Robustness Assessment of Black-box Models

Quantile-constrained Wasserstein Projections and Isotonic Polynomial Approximations

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GdR MASCOT-NUM
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Introduction

Goal: Enhance the **confidence** in the practical usage of a black-box model, by assessing its **robustness to input perturbations.**

Challenges:

1. Define **generic**, but **understandable** input perturbations.
2. Unify ML interpretability and sensitivity analysis (SA)
    - ML: Features are modelled as **empirical probability measures**
    - SA: Inputs are modelled as **probability measures admitting a positive density.**
3. Local/Global robustness assessment of a model, or some of its key characteristics.

Illustrative example: Epistemic uncertainty on a riverbed's roughness near an industrial site.

Context

Let $P \in \mathcal{P}(\mathbb{R}^d)$ be an **initial** probability measure. We seek the solution of the projection problem

$$Q = \underset{G \in \mathcal{P}(\mathbb{R}^d)}{\operatorname{argmin}} \quad \mathcal{D}(P, G)$$
$$\text{s.t.} \quad G \in \mathcal{C}, \text{ and } C_P = C_Q$$

where $\mathcal{C} \subseteq \mathcal{P}(\mathbb{R}^d)$ is a **perturbation class**, and $\mathcal{D}$ a discrepancy between probability measures. Ideally, P and Q must have **the same copula**.

ML interpretability (Bachoc et al. 2020) and SA (Lemaître et al. 2015) work focus on the **Kullback-Leibler divergence** (KL) as a discrepancy, and **generalized moments** perturbations.

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Drawbacks:

- Generalized moments **may not exist**.
- Different results depending on P due to KL.

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Solutions:

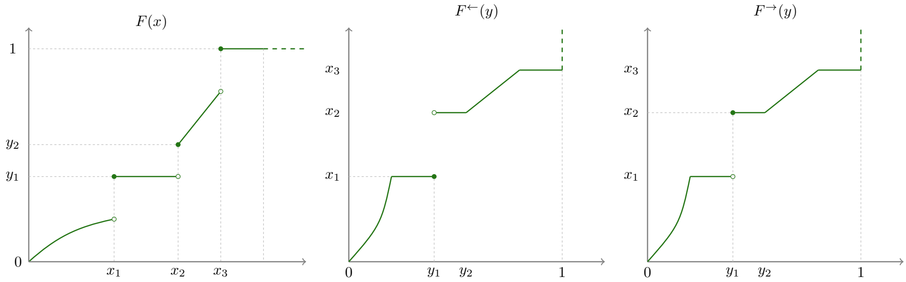
- **Quantile** perturbation class.
- 2-Wasserstein: does not depend on the nature of P.

Why quantiles ?

Generalized quantile functions are the generalized inverses (de la Fortelle 2015) of the cdf of random variables.

$$F_P^{\leftarrow}(a) = \sup\{t \in \mathbb{R} \mid F_P(t) < a\} \qquad F_P^{\rightarrow}(a) = \sup\{t \in \mathbb{R} \mid F_P(t) \leq a\}$$
$$= \inf\{t \in \mathbb{R} \mid F_P(t) \geq a\}. \qquad = \inf\{t \in \mathbb{R} \mid F_P(t) > a\},$$

- They **characterize** probability measures (Dufour 1995)
- Univariate quantiles **always exist**.



Quantile perturbation class

The **quantile perturbation class** $\mathcal{Q}_{\mathcal{V}}$ is defined using constraints of the form

$$F_Q^{\leftarrow}(\alpha) \geq b \geq F_Q^{\rightarrow}(\alpha).$$

with $b \in \mathbb{R}$, and leading to the set

$$\mathcal{Q}_{\mathcal{V}} = \left\{ Q \in \mathcal{P}(\mathbb{R}) \mid F_Q^{\leftarrow} \in \mathcal{V}, \quad F_Q^{\leftarrow}(\alpha_i) \geq b_i \geq F_Q^{\rightarrow}(\alpha_i), i = 1, \ldots, K \right\}.$$

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Collections of perturbations can be driven by an **intensity parameter** $\theta \in [-1, 1]$

- **Quantile shift:** shifting the α-quantile of P between two values.
- **Operating domain dilatation:** widewing or narrowing the bounds of the support of P w.r.t. a scaling parameter $\eta \in \mathbb{R}$.

