Parametric estimation via MMD optimization: robustness to outliers and to dependence

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RIKEN AIP : ABI team

RIKEN AIP Center for Advanced Intelligence Project

Approximate Bayesian Inference team (ABI), lead by Emtiyaz Khan

Please visit the team website

https ://emtiyaz.github.io/

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Letting p_θ denote the density of P_θ, then

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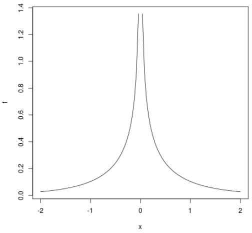
Example : $P_{(m,\sigma)} = \mathcal{N}(m, \sigma^2)$ then

$$\hat{m} = \frac{1}{n} \sum_{i=1}^{n} X_i \text{ and } \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \hat{m})^2.$$

MLE not unique / not consistent

Example :

$$p_\theta(x) = \frac{\exp(-|x-\theta|)}{2\sqrt{\pi|x-\theta|}},$$



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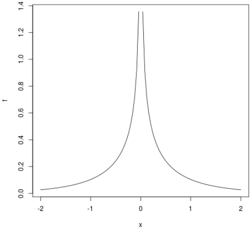
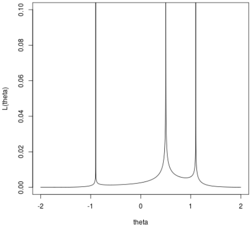


$$L(\theta) = \frac{\exp\left(-\sum_{i=1}^n |X_i-\theta|\right)}{(2\sqrt{\pi})^n \prod_{i=1}^n \sqrt{|X_i-\theta|}}.$$



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Huber proposed the contamination model : with probability ε, X_i is not drawn from P_{θ_0} but from Q that can be anything :

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In the case of the following contamination, the MLE is extremely far from the truth :

$$P_0 = (1-\varepsilon).\mathcal{U}nif[0,1] + \varepsilon.\mathcal{N}(10^{10},1)...$$

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2. in the misspecified case $P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q$, for any Q,
$$\mathbb{E}\left[d(P_{\hat{\theta}_n}, P_0)\right] \leq \underbrace{d(P_0, P_{\theta_0})}_{\xrightarrow[\varepsilon\to\infty]{}0} + \underbrace{r_n(\Theta)}_{\xrightarrow[n\to\infty]{}0} .$$

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The MLE does not satisfy these requirements.

Some examples

Yatracos' skeleton estimate $\hat{\theta}_n^Y$:

$$\mathbb{E}\left[d_{TV}(P_{\hat{\theta}_n^Y}, P_0)\right] \leq 3 d_{TV}(P_0, P_{\theta_0}) + C.\sqrt{\frac{\dim(\Theta)}{n}}$$

where

$$d_{TV}(P,Q) = \sup_E |P(E) - Q(E)|.$$

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More recent work with the Hellinger distance :

Baraud, Y., Birgé, L., & Sart, M. (2017). A new method for estimation and model selection : ρ-estimation. *Inventiones mathematicae*.

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Problem with the aforementioned estimators : they cannot be computed in practice.

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Additional requirement : an estimator must be computable ! ! !

Overview of the talk

1. Estimation via MMD optimization
   - Definition of the estimator
   - Basic properties
   - References and further works
2. Robustness to outliers
   - Application to Huber contamination model
   - Example : estimation of the mean of a Gaussian
   - Numerical experiments
3. Robustness to dependence
   - Extension to non-independent observations
   - A (new ?) dependence coefficient
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Reminder : kernels

Let $\mathcal{H}$ be a Hilbert space and any continuous function $\Phi : \mathcal{X} \to \mathcal{H}$. The function

$$K(x,y) = \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}}$$

is called a kernel.

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is called a kernel. Conversely :

Mercer's theorem

Let $K(x, y)$ be a continuous function such that for any $(x_1, \dots, x_n) \in \mathcal{X}^n$ and $(c_1, \dots, c_n) \neq (0, \dots, 0) \in \mathbb{R}^n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x_i, x_j) > 0,$$

then there is $\mathcal{H}$ and Φ such that $K(x, y) = \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}}$.

