussian process $f_\theta \sim \mathcal{N}(0, C_\theta)$.

- **Noise ε_i :** $\varepsilon_i \stackrel{iid}{\sim} \mathcal{N}(0, \tau^2)$.

■ **BAYESIAN APPROACH**

Bayesian Inference : Estimation of the **hidden state** f_θ and **parameters** $\phi := \{\beta, \theta, \tau^2\}$.

- **Prior distributions :** We assume prior knowledge $p(\beta)$, $p(\theta)$ and $p(\tau^2)$.

- **Likelihood :** $p(y \mid f_\theta, \beta, \tau^2) = \mathcal{N}(X\beta + f_\theta, \tau^2 I)$.

- **Latent GP prior :** $p(f_\theta \mid \theta) = \mathcal{N}(0, C_\theta)$.

Joint posterior distribution :

$$p(f_\theta, \beta, \theta, \tau^2 \mid y) \propto \underbrace{p(y \mid f_\theta, \beta, \tau^2)}_{\text{data likelihood}} \times \underbrace{p(f_\theta \mid \theta)}_{\text{spatial link}} \times \underbrace{p(\beta)p(\theta)p(\tau^2)}_{\text{parameter priors}}.$$

■ COMPUTATIONAL COSTS

Both the predictive mean and variance require **solving linear systems** involving $\Sigma = \sigma^2 I + C_{xx}$.

- **Time complexity :** Matrix inversion $\longrightarrow \mathcal{O}(N^3)$.

- **Space complexity :** Storing covariance matrix $\longrightarrow \mathcal{O}(N^2)$.

Solutions :
- Acting on the **covariance matrix Σ** : compact support, covariance tapering, markovian models $\longrightarrow$ **Sparse matrix**.

- Acting on the **amount of observations N**...

■ INDEPENDANT LOCAL KRIGING

Idea : Split the observations $\mathcal{D}$ into K subsets $\mathcal{D}_1, \ldots, \mathcal{D}_K$, with $\mathcal{D}_k := \{(x_i, y_i) \mid x_i \in \Omega_k\}$.

Region $\Omega_k \longrightarrow$ Local gaussian process $f_k \longrightarrow$ Associated covariance function $C_k(\cdot, \cdot)$.

- **Stationary process :** $C_k(\cdot, \cdot) = C(\cdot, \cdot)$.
- Otherwise : Different covariance functions C_k.
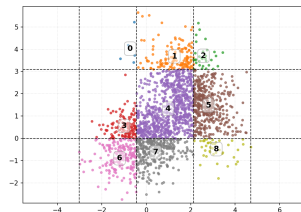
$$y_{k,i} = f_k(x_i) + \varepsilon_{k,i}.$$

Two questions :
- How to split the observations efficiently ?
- How to deal with shared boundaries $\Gamma_{k,\ell} := \overline{\Omega}_k \cap \overline{\Omega}_\ell$?

■ SPLITTING THE OBSERVATIONS

Grid partitioning : Splitting the data using an uniform grid to cover the space.
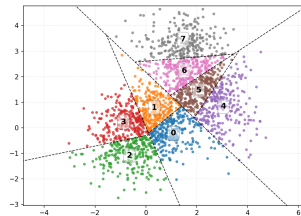
$\oplus$ Very easy implementation.

$\ominus$ High density variance between regions.

Grid partitioning

PCA partitioning : Splitting the data based on principal component projections values.

$\oplus$ Balanced number of points ($N_k \approx$ cst).

$\ominus$ Complex boundary definition.

PCA partitioning

■ BORDER DISCONTINUITY

Issue :

$$f_k(x) \neq f_\ell(x) \text{ at frontier } \Gamma_{k,\ell}.$$
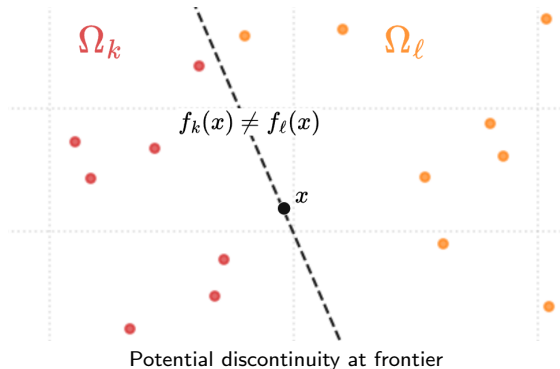
Solution :

