

# Patched Gaussian Processes

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## ■ GAUSSIAN PROCESS

**Gaussian Process** : Random surface  $W(s)$  over a domain  $\mathcal{D}$  such that :

$$\forall \{s_1, \dots, s_n\} \in \mathcal{D}^n, W := (W(s_1), \dots, W(s_n)) \sim \mathcal{N}(\mu, C).$$

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

**Law of  $W$**  :

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

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

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

**Kriging** : Stochastic predictions based on these observations.

- **Responses**  $y$  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  $c_{**} = C(x^*, x^*)$ ,  $c_{x*} = [C(x_1, x^*), \dots, C(x_N, x^*)]^T$ ,  $C_{xx} = [C(x_i, x_j)]_{1 \leq i, j \leq N}$ .

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

## ■ BAYESIAN APPROACH

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

- **Prior distributions** : We assume prior knowledge  $p(\beta)$ ,  $p(\theta)$  and  $p(\tau^2)$ .
- **Likelihood** :  $p(y | f_\theta, \beta, \tau^2) = \mathcal{N}(X\beta + f_\theta, \tau^2 I)$ .
- **Latent GP prior** :  $p(f_\theta | \theta) = \mathcal{N}(0, C_\theta)$ .

**Joint posterior distribution :**

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

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## ■ 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  $\Sigma$**  : 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  $\mathcal{D}_1, \dots, \mathcal{D}_K$ , with  $\mathcal{D}_k := \{(x_i, y_i) \mid x_i \in \Omega_k\}$ .

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

- **Stationary process** :  $C_k(\cdot, \cdot) = C(\cdot, \cdot)$ .
- Otherwise : Different covariance functions  $C_k$ .

$$y_{k,i} = f_k(x_i) + \varepsilon_{k,i}.$$

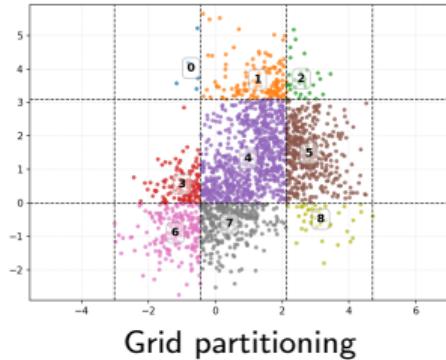
Two questions :

- 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

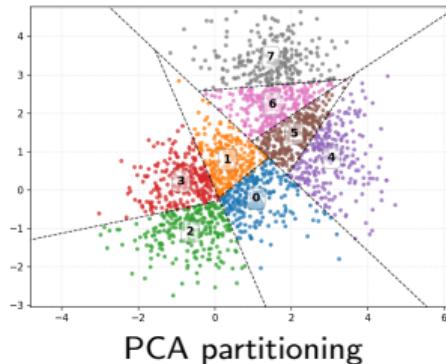
**Grid partitioning** : Splitting the data using an uniform grid to cover the space.

- (+) Very easy implementation.
- (-) High density variance between regions.



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

- (+) Balanced number of points ( $N_k \approx \text{cst}$ ).
- (-) Complex boundary definition.



## BORDER DISCONTINUITY

**Issue :**

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

**Solution :**

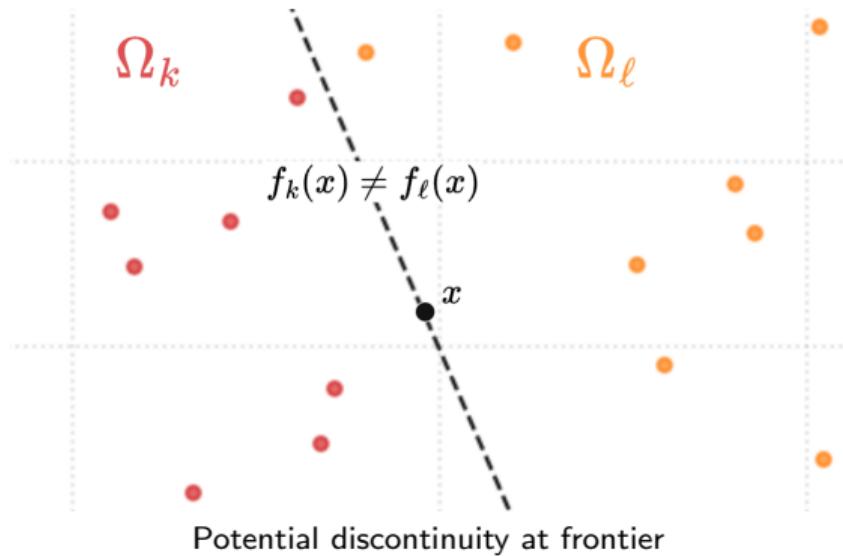
Set  $\delta_{k,\ell} := f_k - f_\ell = 0$  at  $\Gamma_{k,\ell}$ .