Additional ponctual **modelling constraints** can also be added (e.g., preservation of empirical quantiles, expert knowledge).

The Wasserstein distance

For two probability measure $P, Q \in \mathcal{P}(\mathbb{R}^d)$ **having the same copula** (Alfonsi and Jourdain 2014):

$$W_p^p(P, Q) = \sum_{i=1}^{d} W_p^p(P_i, Q_i). \tag{1}$$

where each $P_i, Q_i \in \mathcal{P}(\mathbb{R})$ is a marginal distribution. Each element of the sum reduces to (Santambrogio 2015):

$$W_p^p(P_i, Q_i) = \int_0^1 \left| F_{P_i}^{\rightarrow}(x) - F_{Q_i}^{\rightarrow}(x) \right|^p dx$$

whatever the “nature” of P (empirical, continuous...).

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- **Solving d univariate perturbation problems.**
- **Optimal transportation map preserves the copula:** $T_i = (F_{Q_i}^{\leftarrow} \circ F_{P_i})$

Wasserstein and L^2 projections

Hence, one focuses on the marginal perturbation problem:

$$\begin{aligned} Q = \operatorname*{argmin}_{G \in \mathcal{P}(\mathbb{R})} \quad & W_2\left(P, G\right) \\ \text{s.t.} \quad & G \in \mathcal{Q}_{\mathcal{V}} \end{aligned} \tag{2}$$

Proposition

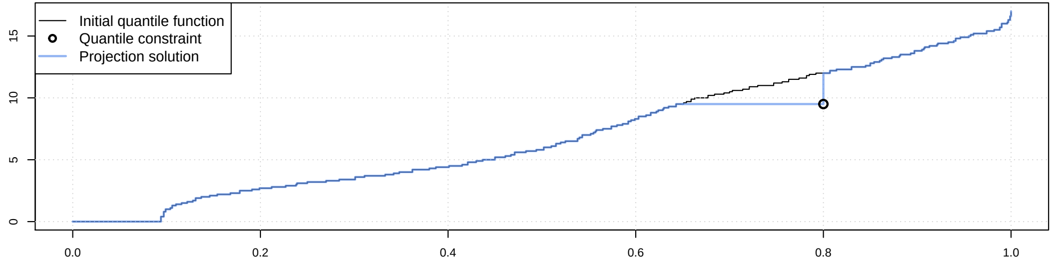
The solution Q of the problem in Eq. (2) is uniquely characterized by its quantile function being the solution

$$\begin{aligned} F_Q^{\leftarrow} = \operatorname*{argmin}_{L \in L^2([0,1])} \quad & \int_0^1 \left(L(x) - F_P^{\rightarrow}(x)\right)^2 \\ s.t. \quad & L(\alpha_i) \leq b_i \leq L\left(\alpha_i^+\right), \quad i = 1, \ldots, K, \\ & L \in \mathcal{V} \end{aligned}$$

Solving the perturbation problem

If $\mathcal{V} = \mathcal{F}^{\leftarrow}$, there exists a **unique analytical solution** Q to the problem:

Q is the same as P, except on the intervals between $F_P^{\leftarrow}(\alpha_i)$ and b_i which have no mass, and an atom is added at b_i, taking the initial mass of the interval.



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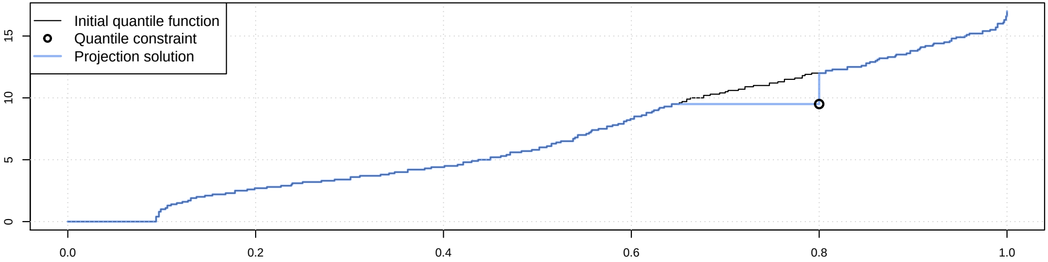


How to explicitly enforce “smoothness” to the resulting perturbed quantile function ?

