Gaussian process regression model for distribution inputs

European Meeting of Statisticians

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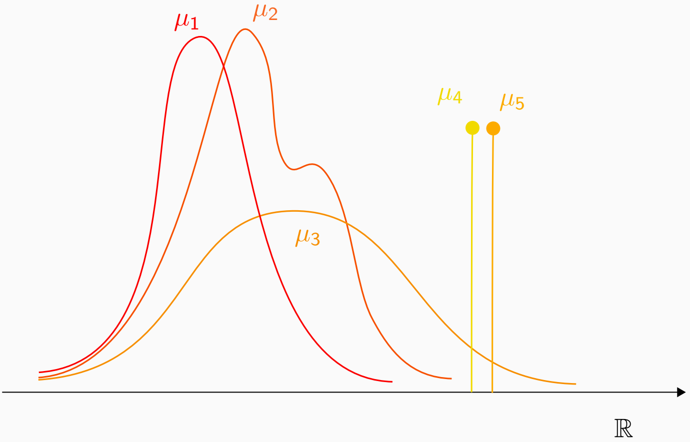
The regression problem for distribution inputs

We are given n *input/output* couples $(\mu_i, y_i) \in \mathcal{P}(\mathbb{R}) \times \mathbb{R}$, and we are looking to associate an output to a new input μ_{n+1}.



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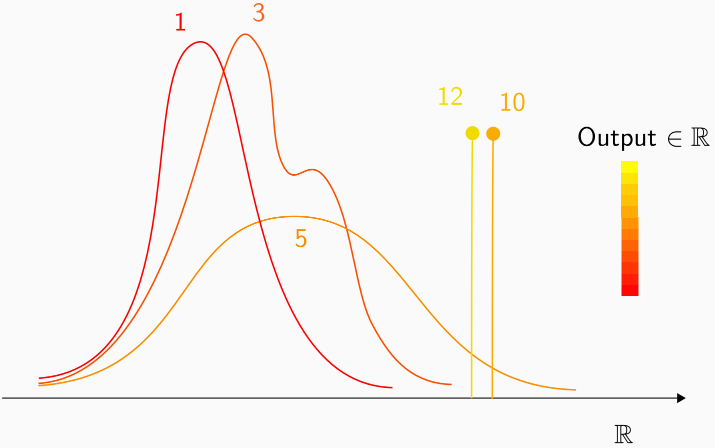

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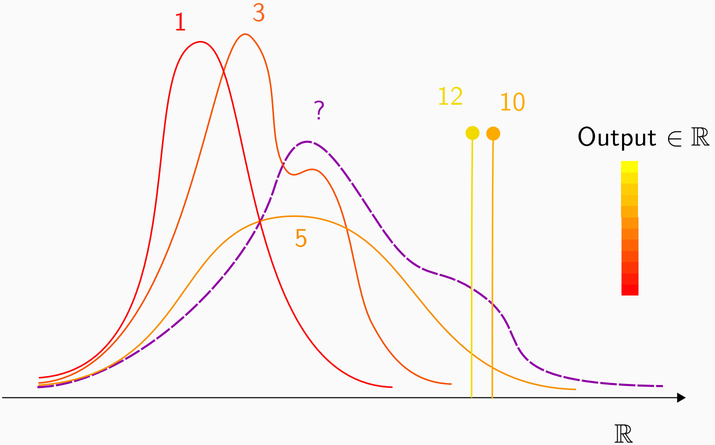


Motivations

Our motivations are threefold: we want to deal with regression problems which inputs are

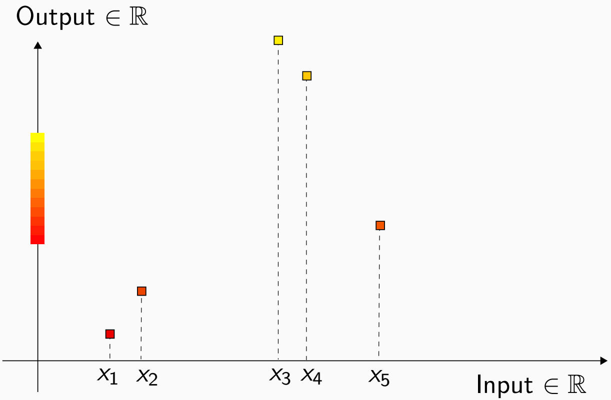
1. probability distributions (ex: blood sampling problem)
2. functional objects (spectra, histograms,...)
    - with the nonnegative values and mass 1 restrictions
    - ... which in turn allow the use of tools such as the Wasserstein distance