In practice : pseudo-observations

$\delta_{k,\ell}(x) = 0$  at the frontiers.

$$\mathbb{E} \left[ f_*^{(k)} \mid y \right] \longrightarrow \mathbb{E} \left[ f_*^{(k)} \mid y, \delta = 0 \right].$$

$$\mathbb{V} \left[ f_*^{(k)} \mid y \right] \longrightarrow \mathbb{V} \left[ f_*^{(k)} \mid y, \delta = 0 \right].$$



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## ■ PSEUDO-OBSERVATIONS

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

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

- **Observations** :  $y := \left( y_1^T, \dots, y_K^T \right)^T$ .
- **Pseudo-observations** :  $\delta := \left( \delta_{1,1}^T, \dots, \delta_{1,K}^T, \dots, \delta_{K,K}^T \right)^T$ .

## ■ PATCHWORK KRIGING

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

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

## ■ PATCHWORK KRIGING

Definitions of the covariance blocks :

$$c_{**} := \text{Cov}(f_*^{(k)}, f_*^{(k)}),$$

$$c_{*\mathcal{D}}^{(k)} := \left( \text{Cov}(f_*^{(k)}, y_1), \dots, \text{Cov}(f_*^{(k)}, y_K) \right),$$

$$c_{*\delta}^{(k)} := \left( \text{Cov}(f_*^{(k)}, \delta_{1,1}), \dots, \text{Cov}(f_*^{(k)}, \delta_{K,K}) \right),$$

$$C_{\mathcal{D}\mathcal{D}} := \begin{bmatrix} \text{Cov}(y_1, y_1) & \dots & \text{Cov}(y_1, y_K) \\ \dots & \ddots & \dots \\ \text{Cov}(y_K, y_1) & \dots & \text{Cov}(y_K, y_K) \end{bmatrix}, \quad C_{\mathcal{D}\delta} := \begin{bmatrix} \text{Cov}(y_1, \delta_{1,1}) & \dots & \text{Cov}(y_1, \delta_{K,K}) \\ \dots & \ddots & \dots \\ \text{Cov}(y_K, \delta_{1,1}) & \dots & \text{Cov}(y_K, \delta_{K,K}) \end{bmatrix} \quad \text{and}$$

$$C_{\delta\delta} := \begin{bmatrix} \text{Cov}(\delta_{1,1}, \delta_{1,1}) & \dots & \text{Cov}(\delta_{1,1}, \delta_{K,K}) \\ \dots & \ddots & \dots \\ \text{Cov}(\delta_{K,K}, \delta_{1,1}) & \dots & \text{Cov}(\delta_{K,K}, \delta_{K,K}) \end{bmatrix}.$$

## ■ 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 :**

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

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

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

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

## ■ PROOF

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 :

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

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

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

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

and

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

## ■ PROOF

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

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

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

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

Taking  $\delta = 0$  finally leads to :

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

# ■ PROOF

Concerning the predictive variance, the inversion formula also gives :

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

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  $\rightarrow c_k(\cdot, \cdot)$  for  $k \in \{1, \dots, K\}$ .
- 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  $K = 2^D$  (where  $D$  is the depth of the PCA partitioning).
  - $K \nearrow \Rightarrow$  Less accurate predictions.
- Number of pseudo-observations  $B$  per frontier.
  - $B \nearrow \Rightarrow$  More accurate predictions.

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## ■ INTUITIVE IDEA

idk

## ■ THEORETICAL DEFINITION

- Item
- Item

## ■ PROPER SOLUTION

- Item
- Item

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