$$\text{Set } \delta_{k,\ell} := f_k - f_\ell = 0 \text{ at } \Gamma_{k,\ell}.$$

In practice : pseudo-observations
$\delta_{k,\ell}(x) = 0$ at the frontiers.
$$\mathbb{E}\left[f_*^{(k)} \mid y\right] \longrightarrow \mathbb{E}\left[f_*^{(k)} \mid y, \delta = 0\right].$$
$$\mathbb{V}\left[f_*^{(k)} \mid y\right] \longrightarrow \mathbb{V}\left[f_*^{(k)} \mid y, \delta = 0\right].$$

Potential discontinuity at frontier

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For two neighbor regions Ω_k, Ω_ℓ, place B observations on the border $\Gamma_{k,\ell}$:

- **Pseudo-locations :** $x^{(k,\ell)} := \left(x_1^{(k,\ell)}, \ldots, x_B^{(k,\ell)}\right)^T$.

- **Pseudo-values :** $\delta_{k,\ell} := \left(\delta_{k,\ell}(x_1^{(k,\ell)}), \ldots, \delta_{k,\ell}(x_B^{(k,\ell)})\right)^T$.

▶ **Observations :** $y := \left(y_1^T, \ldots, y_K^T\right)^T$.

▶ **Pseudo-observations :** $\delta := \left(\delta_{1,1}^T, \ldots, \delta_{1,K}^T, \ldots, \delta_{K,K}^T\right)^T$.

Predict $f_*^{(k)} := f_k(x^*)$ at $x^* \in \Omega_k \longrightarrow$ **Joint law of $(f_*^{(k)}, y, \delta)$** :

$$\begin{bmatrix} f_*^{(k)} \\ y \\ \delta \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} c_{**} & c_{*\mathcal{D}}^{(k)} & c_{*\delta}^{(k)} \\ c_{\mathcal{D}*}^{(k)} & C_{\mathcal{D}\mathcal{D}} & C_{\mathcal{D}\delta} \\ c_{\delta*}^{(k)} & C_{\delta\mathcal{D}} & C_{\delta\delta} \end{bmatrix} \right).$$

- On the border between regions k and l $\delta_{k,l} = f_k - f_l$

- Under the asumption f_k and f_l are independent gaussian processes, $\delta_{k,l}$ is one too

- Specifically, we can easily compute its covariance with $f_j(x)$, for a certain $x \in \mathcal{D}_j$
$$\mathbb{C}\text{ov}(\delta_{k,l}(x_1), f_j(x_2)) = \mathbb{C}\text{ov}(f_k(x_1), f_j(x_2)) - \mathbb{C}\text{ov}(f_l(x_1), f_j(x_2))$$

Definitions of the covariance blocks :

$$c_{**} := \mathbb{C}\text{ov}(f_*^{(k)}, f_*^{(k)}),$$

$$c_{*\mathcal{D}}^{(k)} := \left(\mathbb{C}\text{ov}(f_*^{(k)}, y_1), \ldots, \mathbb{C}\text{ov}(f_*^{(k)}, y_K) \right),$$

$$c_{*\delta}^{(k)} := \left(\mathbb{C}\text{ov}(f_*^{(k)}, \delta_{1,1}), \ldots, \mathbb{C}\text{ov}(f_*^{(k)}, \delta_{K,K}) \right),$$

$$C_{\mathcal{DD}} := \begin{bmatrix} \mathbb{C}\text{ov}(y_1, y_1) & \ldots & \mathbb{C}\text{ov}(y_1, y_K) \\ \ldots & \ddots & \ldots \\ \mathbb{C}\text{ov}(y_K, y_1) & \ldots & \mathbb{C}\text{ov}(y_K, y_K) \end{bmatrix}, \quad C_{\mathcal{D}\delta} := \begin{bmatrix} \mathbb{C}\text{ov}(y_1, \delta_{1,1}) & \ldots & \mathbb{C}\text{ov}(y_1, \delta_{K,K}) \\ \ldots & \ddots & \ldots \\ \mathbb{C}\text{ov}(y_K, \delta_{1,1}) & \ldots & \mathbb{C}\text{ov}(y_K, \delta_{K,K}) \end{bmatrix} \text{ and}$$