Isotonic interpolating piece-wise continuous polynomials

Idea: Using piece-wise continuous polynomials of degree p to ensure continuity.

Partition $[0,1]$ according into interval $[t_j, t_{j+1}]$, $i = 0, \ldots, K$ with $t_0 = 0$, $t_{K+1} = 1$, and $t_i = \alpha_i$ (ordered increasingly), and solve for

$$
\begin{aligned}
S = \underset{G \in \mathbb{R}[x]_{\leq p}}{\text{argmin}} \quad & \int_{t_i}^{t_{i+1}} (F_P^{\rightarrow}(x) - G(x))^2 dx \\
\text{s.t.} \quad & G(t_i) = b_i, G(t_{i+1}) = b_{i+1} \\
& G'(x) \geq 0, \quad \forall x \in [t_0, t_1]
\end{aligned}
\tag{3}
$$

Proposition

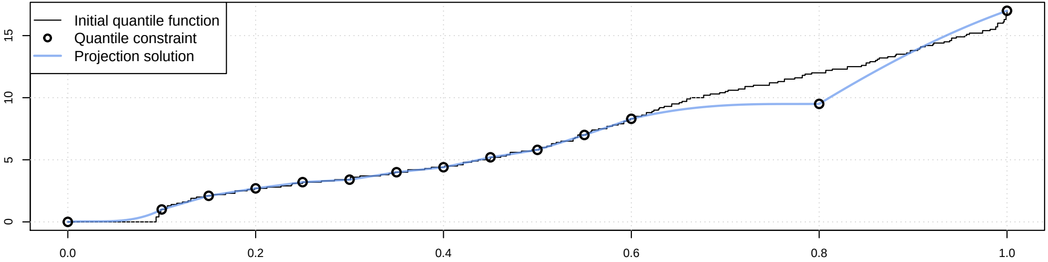
The polynomial solution of Eq. (3) admits as coefficients

$$
\begin{aligned}
s^* = \underset{s \in \mathbb{R}^{p+1}}{\text{argmin}} \quad & s^\top M s - 2 s^\top r \\
\text{s.t.} \quad & s \in \mathcal{K}
\end{aligned}
$$

where M is the moment matrix of the Lebesgue measure on $[t_i, t_{i+1}]$, r is the moment vector of $F_P^{\rightarrow}$, and $\mathcal{K}$ is a closed convex subset of $\mathbb{R}^{p+1}$.

Isotonic interpolation piece-wise continuous polynomials

It is a **Convex Constrained Quadratic Problem** which can be solved using numerical solvers (e.g., `CVXR` (Fu, Narasimhan, and Boyd 2020)).



Each marginal input $X_i \sim P_i$ can be perturbed using the optimal monotone perturbation map

$$\widetilde{X}_i = T_i(X_i) = (F_{Q_i}^{\leftarrow} \circ F_{P_i})(X_i)$$

preserving the (empirical) copula between all the inputs.

SIPA framework for model-agnostic interpretation

Our methodology follows the **SIPA** framework (Scholbeck et al. 2020):

1. **Sampling**: **Observed** (ML) or **simulated** (UQ) values of P.
2. **Intervention**: Define **optimal perturbations** under **quantile constraints** and apply the **perturbation map**, resulting in perturbed inputs $\widetilde{X} = T(X)$ with the **same dependence structure**.
3. **Prediction**: Evaluate the model G (numerical in UQ, learned in ML) on the perturbed inputs.
4. **Aggregation**: Estimate **local** or **global** statistics on the perturbed output $\widetilde{Y} = G(\widetilde{X})$.