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$$\mu_K(P) = \mathbb{E}_{X \sim P}\left[\Phi(x)\right].$$

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Consider, for any probability distribution P on $\mathcal{X}$,

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The kernel K is said to be characteristic if

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Theorem

$K(x, y) = \exp(-\frac{\|x-y\|^2}{\gamma^2})$ and $\exp(-\frac{\|x-y\|}{\gamma})$ are char. kernels.

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Theorem

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Definition : the MMD distance

$$\mathbb{D}_K(P,Q) = \left\|\mu_K(P) - \mu_K(Q)\right\|_{\mathcal{H}}.$$

MMD-based estimator

Reminder of the context :

1. $X_1, \ldots, X_n$ be i.i.d in $\mathcal{X}$ from a probability distribution P_0,
2. model $(P_\theta, \theta \in \Theta)$.

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Definition - MMD based estimator

$$\hat{\theta}_n^{MMD} = \arg\min_{\theta \in \Theta} \mathbb{D}_K \left(P_\theta, \hat{P}_n \right) \text{ where } \hat{P}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}.$$

A preliminary lemma

Lemma

For any P_0, when $X_1, \dots, X_n$ are i.i.d from P_0,

$$\mathbb{E}\left[\mathbb{D}_K\left(\hat{P}_n, P^0\right)\right] \leq \frac{1}{\sqrt{n}}.$$

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$$\begin{aligned}\left\{\mathbb{E}\left[\mathbb{D}_K\left(\hat{P}_n, P^0\right)\right]\right\}^2 &\leq \mathbb{E}\left[\mathbb{D}_K^2\left(\hat{P}_n, P^0\right)\right] \\ &= \mathbb{E}\left[\left\|(1/n)\sum(\mu(\delta_{X_i}) - \mu(P_0))\right\|_{\mathcal{H}}^2\right] \\ &= (1/n)\mathbb{E}\left[\|\mu(\delta_{X_1}) - \mu(P_0)\|_{\mathcal{H}}^2\right] \\ &\leq 1/n.\end{aligned}$$

A bound in expectation

$$
\begin{aligned}
\forall\theta,\ \mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, P^0\right) &\leq \mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, \hat{P}_n\right) + \mathbb{D}_K\left(\hat{P}_n, P^0\right) \\
&\leq \mathbb{D}_K\left(P_\theta, \hat{P}_n\right) + \mathbb{D}_K\left(\hat{P}_n, P^0\right) \\
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Theorem

For any P_0, when $X_1, \dots, X_n$ are i.i.d from P_0,

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\mathbb{E}\left[\mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, P_0\right)\right] \leq \inf_{\theta\in\Theta} \mathbb{D}_K(P_\theta, P_0) + \frac{2}{\sqrt{n}}.
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A bound in probability

We can replace the control on the expectation of $\mathbb{D}_K\left(\hat{P}_n, P^0\right)$ by a bound that holds with large probability, thanks to McDiarmid's inequality.

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Theorem

For any P_0, when $X_1, \dots, X_n$ are i.i.d from P_0, with probability at least $1-\delta$,

$$\mathbb{D}_K\left(P_{\hat{\theta}_n}, P^0\right) \leq \inf_{\theta \in \Theta} \mathbb{D}_K\left(P_\theta, P^0\right) + \frac{2 + 2\sqrt{2\log\left(\frac{1}{\delta}\right)}}{\sqrt{n}}.$$

How to compute $\hat{\theta}_n^{MMD}$?

We actually have

$$\mathbb{D}_K^2(P_\theta, \hat{P}_n) = \mathbb{E}_{X,X'\sim P_\theta}[K(X,X')] - \frac{2}{n}\sum_{i=1}^{n}\mathbb{E}_{X\sim P_\theta}[K(X_i,X)] + \frac{1}{n^2}\sum_{1\leq i,j\leq n} K(X_i,X_j)$$

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and so

$$\nabla_\theta \mathbb{D}_K^2(P_\theta, \hat{P}_n) = 2\mathbb{E}_{X,X'\sim P_\theta}\left\{\left[K(X,X') - \frac{1}{n}\sum_{i=1}^{n} K(X_i,X)\right]\nabla_\theta[\log p_\theta(X)]\right\}$$

that can be approximated by sampling from P_θ.