Outline of the presentation

1. Gaussian Process Regression
2. Existence of models – Stationary kernels on the Wasserstein space
3. Maximum-likelihood model selection – Asymptotic results
4. Numerical results

Gaussian Process Regression

Gaussian Process Regression (Kriging)



We chose a random process $(Y_x)_{x\in\mathbb{R}}$ and consider

$$\hat{Y}(x) := \mathbb{E}(Y_x | Y_{x_1} = y_1, \cdots, Y_{x_n} = y_n)$$

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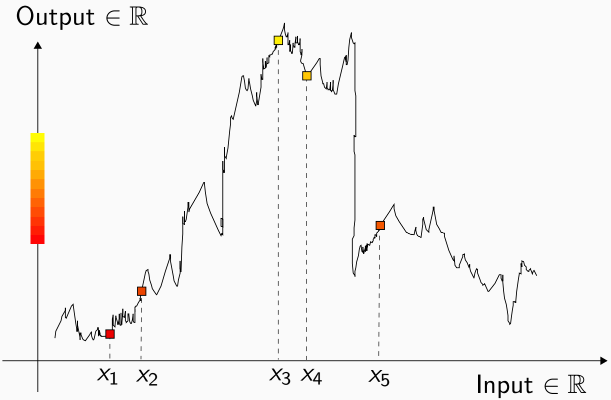

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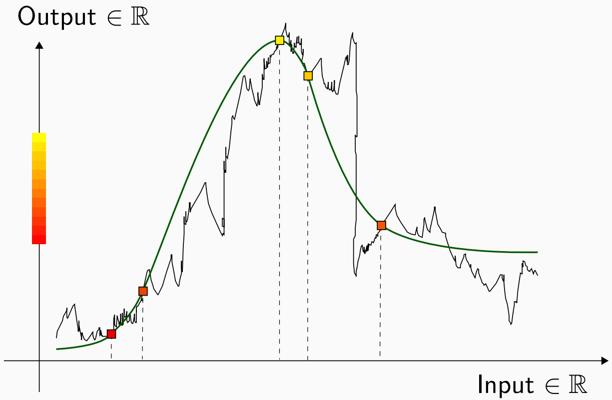

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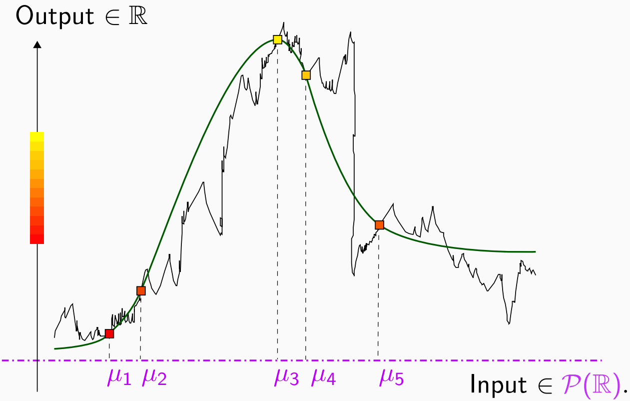


Here we need a random process $(Y_\mu)_{\mu \in \mathcal{P}(\mathbb{R})}$ to consider

$$\hat{Y}(\mu) := \mathbb{E}(Y_\mu | Y_{\mu_1} = y_1, \cdots, Y_{\mu_n} = y_n)$$

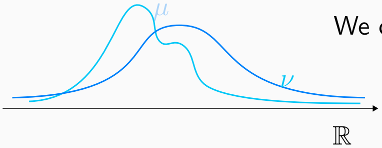
Existence of models – Stationary kernels on the Wasserstein space

The Wasserstein distance

The *Wasserstein distance* between two probability distributions μ and ν that admit a second order moment is defined by:

$$W_2(\mu,\nu) := \left(\inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathbb{R}^2} |x-y|^2 \, d\pi(x,y) \right)^{1/2},$$

where $\Pi(\mu,\nu)$ is the set of probability distributions on $\mathbb{R}^2$ with margins μ and ν.