Simplified hydrological model

Model of the water level of a river. Simplification of the one-dimensional Saint-Venant equation, with a uniform and constant flow rate (Iooss and Lemaître 2015; Fu, Couplet, and Bousquet 2017)

- Q: River maximum annual water flow rate.
- K_s: Strickler riverbed roughness coefficient.
- Z_v: Downstream river level.
- Z_m: Upstream river level.
- L: River length.
- B: River width.

Input	Distribution	Application Domain
Q	$\mathcal{G}(1013, 558)$ trunc.	$[500, 3000]$
K_s	$\mathcal{N}(35, 5)$ trunc.	$[20, 50]$
Z_v	$\mathcal{T}(49, 50, 51)$	$[49, 51]$
Z_m	$\mathcal{T}(54, 55, 56)$	$[54, 56]$
L	$\mathcal{T}(4990, 5000, 5010)$	$[4990, 5010]$
B	$\mathcal{T}(295, 300, 305)$	$[295, 305]$

Model:

$$Y = Z_v + \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}} \right)^{3/5}$$

Gaussian copula with covariance matrix :

$$R_P = \begin{pmatrix} 1 & 0.5 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0.3 & 0 & 0 \\ 0 & 0 & 0.3 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0.3 \\ 0 & 0 & 0 & 0 & 0.3 & 1 \end{pmatrix}$$

Perturbation strategy

Ponctual perturbations

Q:

- Shift of the application domain from $[500, 3000]$ to $[500, 3200]$.
- Preserve the median of the distribution.
- Increase the initial 0.15-quantile by 75.
- Decrease the initial 0.75-quantile by 125.

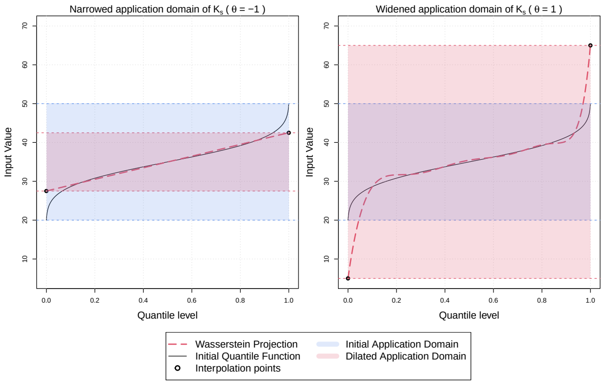
L:

- Shift the application domain from $[4990, 5010]$ to $[4988, 5012]$.
- Preserve the median of the distribution.

Z_m:

- Preserve the application domain and the median of the initial distribution.
- Increase the 0.8 and 0.9-quantiles by 0.1.
- Decrease the 0.25-quantile by 0.05.

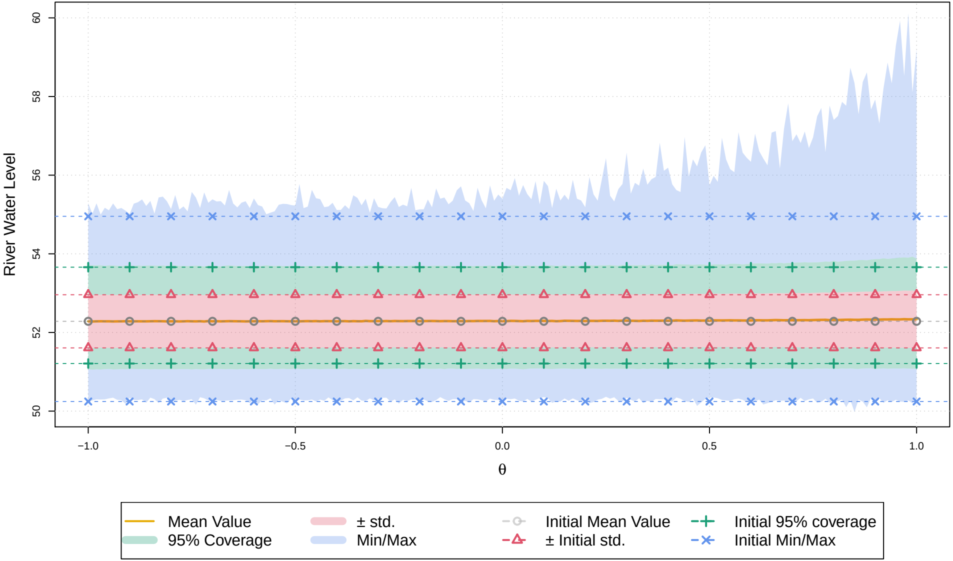
Application domain dilatation on K_s $(\eta = 2)$



