Estimation of deformation between distributions by minimal Wasserstein distance

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Summary

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- We observe a random variable and a deformation of this variable

$$\begin{cases} \varepsilon \\ X = \varphi(\varepsilon) \end{cases}$$

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- How to extract information? : estimation of the deformation, study of a mean distribution if several deformations are observed...

Warped curves

- Dynamic Time Warping. **Sakoe-Chiba-[1978]**
  Align two signals $(f(i))_{1\leqslant i\leqslant N}$ and $(g(j))_{1\leqslant j\leqslant M}$ by a time axis re normalization.
  Idea : to consider some "warping operators" between $1 \leqslant i \leqslant N$ and $1 \leqslant j \leqslant M$.
  $\rightsquigarrow$ Minimize a cost

$$C(w, f, g) = \sum_{(i,j)\in w} (f(i) - g(j))^2 .$$

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- Extension to warped curves in a regression scheme : **Wang-Gasser-[1999]**, **Gamboa-Loubes-Maza-[2007]**. Different cost functions.

Deformation of distributions

- Observations $X_j = \varphi_j(\varepsilon)$, $1 \leqslant j \leqslant J$ where φ_j are realizations of a random process.
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- Test for a parametric relationship between two distributions in terms of quantile functions $F^{-1} = \mathcal{F}\left(G^{-1}, \theta\right)$. Test statistic based on the L^2 norm between quantile functions in **Freitag-Munk-[2005]**.

Model studied

Semi parametric framework

$$\begin{cases} \varepsilon \\ X = \varphi_{\theta^\star}(\varepsilon) \end{cases}$$

- shape of the deformation φ assumed **known**,
- deformation parameter $\theta^\star$ and template measure μ of ε to estimate.

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- shape of the deformation φ assumed **known**,
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Idea: **Align** the distribution of X on the distribution of ε.
$\rightsquigarrow$ Study of $Z(\theta) = \varphi_\theta^{-1}(X) = \varphi_\theta^{-1} \circ \varphi_{\theta^\star}(\varepsilon)$.

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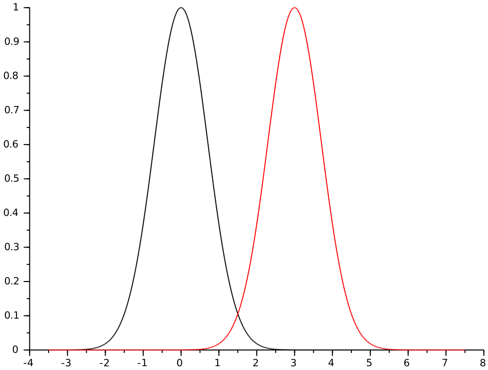

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$\rightarrow$ Align the distribution of $Z(\theta)$ on the distribution of ε by varying θ. Minimization of a D.T.W. criterion.

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$\rightarrow$ Which cost function? Requires a distance between probabilities. Utilization of the **Wasserstein distance** related to problems of mass transport.

Summary

Presentation of the model

Observations :

$$\begin{cases} \varepsilon_{i1} & 1 \leqslant i \leqslant n \\ X_i = \varphi_{\theta^\star}(\varepsilon_{i2}) & 1 \leqslant i \leqslant n \end{cases} \tag{1}$$

- structure : $(\varepsilon_{ij})_{\substack{1 \leqslant i \leqslant n \\ j=1,2}}$ i.i.d. following the law μ,
- deformation parameter : $\theta^\star$ where $\theta^\star \in \Theta \subset \mathbb{R}^d$,
- deformation function : $\varphi_\theta :]a;b[\to]c;d[$ invertible for $\theta \in \Theta$,
- Empirical distribution of the i.i.d. sample $(\varepsilon_{i1})_{1 \leqslant i \leqslant n}$: μ_1^n .

For $\theta \in \Theta$ we define

$$Z_i(\theta) = \varphi_\theta^{-1}(X_i) = \varphi_\theta^{-1} \circ \varphi_{\theta^\star}(\varepsilon_{i2})$$

- Distribution of $Z_1(\theta)$: $\mu_\star(\theta) = \mu \circ \varphi_{\theta^\star}^{-1} \circ \varphi_\theta$,
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$\Rightarrow$ Recover $\theta^\star$ by minimizing the energy needed to align the distribution $\mu_\star(\theta)$ on μ :$\mu_\star(\theta^\star) = \mu$.
Wasserstein distance to quantify the alignment.