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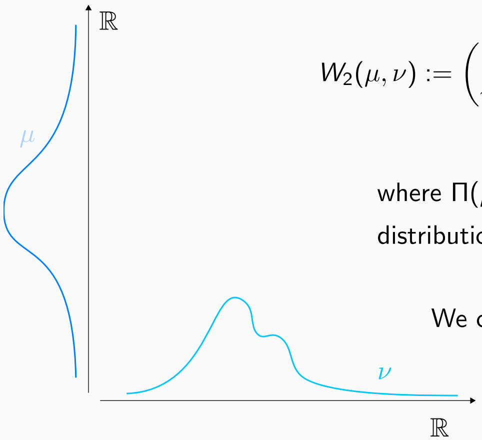

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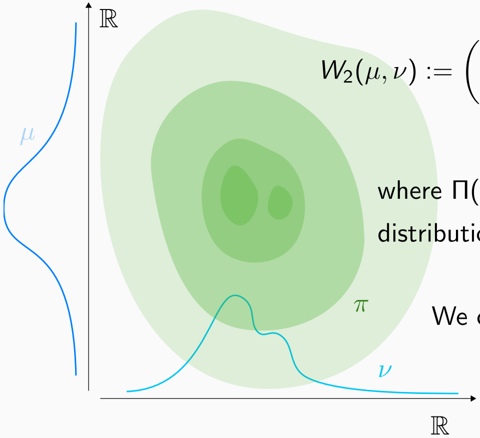

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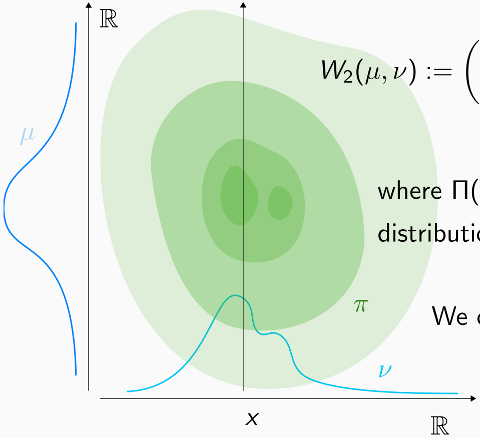

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A remark

For $\mu, \nu \in \mathcal{W}_2(\mathbb{R})$ and F_μ^{-1}, F_ν^{-1} the associated quantile functions,

$$W_2(\mu,\nu) = \left(\int_{[0,1]} \left(F_\mu^{-1}(u) - F_\nu^{-1}(u) \right)^2 du \right)^{1/2}. \tag{1}$$

- This optimal coupling, which is specific to the dimension 1 case, allows the numerical evaluation of Wasserstein distances.
- It is also the main ingredient of the proofs of Theorems 1 and 2.

Existence of Wasserstein-indexed models i

Theorem 1 (Fractional Brownian fields)

For ever $0 \leq H \leq 1$ *and* $\sigma_0 \in \mathcal{W}_2(\mathbb{R})$*,*

$$K^{H,\sigma}(\mu,\nu) = \frac{1}{2}\left(W_2^{2H}(\sigma_0,\mu) + W_2^{2H}(\sigma_0,\nu) - W_2^{2H}(\mu,\nu)\right) \tag{2}$$

is a covariance function on $\mathcal{W}_2(\mathbb{R})$*. Moreover, it is nondegenerated if and only if* $0 < H < 1$*.*

- We get a fractional Brownian field indexed by $\mathcal{W}_2(\mathbb{R})$. It is a generalisation of the time-indexed fractional Brownian motion, which inherits many enjoyable properties:
- Statistical auto-similarity, path-regularity and long distance memory that are governed by the *Hurst parameter* H.