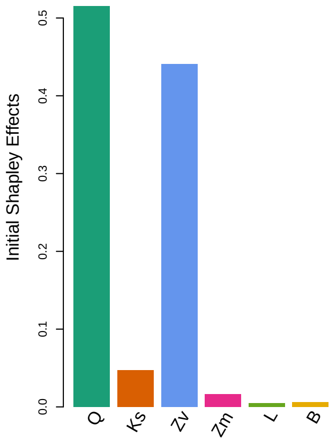
- $\theta = -1$: Riverbed between a slow winding natural river, up to a plain river without shrub vegetation ($K_s \in [27.5, 42.5]$).
- $\theta = 1$: Riverbed roughness from proliferating algae up to smooth concrete ($K_s \in [5, 65]$).

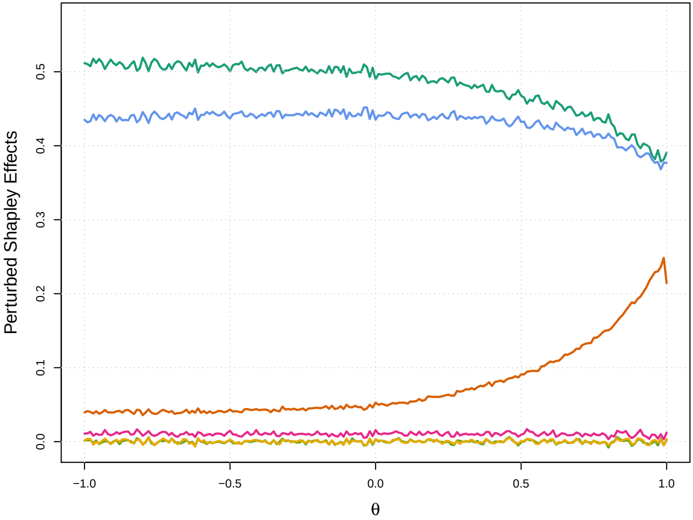
Optimal perturbation problems are solved with polynomial smoothing (arbitrary degree equal to 12).

Global statistics



Shapley effects





Double Monte Carlo estimation with $N_v = 10^5$, $N_o = 3 \times 10^3$ and $N_i = 300$.

Conclusion & perspectives

Generic and interpretable **marginal perturbation scheme**.

Local and global robustness assessment of black-box numerical (SA) and predictive models (ML).

Perspectives:

- Optimal degree selection, and derivability of the resulting polynomial.
- Multivariate quantile perturbation.
- More general smoothing spaces (monotone Sobolev functions, RKHS).

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More details and ML application (Acoustic Fire Extinguisher) in our pre-print (HAL/arXiv) (I. et al. 2022):

Quantile-constrained Wasserstein projections for robust interpretability of numerical and machine learning models

Marouane Il Idrissi[a,b,c,e], Nicolas Bousquet[a,b,d], Fabrice Gamboa[c], Bertrand Iooss[a,b,c], Jean-Michel Loubes[c]

References i

Alfonsi, A., and B. Jourdain. 2014. "A remark on the optimal transport between two probability measures sharing the same copula" [in en]. *Statistics & Probability Letters* 84 (January): 131–134. ISSN: 0167-7152. https://doi.org/10.1016/j.spl.2013.09.035. https://www.sciencedirect.com/science/article/pii/S0167715213003337.