$$C_{\delta\delta} := \begin{bmatrix} \mathbb{C}\text{ov}(\delta_{1,1}, \delta_{1,1}) & \ldots & \mathbb{C}\text{ov}(\delta_{1,1}, \delta_{K,K}) \\ \ldots & \ddots & \ldots \\ \mathbb{C}\text{ov}(\delta_{K,K}, \delta_{1,1}) & \ldots & \mathbb{C}\text{ov}(\delta_{K,K}, \delta_{K,K}) \end{bmatrix}.$$

■ PATCHWORK KRIGING

Predictive mean :

$$\mathbb{E}\left[f_*^{(k)} \mid y, \delta = 0\right] = \left(c_{*\mathcal{D}}^{(k)} - c_{*\delta}^{(k)} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}}\right)\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}}\right)^{-1} y.$$

Predictive variance :

$$\mathbb{V}\left[f_*^{(k)} \mid y, \delta = 0\right] = c_{**} - c_{*\delta}^{(k)} C_{\delta\delta}^{-1} c_{\delta*}^{(k)}$$
$$- \left(c_{*\mathcal{D}}^{(k)} - c_{*\delta}^{(k)} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}}\right)\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}}\right)^{-1}\left(c_{\mathcal{D}*}^{(k)} - c_{\delta*}^{(k)} C_{\delta\delta}^{-1} C_{\mathcal{D}\delta}\right)$$

Noting $Q := \left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}}\right)^{-1}, v := L^{-1} C_{\delta\mathcal{D}}$ and $w_* := L^{-1} c_{\delta*}^{(k)}$ (where $C_{\delta\delta} = LL^T$),

$$\boxed{\begin{aligned}
\mathbb{E}\left[f_*^{(k)} \mid y, \delta = 0\right] &= (c_{*\mathcal{D}}^{(k)} - w_*^T v)Qy. \\
\mathbb{V}\left[f_*^{(k)} \mid y, \delta = 0\right] &= c_{**} - w_*^T w_* - (c_{*\mathcal{D}}^{(k)} - w_*^T v)Q(c_{*\mathcal{D}}^{(k)} - w_*^T v)^T.
\end{aligned}}$$

For two gaussian vectors $\mathbf{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$ and $\mathbf{x}_2 \sim \mathcal{N}(\mu_2, \Sigma_2)$, the conditional distribution $p(\mathbf{x}_1 \mid \mathbf{x}_2)$ is gaussian and verifies :

$$\mathbb{E}\left[\mathbf{x}_1 \mid \mathbf{x}_2\right] = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2 - \mu_2).$$

$$\mathbb{V}\left[\mathbf{x}_1 \mid \mathbf{x}_2\right] = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}.$$

Applying this to $\mathbf{x}_1 = f_*^{(k)}$ and $\mathbf{x}_2 = (y, \delta)$ gives :

$$\mathbb{E}\left[f_*^{(k)} \mid y, \delta\right] = \left[c_{*\mathcal{D}}^{(k)}, c_{*\delta}^{(k)}\right] \left[\begin{array}{cc} C_{\mathcal{D}\mathcal{D}} & C_{\mathcal{D}\delta} \\ C_{\delta\mathcal{D}} & C_{\delta\delta} \end{array}\right]^{-1} \left[\begin{array}{c} y \\ \delta \end{array}\right]$$

and

$$\mathbb{V}\left[f_*^{(k)} \mid y, \delta\right] = c_{**} - \left[c_{*\mathcal{D}}^{(k)}, c_{*\delta}^{(k)}\right] \left[\begin{array}{cc} C_{\mathcal{D}\mathcal{D}} & C_{\mathcal{D}\delta} \\ C_{\delta\mathcal{D}} & C_{\delta\delta} \end{array}\right]^{-1} \left[\begin{array}{c} c_{\mathcal{D}*}^{(k)} \\ c_{\delta*}^{(k)} \end{array}\right].$$