Existence of Wasserstein-indexed models ii

Theorem 2 (Stationary processes)

For every completely monotone $F : \mathbb{R}^+ \to \mathbb{R}^+$ *and* $0 < H \leq 1$,

$$(\mu, \nu) \mapsto F\left(W_2^{2H}(\mu, \nu)\right) \tag{3}$$

is a stationary covariance function on $\mathcal{W}_2(\mathbb{R})$.

- Recall that $F \in C^\infty(\mathbb{R}^+, \mathbb{R}^+)$ is completely monotone if $(-1)^n F^{(n)}$ is nonnegatively valued for every $n \in \mathbb{N}$.
- In particular for every $\sigma^2, \ell > 0$ and $0 \leq H \leq 1$,

$$K_{\sigma^2,\ell,H}(\nu_1, \nu_2) = \sigma^2 \exp\left(-\frac{W_2(\nu_1, \nu_2)^{2H}}{\ell}\right) \tag{M}$$

is a valid covariance.

Maximum-likelihood model selection – Asymptotic results

Conditions for our results i

Condition 1 (Asymptotic expansion framework)

We consider a triangular array of observation points $\{\mu_1, ..., \mu_n\} = \{\mu_1^{(n)}, ..., \mu_n^{(n)}\}$ *so that for all* $n \in \mathbb{N}$ *and* $1 \leq i \leq n$, μ_i *has support in* $[i, i+K]$ *with a fixed* $K < \infty$.

Condition 2 (Parametric stationary model)

The model of covariance functions $\{K_\theta, \theta \in \Theta\}$ *satisfies*

$$\forall \theta \in \Theta, \ K_\theta(\mu, \nu) = F_\theta\left(W_2(\mu, \nu)\right),$$

with $F_\theta : \mathbb{R}^+ \to \mathbb{R}$ *and* $\sup_{\theta \in \Theta} |F_\theta(t)| \leq \frac{A}{1+|t|^{1+\tau}}$ *with a fixed* $A < \infty$, $\tau > 1$.

Conditions for our results ii

Condition 3 (Well-specified case)

We have observations $y_i = Y(\mu_i)$, $i = 1, \cdots, n$ *of the centered Gaussian Process* Y *with covariance function* K_{θ_0} *for some* $\theta_0 \in \Theta$.

Condition 4 (Asymptotical nondegeneracy)

The sequence of matrices $R_\theta = (K_\theta(\mu_i, \mu_j))_{1 \le i,j \le n}$ *satisfies*

$$\lambda_{\inf}(R_\theta) \ge c$$

for a fixed $c > 0$, *where* $\lambda_{\inf}(R_\theta)$ *denotes the smallest eigenvalue of* R_θ.

Conditions for our results iii

Condition 5

$\forall \alpha > 0$,

$$\liminf_{n\to\infty} \inf_{\|\theta-\theta_0\|\geq\alpha} \frac{1}{n} \sum_{i,j=1}^{n} \left[K_\theta(\mu_i, \mu_j) - K_{\theta_0}(\mu_i, \mu_j)\right]^2 > 0.$$

Consistency of the maximum-likelihood estimator

Theorem 3 (Consistency of MLE)

Under conditions 1 to 5, the maximum-likelihood estimator is consistent, that is to say:

$$\hat{\theta}_{ML} \xrightarrow[n\to\infty]{\mathbb{P}} \theta_0.$$

Supplementary conditions

Condition 6 (Model regularity)

- *$\forall t \geq 0$, $F_\theta(t)$ is $\mathcal{C}^1$ with respect to θ and verifies* $\sup_{\theta \in \Theta} \max_{i=1,\cdots,p} \left| \frac{\partial}{\partial \theta_i} F_\theta(t) \right| \leq \frac{A}{1+t^{1+\tau}}$*, where A, τ are defined in Condition 2.*
- *For every $t \geq 0$, $F_\theta(t)$ is $\mathcal{C}^3$ with respect to θ and $\forall q \in \{2,3\}$,* $\forall i_1 \cdots i_q \in \{1, \cdots p\}$,

$$\sup_{\theta \in \Theta} \max_{i=1,\cdots,p} \left| \frac{\partial}{\partial \theta_{i_1}} \cdots \frac{\partial}{\partial \theta_{i_q}} F_\theta(t) \right| \leq \frac{A}{1+|t|^{1+\tau}}.$$