Bachoc, F., F. Gamboa, M. Halford, J-M. Loubes, and L. Risser. 2020. "Explaining Machine Learning Models using Entropic Variable Projection" [in en]. ArXiv: 1810.07924, *arXiv:1810.07924* [*cs, stat*] (December). http://arxiv.org/abs/1810.07924.

de la Fortelle, A. 2015. "A study on generalized inverses and increasing functions Part I: generalized inverses" [in en], 14. https://hal-mines-paristech.archives-ouvertes.fr/hal-01255512.

Dufour, J-M. 1995. *Distribution and quantile functions* [in en]. https://jeanmariedufour.github.io/ResE/Dufour_1995_C_Distribution_Quantile_W.pdf.

Fu, A., B. Narasimhan, and S. Boyd. 2020. "CVXR: An R Package for Disciplined Convex Optimization." *Journal of Statistical Software* 94 (14): 1–34. https://doi.org/10.18637/jss.v094.i14.

Fu, S., M. Couplet, and N. Bousquet. 2017. "An adaptive kriging method for solving nonlinear inverse statistical problems" [in en]. *Environmetrics* 28 (4): e2439. ISSN: 1099-095X. https://doi.org/10.1002/env.2439. https://onlinelibrary.wiley.com/doi/abs/10.1002/env.2439.

I., M., N. Bousquet, F. Gamboa, B. Iooss, and J-M. Loubes. 2022. "Quantile-constrained Wasserstein projections for robust interpretability of numerical and machine learning models." September. https://hal.archives-ouvertes.fr/hal-03784768.

References ii

Iooss, B., and P. Lemaître. 2015. "A Review on Global Sensitivity Analysis Methods." In *Uncertainty Management in Simulation-Optimization of Complex Systems: Algorithms and Applications,* edited by G. Dellino and C. Meloni, 101–122. Springer US. https://doi.org/10.1007/978-1-4899-7547-8_5. https://doi.org/10.1007/978-1-4899-7547-8_5.

Lemaître, P., E. Sergienko, A. Arnaud, N. Bousquet, F. Gamboa, and B. Iooss. 2015. "Density modification-based reliability sensitivity analysis." *Journal of Statistical Computation and Simulation* 85 (6): 1200–1223. https://doi.org/10.1080/00949655.2013.873039. eprint: https://doi.org/10.1080/00949655.2013.873039. https://doi.org/10.1080/00949655.2013.873039.

Santambrogio, F. 2015. *Optimal Transport for Applied Mathematicians.* Vol. 87. Progress in Nonlinear Differential Equations and Their Applications. Cham: Springer International Publishing. ISBN: 978-3-319-20827-5 978-3-319-20828-2. https://doi.org/10.1007/978-3-319-20828-2. http://link.springer.com/10.1007/978-3-319-20828-2.

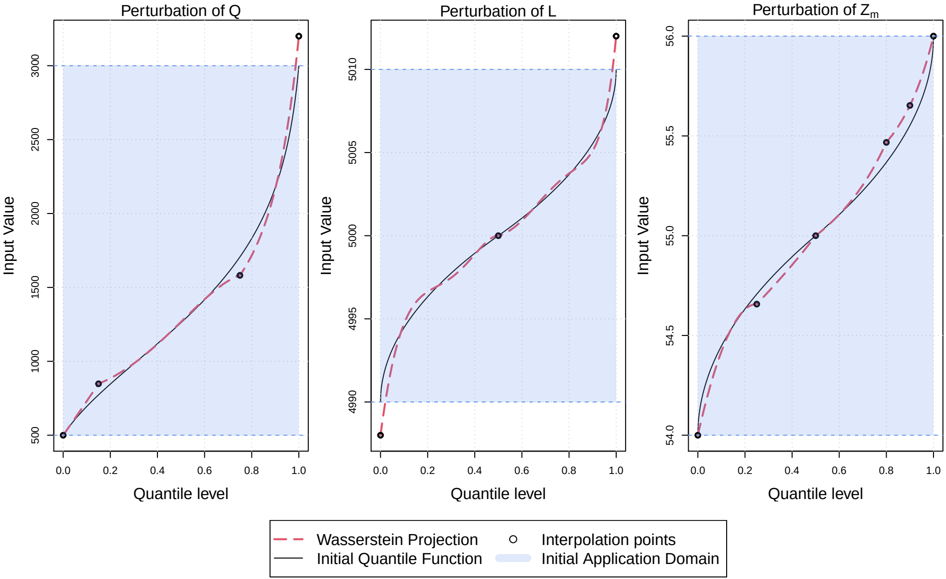
Scholbeck, Christian A., Christoph Molnar, Christian Heumann, Bernd Bischl, and Giuseppe Casalicchio. 2020. "Sampling, Intervention, Prediction, Aggregation: A Generalized Framework for Model-Agnostic Interpretations" [in en]. In *Machine Learning and Knowledge Discovery in Databases,* edited by Peggy Cellier and Kurt Driessens, 205–216. Communications in Computer and Information Science. Cham: Springer International Publishing. ISBN: 978-3-030-43823-4. https://doi.org/10.1007/978-3-030-43823-4_18.