■ PROOF

For invertible matrix A, B, D, the following inversion formula holds true :

$$\begin{bmatrix} A & B \\ B^T & D \end{bmatrix}^{-1} = \begin{bmatrix} \left(A - BD^{-1}B^T\right)^{-1} & -\left(A - BD^{-1}B^T\right)^{-1} BD^{-1} \\ -D^{-1}B^T\left(A - BD^{-1}B^T\right)^{-1} & \left(D - B^T A^{-1}B\right)^{-1} \end{bmatrix}.$$

Applying this to $A = C_{\mathcal{D}\mathcal{D}}$, $B = C_{\mathcal{D}\delta}$, $D = C_{\delta\delta}$ gives, for the predictive mean :

$$\mathbb{E}\left[f_*^{(k)} \mid y, \delta\right] = \begin{bmatrix} c_{*\mathcal{D}}^{(k)} \\ c_{*\delta}^{(k)} \end{bmatrix}^T \begin{bmatrix} \left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} & -\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} C_{\mathcal{D}\delta}C_{\delta\delta}^{-1} \\ -C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} & \left(C_{\delta\delta} - C_{\delta\mathcal{D}}C_{\mathcal{D}\mathcal{D}}^{-1}C_{\mathcal{D}\delta}\right)^{-1} \end{bmatrix} \begin{bmatrix} y \\ \delta \end{bmatrix}$$

$$= c_{*\mathcal{D}}^{(k)}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} y - c_{*\delta}^{(k)}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}^T\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} y$$

$$- c_{*\mathcal{D}}^{(k)}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}\delta + c_{*\delta}^{(k)}\left(C_{\delta\delta} - C_{\delta\mathcal{D}}C_{\mathcal{D}\mathcal{D}}^{-1}C_{\mathcal{D}\delta}\right)^{-1}\delta.$$

Taking $\delta = 0$ finally leads to :

$$\mathbb{E}\left[f_*^{(k)} \mid y, \delta = 0\right] = \left(c_{*\mathcal{D}}^{(k)} - c_{*\delta}^{(k)}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} y.$$

Concerning the predictive variance, the inversion formula also gives :

$$
\mathbb{V}\left[f_*^{(k)} \mid y, \delta\right]
$$

$$
= c_{**} - \left[\begin{array}{c} c_{*\mathcal{D}}^{(k)} \\ c_{*\delta}^{(k)} \end{array}\right]^T \left[\begin{array}{cc} \left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} & -\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1}C_{\mathcal{D}\delta}C_{\delta\delta}^{-1} \\ -C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1} & \left(C_{\delta\delta} - C_{\delta\mathcal{D}}C_{\mathcal{D}\mathcal{D}}^{-1}C_{\mathcal{D}\delta}\right)^{-1} \end{array}\right] \left[\begin{array}{c} c_{\mathcal{D}*}^{(k)} \\ c_{\delta*}^{(k)} \end{array}\right]
$$

$$
= c_{**} - c_{*\mathcal{D}}^{(k)}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1}c_{\mathcal{D}*}^{(k)} + c_{*\mathcal{D}}^{(k)}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1}C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}c_{\delta*}^{(k)}
$$

$$
+ c_{*\delta}^{(k)}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1}c_{\mathcal{D}*}^{(k)} - c_{*\delta}^{(k)}\left(C_{\delta\delta} - C_{\delta\mathcal{D}}C_{\mathcal{D}\mathcal{D}}^{-1}C_{\mathcal{D}\delta}\right)^{-1}c_{\delta*}^{(k)}.
$$

This finally yields to :

$$
\mathbb{V}\left[f_*^{(k)} \mid y, \delta = 0\right] = c_{**} - c_{*\delta}^{(k)}C_{\delta\delta}^{-1}c_{\delta*}^{(k)} - \left(c_{*\mathcal{D}}^{(k)} - c_{*\delta}^{(k)}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)\left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}C_{\delta\mathcal{D}}\right)^{-1}\left(c_{\mathcal{D}*}^{(k)} - C_{\mathcal{D}\delta}C_{\delta\delta}^{-1}c_{\delta*}^{(k)}\right).
$$

■ CHOICE OF THE PARAMETERS

Covariance function :

- Different for each region $\longrightarrow C_k(\cdot, \cdot)$ for $k \in \{1, \ldots, K\}$.