- $\forall (\lambda_1 \cdots, \lambda_p) \neq (0, \cdots, 0)$,

$$\liminf_{n \to \infty} \frac{1}{n} \sum_{i,j=1}^{n} \left(\sum_{k=1}^{p} \lambda_k \frac{\partial}{\partial_{\theta_k}} K_{\theta_0}(\mu_i, \mu_j) \right)^2 > 0.$$

Asymptotic normality of the maximum-likelihood estimator

Theorem 4

Let M_{ML} be the $p \times p$ matrix defined by

$$(M_{ML})_{i,j} = \frac{1}{2n} Tr \left(K_{\theta_0}^{-1} \frac{\partial K_{\theta_0}}{\partial \theta_i} K_{\theta_0}^{-1} \frac{\partial K_{\theta_0}}{\partial \theta_j} \right).$$

Under conditions 1 to 6, the maximum-likelihood estimator is asymptotically normal:

$$\sqrt{n}\ M_{ML}^{1/2} \left(\hat{\theta}_{ML} - \theta_0 \right) \xrightarrow[n \to \infty]{\mathcal{L}} \mathcal{N}(0, I_p).$$

Moreover

$0 < \liminf_{n \to \infty} \lambda_{min}(M_{ML}) \leq \limsup_{n \to \infty} \lambda_{max}(M_{ML}) < +\infty.$

Kriging under the ML-estimated parameter

Theorem 5

Under conditions 1 to 6, the Kriging estimator under the ML-estimated parameter $\hat{\theta}_{ML}$ is asymptotically optimal:

$$\forall \mu \in \mathcal{W}_2(\mathbb{R}), \ \left| \hat{Y}_{\hat{\theta}_{ML}}(\mu) - \hat{Y}_{\theta_0}(\mu) \right| = o_{\mathbb{P}}(1).$$

Numerical results

Performances on simulated data

- Denote by $m_k(\nu)$ the order k moment of ν. We consider

$$F : \mathcal{W}_2(\mathbb{R}) \to \mathbb{R}$$

$$F(\nu) = \frac{m_1(\nu)}{0.05 + \sqrt{m_2(\nu) - m_1(\nu)^2}}, \tag{4}$$

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- Let us generate normal random variables $\nu_1, \cdots, \nu_{100}$, with means and variances drawn uniformly at random, randomly perturbed to exhibit irregularities.
- We estimate $\hat{\sigma}^2, \hat{\ell}, \hat{H}$ by maximising the maximum likelihood for the parametric model:

$$K_{\sigma^2,\ell,H}(\nu_1, \nu_2) = \sigma^2 \exp\left(-\frac{W_2(\nu_1, \nu_2)^{2H}}{\ell}\right). \tag{5}$$

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$$RMSE^2 = \frac{1}{500} \sum_{i=1}^{500} \left(F(\nu_{t,i}) - \hat{F}(\nu_{t,i}) \right)^2,$$

$$CIR_\alpha = \frac{1}{500} \sum_{i=1}^{500} \mathbf{1} \left\{ \left| F(\nu_{t,i}) - \hat{F}(\nu_{t,i}) \right| \leq q_\alpha \hat{\sigma}(\nu_{t,i}) \right\}.$$

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modèle	RMSE	$CIR_{0.9}$
"Wasserstein"	0.094	0.92
"Legendre" ordre 5	0.49	0.92
"Legendre" ordre 10	0.34	0.89
"Legendre" ordre 15	0.29	0.91
"PCA" ordre 5	0.63	0.82
"PCA" ordre 10	0.52	0.87
"PCA" ordre 15	0.47	0.93

Thank you for your attention

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Wanted:

Dataset with inputs on the cylinder $\mathbb{S}^1 \times \mathbb{R}$.