Wasserstein distance

Set $\mathcal{W}_2(\mathbb{R}) = \left\{P \text{ probability on } \mathbb{R}, \int_{\mathbb{R}} x^2 dP < \infty\right\}$.
For $P, Q \in \mathcal{W}_2(\mathbb{R})$ with respective distribution function F and G, their Wasserstein distance is

$$W_2^2(P, Q) = \int_0^1 \left(F^{-1}(t) - G^{-1}(t)\right)^2 dt. \tag{2}$$

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If P and Q are defined on more general metric space (S, d) with a moment of order 2 :

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- Set $X_n \sim P_n, X \sim P$.
  Then $W_2(P_n, P) \to 0 \iff \begin{cases} X_n \rightharpoonup X \\ \mathbb{E}\left[X_n^2\right] \to \mathbb{E}\left[X^2\right] \end{cases}$

The estimators

To quantify the alignment of the measures, consider the criterion

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$\rightarrow$ Empirical version :

$$M_n(\theta) = W_2^2(\mu_\star^n(\theta), \mu_1^n)$$

with the order statistics

$$M_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left[Z_{(i)}(\theta) - \varepsilon_{(i)1} \right]^2 . \tag{4}$$

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Estimator of $\theta^\star$

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We have $\varphi_{\widehat{\theta}^n}^{-1}(X_i) = \varphi_{\widehat{\theta}^n}^{-1} \circ \varphi_{\theta^\star}(\varepsilon_{i2}) \approx \varepsilon_{i2}$, following the unknown law μ.

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Estimator of $\theta^\star$

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We have $\varphi^{-1}_{\widehat{\theta}^n}(X_i) = \varphi^{-1}_{\widehat{\theta}^n} \circ \varphi_{\theta^\star}(\varepsilon_{i2}) \approx \varepsilon_{i2}$, following the unknown law μ.

- Plugg-in estimator of μ

$$\widehat{\mu}^n = \frac{1}{n} \sum_{i=1}^{n} 1_{\varphi^{-1}_{\widehat{\theta}^n}(X_i)} \tag{6}$$

Idea : "increase" the size of $(\varepsilon_{i1})_{1 \leqslant i \leqslant n} \rightsquigarrow \widetilde{\mu}^n = \frac{1}{2}\left(\widehat{\mu}^n + \mu_1^n\right)$

Summary

Principle of M-estimation

→ Convergence criterion for estimators defined as minimizers of a random functional M_n on a set Θ.

$$
\begin{array}{ccc}
M_n(\theta) & \xrightarrow{n\to\infty} & M(\theta) \\
\min \uparrow & & \min \uparrow \\
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<u>Consistency criterion</u>

- If M is a deterministic function,
- $sup_{\theta\in\Theta} |M_n(\theta) - M(\theta)| \xrightarrow{n\to\infty} 0$ in probability,
- $\forall\delta > 0 \quad \inf_{\theta\in\Theta\cap B(\theta^\star,\delta)^c} M(\theta) > M(\theta^\star)$

then $\widehat{\theta}^n \xrightarrow{n\to\infty} \theta^\star$ in probability.

Assumptions

- Laws considered are defined on subsets of $\mathbb{R}$ and $\forall\theta \in \Theta$, $\mu_\star(\theta) \in \mathcal{W}_2(\mathbb{R})$.
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$$\sup_{\theta\in\Theta} \left\|\partial\varphi_\theta^{-1}(x)\right\| \leqslant H(x) \text{ with } H \in L^2(X)$$

  $\Rightarrow$ Control the distance between $\mu_\star\left(\theta^1\right)$ and $\mu_\star\left(\theta^2\right)$ for $\theta^1, \theta^2 \in \Theta$.

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  $\Rightarrow$ Uniform convergence and Taylor expansion.
- Identifiability condition : for all $\theta \neq \theta^\star$, $\varphi_\theta^{-1} \circ \varphi_{\theta^\star} \neq Id$ on a set of positive μ-measure.
  $\Rightarrow$ Uniqueness of the minimizer of the function M.

Consistency results

Deformation estimator

$$\widehat{\theta}^n \in argmin_{\theta\in\Theta} M_n\left(\theta\right) :$$

Theorem

Under previous assumptions $\widehat{\theta}^n$ converges in probability to $\theta^\star$.