- Obtained by minimizing the negative log-likelihood :

$$NL(\theta) := -\log p(y, \delta = 0 \mid \theta)$$

$$= \frac{N}{2} \log(2\pi) + \frac{1}{2} \log \begin{vmatrix} C_{\mathcal{D}\mathcal{D}} & C_{\mathcal{D}\delta} \\ C_{\delta\mathcal{D}} & C_{\delta\delta} \end{vmatrix} + \frac{1}{2} \begin{bmatrix} y \\ 0 \end{bmatrix}^T \begin{bmatrix} C_{\mathcal{D}\mathcal{D}} & C_{\mathcal{D}\delta} \\ C_{\delta\mathcal{D}} & C_{\delta\delta} \end{bmatrix}^{-1} \begin{bmatrix} y \\ 0 \end{bmatrix}.$$

Hyperparameters :

- Number of regions $\boldsymbol{K} = 2^D$ (where D is the depth of the PCA partitioning).
  - ➤ $K \nearrow \implies$ Less accurate predictions.

- Number of pseudo-observations $\boldsymbol{B}$ per frontier.
  - ➤ $B \nearrow \implies$ More accurate predictions.

Steps :
1. Partition the domain : $\Omega = \bigcup_{k=1}^{K} \Omega_k$.
2. Create the pseudo-observations $\delta_{k,\ell}$ on each $\Gamma_{k,\ell}$.
3. Use MLE to choose each covariance function $C_k(\cdot, \cdot)$.
4. Compute $\mathbb{E}\left[f_*^{(k)} \mid y, \delta = 0 \right]$ and $\mathbb{V}\left[f_*^{(k)} \mid y, \delta = 0 \right]$:
   - Comptute $Q = \left(C_{\mathcal{D}\mathcal{D}} - C_{\mathcal{D}\delta} C_{\delta\delta}^{-1} C_{\delta\mathcal{D}} \right)^{-1}$.
   - Compute Cholesky decomposition of $C_{\delta\delta} = LL^T$
   - Deduce $v = L^{-1} C_{\delta\mathcal{D}}$ and $w_* = L^{-1} c_{\delta*}^{(k)}$.
5. Be happy ☺

■ INTUITIVE IDEA

- It seems logical to assume that far away observations have little impact on the Kriging.

- We now consider:

$$f_\theta \sim \mathcal{N}(0, K_\theta)$$

$$f(x^*) = \sum_{j=1}^{n} A_j y_j + \varepsilon$$

- With $A_j = \delta_{N(x^*)}$ Where $N(x^*)$ is the set of x^* nearest neighbors.

- Restraining the Kriging to the m nearest neighbors of each prediction location x^* leads to a sub-optimal prediction.

- Our Kriging variance is now $c_{**} - c_{N(x^*)*}^T (C_{N(x^*)N(x^*)})^{-1} c_{N(x^*)*}$. for the given x^*.

■ NEAREST-NEIGHBORS

Nearest-Neighbors are the points that have the highest spatial correlation with the prediction location x^*:

- In the case of stationary covariance functions, these are simply the closest points to x^*.

- For non-stationary covariance functions, the nearest neighbors are the maxima of the covariance function with respect to x^*.

■ CHOOSING M

- First idea : running cross-validation for different values of m and choosing the one that minimizes the prediction error.

- In Bayesian Inference, m is treated as a parameter and updated in the MCMC algorithm.

$$p(f_\theta, \beta, \theta, \tau^2, m \mid y) \propto p(y \mid f_\theta, \beta, \tau^2) \times p(f_\theta \mid \theta) \times p(\beta)p(\theta)p(\tau^2)p(m)$$

■ COMPLEXITY ANALYSIS I

For Method I (**Patchwork Kriging**), the expense is located in the computation of:

$$(C_{\delta\delta} - C_{\mathcal{D}\delta}^T C_{\mathcal{D}\mathcal{D}}^{-1} C_{\mathcal{D}\delta})^{-1}$$

Reminder

- N observations in a space of dimension d

- Split into K regions of $M = \frac{N}{K}$ points, with B pseudo-observations at each boundary

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Complexity

- $C_{\mathcal{D}\mathcal{D}}^{-1}$ block diagonal $\rightarrow \mathcal{O}(\boldsymbol{KM^3})$