Villani, C. 2003. *Topics in Optimal Transportation* [in en]. Vol. 58. Graduate Studies in Mathematics. ISSN: 1065-7339. American Mathematical Society, March. ISBN: 978-0-8218-3312-4 978-0-8218-7232-1 978-1-4704-1804-5, accessed June 23, 2021. https://doi.org/10.1090/gsm/058. http://www.ams.org/gsm/058.

Thank you for your attention!

Any questions?

River water level ponctual perturbations



Copula preservation

Let $\mathcal{X} \subseteq \mathbb{R}^d$, for d a positive integer, and $P \in \mathcal{P}(\mathcal{X})$. Let Q_i be the solution of the optimal projection problem with $\mathcal{C} = \mathcal{C}_{\mathcal{V}}$, for every marginal distribution P_i of P, $i = 1, \ldots, d$, and where $\mathcal{V} \subseteq \otimes_{j=1}^{d} \mathcal{F}_j^{\leftarrow}$. Let the random vectors

$$X \sim P, \quad \widetilde{X} := T(X)$$

where

$$\begin{aligned} T : \quad & \mathcal{X} & \to \quad & \mathcal{X} \\ & \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} & \mapsto \quad & \begin{pmatrix} T_1(x_1) \\ \vdots \\ T_d(x_d) \end{pmatrix} \end{aligned} \tag{4}$$

where

$$T_j = \left(F_{Q_j}^{\leftarrow} \circ F_{P_j} \right), \quad j = 1, \ldots, d.$$

1. If P is an empirical measure (i.e., X represents a dataset), then X and the perturbed dataset $\widetilde{X}$ have the same empirical copula. Moreover, the empirical measure of every perturbed marginal sample $\widetilde{X}_i$ converges towards Q_i, $i = 1, \ldots, d$.
2. If P is atomless, and assuming additionally that $\mathcal{V}$ is such that every $F_{Q_i}^{\leftarrow}$, $i = 1, \ldots, d$ is strictly increasing, then the random vectors X and $\widetilde{X}$ have the same copula. Moreover, each perturbed marginal $\widetilde{X}_i \sim Q_i$.

Projecting without smoothing

Let P be a probability measure in $\mathcal{P}_2(\mathbb{R})$. Let $\mathcal{C}$ be a non-empty perturbation class characterized by a set of K quantile constraints. Assume, without loss of generality, for $i = 1, \ldots, K$, that $\alpha_1 < \cdots < \alpha_K$ along with $b_1 < \cdots < b_K$. Let $\beta_i = F_P(b_i)$ for $i = 1, \ldots, K$. Define the intervals $A_i = (c_i, d_i]$ for $i = 1, \ldots, K$, such that:

$$c_1 = \min(\beta_1, \alpha_1), \quad c_i = \min\left[\max(\alpha_{i-1}, \beta_i), \alpha_i\right], i = 2, \ldots, K,$$
$$d_K = \max(\beta_K, \alpha_K), \quad d_j = \max\left[\min(\beta_j, \alpha_{j+1}), \alpha_j\right], j = 1, \ldots, K-1.$$