Measure estimator

$$\widehat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} 1_{\varphi^{-1}_{\widehat{\theta}^n}(X_i)}$$

Theorem

Under previous assumptions

$$W_2\left(\widehat{\mu}_n, \mu\right) \xrightarrow{n\to\infty} 0 \text{ in probability.}$$

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In addition to the previous assumptions, we assume

- More regularity : φ^{-1} is C^2 with respect to its two variables (θ, x).

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- More regularity : φ^{-1} is C^2 with respect to its two variables (θ, x).
- The distribution of X has a compact support with distribution function $F_\star$ C^1. We assume $F'_\star := f_\star > 0$ on its support.

$\Rightarrow$ The distribution function F associated with the law μ (law of ε) has a compact support and is C^1 with $F' = f > 0$.

Result

Set $\Phi = \int_0^1 \partial\varphi_{\theta^\star}^{-1}\left(F_\star^{-1}(t)\right)^2 dt \in \mathbb{R}^{d\times d}$.

Theorem

Under previous assumptions and if Φ is invertible, then

$$\sqrt{n}\left(\widehat{\theta}^n - \theta^\star\right) \rightharpoonup \Phi^{-1}\int_0^1 \frac{\partial\varphi_{\theta^\star}^{-1}\left(F_\star^{-1}(t)\right)}{f(F^{-1}(t))}\left[\mathbb{G}_2(t) - \mathbb{G}_1(t)\right] dt$$

where $\mathbb{G}_1$ and $\mathbb{G}_2$ are independent standard Brownian bridges.

Idea of proof

$\rightarrow$ Remains to study $\Psi\left(F^n, F_\star^n\right)$ where F^n (resp. $F_\star^n$) is the empirical distribution function associated with the sample $(\varepsilon_{i1})_{1\leqslant i\leqslant n}$ (resp. $(X_i)_{1\leqslant i\leqslant n}$).

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Convergence of the empirical distribution functions :

Theorem (Donsker)

If $Y_1, \ldots, Y_n$ are i.i.d. random variables with distribution function F and empirical distribution function F_n, the sequence $\sqrt{n}\,(F_n - F)$ converges in law in $\mathbb{S}$, the space of function cadlag on $\bar{\mathbb{R}}$ endowed with the norm $\|\cdot\|_{\infty}$ to $\mathbb{G}\circ F$ where $\mathbb{G}$ is a standard Brownian bridge.

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$\Rightarrow$ Application of a **Delta-method**.

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Examples

- Example 1 : Translation model

$$\varphi_\theta(x) = x + \theta$$

$\Rightarrow \mu \in \mathcal{W}_2(\mathbb{R})$, and $\Theta \subset \mathbb{R}$ compact interval.

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$$\begin{cases} \varepsilon_{i1} \\ X_i = \theta^\star + \varepsilon_{i2} \end{cases} \quad 1 \leqslant i \leqslant n$$

$$\widehat{\theta}^n = \frac{1}{n}\sum_{i=1}^n X_i - \frac{1}{n}\sum_{i=1}^n \varepsilon_{i1} = \theta^\star - \left[\frac{1}{n}\sum_{i=1}^n \varepsilon_{i2} - \frac{1}{n}\sum_{i=1}^n \varepsilon_{i1}\right]$$

- Example 2 : Logit model

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$$\widehat{\theta}^n = \frac{\sum_{i=1}^n \ln\left(\frac{1-X_{(i)}}{X_{(i)}}\right)^2}{\sum_{i=1}^n \ln\left(\frac{1-X_{(i)}}{X_{(i)}}\right)\varepsilon_{(i)1}} = \theta^\star \frac{\sum_{i=1}^n \varepsilon_{(i)2}^2}{\sum_{i=1}^n \varepsilon_{(i)2}\varepsilon_{(i)1}}$$

- Example 3: Location/scale model

$$\varphi_\theta(x) = \theta_2 x + \theta_1$$

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$\rightarrow$ Scale model

$$\begin{cases} \varepsilon_{i1} \\ X_i = \theta^\star \varepsilon_{i2} \end{cases} \quad 1 \leqslant i \leqslant n$$

$$\widehat{\theta}^n = \frac{\sum_{i=1}^n X_{(i)}^2}{\sum_{i=1}^n X_{(i)} \varepsilon_{(i)1}} = \theta^\star \frac{\sum_{i=1}^n \varepsilon_{(i)2}^2}{\sum_{i=1}^n \varepsilon_{(i)2} \varepsilon_{(i)1}}$$

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