- $C_{\mathcal{D}\mathcal{D}}^{-1} C_{\mathcal{D}\delta} \rightarrow \mathcal{O}(\boldsymbol{KBM^2})$

- Inverting $C_{\delta\delta} - C_{\mathcal{D}\delta}^T C_{\mathcal{D}\mathcal{D}}^{-1} C_{\mathcal{D}\delta}$. As it is very sparse, we can use efficient methods to invert sparse matrix (Chan and George (1980)) $\longrightarrow \mathcal{O}(\boldsymbol{d^3B^3K})$

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- Inverting $C_{\delta\delta} - C_{\mathcal{D}\delta}^T C_{\mathcal{D}\mathcal{D}}^{-1} C_{\mathcal{D}\delta}$. As it is very sparse, we can use efficient methods to invert sparse matrix (Chan and George (1980)) $\longrightarrow \mathcal{O}(\boldsymbol{d^3 B^3 K})$

$$\longrightarrow \mathcal{O}(\boldsymbol{KM^3 + KBM^2 + d^3 B^3 K}) \approx \mathcal{O}(\boldsymbol{\frac{N^3}{K^2} + d^3 B^3 K})$$

■ ACCURACY

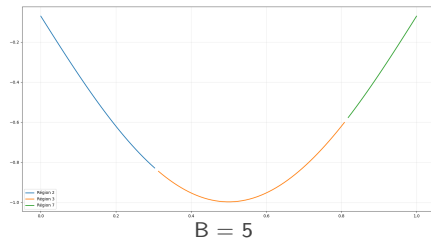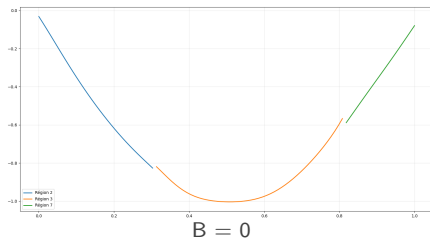For Method I (**Patchwork Kriging**), the accuracy concerns :

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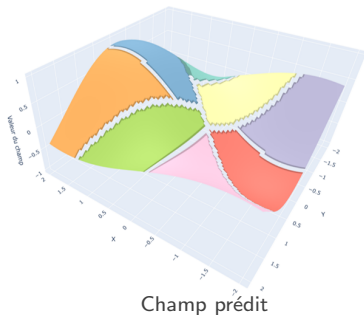- Quality of "stiches" (junctions of regions)
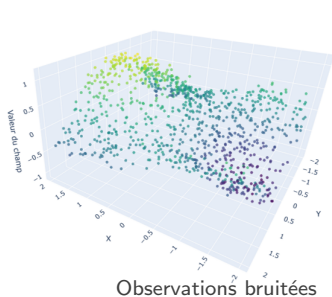

B = 0

B = 5

In Park and Apley (2018), Tests have been made to understand the extent of the Patchwork Kriging Technique

- Result are the most accurate for **long-range, stationary** covariance functions.

- Stitching accuracy is **conditioned by** B, but stops for $B \geq 8$

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Observations bruitées

Champ prédit

In Park and Apley (2018), Tests have been made to understand the extent of the Patchwork Kriging Technique

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High dimensionality ?
- Recall the complexity $\longrightarrow \mathcal{O}(\frac{N^3}{K^2} + d^3 B^3 K)$

- Experimentally, for $d > 10$, dimension is a determining factor for computation time

$$\rightarrow \text{Trade-of quality/speed} : \text{keep } \frac{N}{K} \text{ and } dB \text{ as low as possible.}$$

For Method II (**NN-Kriging**), the expense is located in the computation of

$$c_{**} - c_{N(x^*)*}^T (C_{N(x^*)N(x^*)})^{-1} c_{N(x^*)*}.$$

Reminder

- N observations of a space of dimension d

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Complexity

- Computing a new location$(C_{N(x^*)N(x^*)})^{-1} \to \mathcal{O}(m^3)$

- Computing n new location$(C_{N(x^*)N(x^*)})^{-1} \to \mathcal{O}(nm^3)$

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"On ne peut pas inverser une matrice de taille 20000 une fois, mais on peut inverser 20000 matrice de taille 20 une fois... enfin je crois"

— *L. Lambert*

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