Let $A = \bigcup_{i=1}^{K} A_i$ and $\overline{A} = [0,1] \setminus A$. Then the problem has a unique solution which can be written as, for any $y \in [0,1]$:

$$F_Q^{\leftarrow}(y) = \begin{cases} F_P^{\rightarrow}(y) & \text{if } y \in \overline{A}, \\ b_i & \text{if } y \in A_i, \quad i = 1, \ldots, K. \end{cases} \tag{5}$$

Non-negativity of polynomials on closed intervals

Theorem (Non-negativity of polynomials on closed intervals)

Let $t_0, t_1 \in \mathbb{R}$ such that $t_0 < t_1$, and let $p \in \mathbb{N}^*$.

A univariate polynomial S of even degree $d = 2p$ is non-negative on $[t_0, t_1]$ if and only if it can be written as, $\forall x \in [t_0, t_1]$

$$S(x) = Z(x) + (x - t_0)(t_1 - x)W(x)$$

where Z is an SOS polynomial of degree at most equal to d, and W is an SOS polynomial of degree at most equal to $d - 2$.

A univariate polynomial S of odd degree $d = 2p + 1$ is non-negative on $[t_0, t_1]$ if and only if it can be written as, $\forall x \in [t_0, t_1]$

$$S(x) = (x - t_0)Z(x) + (t_1 - x)W(x)$$

where Z, W are SOS polynomials of degree at most equal to d.

SDP representation of SOS polynomials

Let S be an univariate polynomial of even degree $d = 2p$, with coefficients $s = (s_0, \dots, s_d)$, and denote x_p the usual monomial basis of polynomials of degree at most equal to p, i.e., $x_p = (1, x, x^2, \dots, x^{p-1}, x^p)^\top$. S is an SOS polynomial if and only if there exists a $(p \times p)$ symmetric semi definite positive (SDP) matrix

$$\Gamma = \left[\Gamma_{ij}\right]_{i,j=1,\dots,p}$$

that satisfies, $\forall x \in \mathbb{R}$,

$$S(x) = x_p^\top \Gamma x_p.$$

Moreover, for $k = 0, \dots, d$, let $\mathbb{I}_k^p$ be the $(p \times p)$ matrix defined by, for $i, j = 1, \dots, p$:

$$\left[\mathbb{I}_k^p\right]_{i,j} = \mathbb{1}_{\{i+j=k+2\}}(i,j).$$

If there exists a matrix Γ such that S is SOS, then one has that, for $i = 0, \dots, d$

$$s_i = \langle \mathbb{I}_i^p, \Gamma \rangle_F = \sum_{j+k=i+2} \Gamma_{j,k}$$

where, $\langle ., . \rangle_F$ denotes the Frobenius norm on matrices.

Equivalent optimization formulation

Let $[t_0, t_1] \subset [0, 1]$, and let $s = (s_0, \dots, s_d)^\top \in \mathbb{R}^{d+1}$, M be the symmetric $((d+1 \times d+1))$ moment matrix of the Lebesgue measure on $[t_0, t_1]$, i.e. for $i, j = 1, \dots, d+1$,

$$M_{ij} = \int_{t_0}^{t_1} x^{i+j-2} dx = \frac{(t_1)^{i+j-1} - (t_0)^{i+j-1}}{i+j-1},$$

and denote $r \in \mathbb{R}^{d+1}$ the moment vector of $A(x)$, i.e., for $i = 0, \dots, d$

$$r_i = \int_{t_0}^{t_1} x^i F_P^{\leftarrow}(x) dx$$

Then, the optimization problem can be equivalently solved by finding s as being the solution of the following convex constrained quadratic program,

$$s^* = \operatorname*{argmin}_{s \in \mathbb{R}^{p+1}} s^\top M s - 2 s^\top r$$
$$\text{s.t. } s \in \mathcal{K}$$

where $\mathcal{K}$ is a closed convex subset of $\mathbb{R}^{p+1}$.