Short bibliography

Dziugaite, G. K., Roy, D. M., & Ghahramani, Z. (2015). Training generative neural networks via maximum mean discrepancy optimization. *UAI 2015*.

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application to the estimation of copulas.

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Huber contamination model

Reminder

$$\mathbb{E}\left[\mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, P_0\right)\right] \leq \inf_{\theta\in\Theta} \mathbb{D}_K(P_\theta, P_0) + \frac{2}{\sqrt{n}}.$$

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Huber contamination model : $P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q$.

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Huber contamination model : $P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q$.

$$\begin{aligned}\mathbb{D}_K(P_{\theta_0}, P_0) &= \|P_{\theta_0} - [(1-\varepsilon)P_{\theta_0} + \varepsilon Q]\|_{\mathcal{H}} \\ &\leq \varepsilon\|P_{\theta_0}\|_{\mathcal{H}} + \varepsilon\|Q\|_{\mathcal{H}} \\ &= 2\varepsilon.\end{aligned}$$

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Huber contamination model : $P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q$.

$$\mathbb{D}_K(P_{\theta_0}, P_0) \leq 2\varepsilon.$$

Corollary

When $X_1, \dots, X_n$ are i.i.d from $(1-\varepsilon)P_{\theta_0} + \varepsilon Q$,

$$\mathbb{E}\left[\mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, P_{\theta_0}\right)\right] \leq 4\varepsilon + \frac{2}{\sqrt{n}}.$$

Example : Gaussian mean estimation

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Using a Gaussian kernel $K(x,y) = \exp(-\|x - y^2\|/\gamma^2)$, from the previous theorem and from the equality

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we obtain

$$\mathbb{E}\left[\|\hat{\theta}_n^{MMD} - \theta_0\|^2\right]$$
$$\leq -(4\sigma^2+\gamma^2)\log\left[1 - 4\left(\frac{1}{n}+\varepsilon^2\right)\left(\frac{4\sigma^2+\gamma^2}{\gamma^2}\right)^{\frac{d}{2}}\right].$$

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we obtain

$$\mathbb{E}\left[\|\hat{\theta}_n^{MMD}-\theta_0\|^2\right] \lesssim d\sigma^2\left(\frac{1}{n}+\varepsilon^2\right).$$

Example : Gaussian mean estimation, simulations

Model : $\mathcal{N}(\theta, 1)$, and $X_1, \dots, X_n$ i.i.d $\mathcal{N}(\theta_0, 1)$, $n = 100$ and we repeat the experiment 200 times.

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Now, $\varepsilon = 1\%$ are replaced by $1,000$.

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1 Estimation via MMD optimization
- Definition of the estimator
- Basic properties
- References and further works

2 Robustness to outliers
- Application to Huber contamination model
- Example : estimation of the mean of a Gaussian
- Numerical experiments

3 Robustness to dependence
- Extension to non-independent observations
- A (new ?) dependence coefficient
- Example : auto-regressive observations

And now, non-independent observations

Lemma

When $X_1, \dots, X_n$ are identically distributed from P_0,

$$\mathbb{E}\left[\mathbb{D}_K\left(\hat{P}_n, P^0\right)\right] \leq ?$$

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$$\begin{aligned}
&\mathbb{E}\left[\mathbb{D}_K^2\left(\hat{P}_n, P^0\right)\right] \\
&= \mathbb{E}\left[\left\|(1/n)\sum(\mu(\delta_{X_i}) - \mu(P_0))\right\|_{\mathcal{H}}^2\right] \\
&= \frac{1}{n} + \frac{2}{n^2} \sum_{1\leq i<j\leq n} \mathbb{E}\left\langle \mu(\delta_{X_i}) - \mu(P_0), \mu(\delta_{X_j}) - \mu(P_0)\right\rangle_{\mathcal{H}}
\end{aligned}$$

Mesure of dependence via covariance in $\mathcal{H}$

Definition

When $(X_1, \dots, X_n, \dots)$ is a stationary process with marginal distribution P_0, we put :

$$\varrho_h = \left| \mathbb{E} \left\langle \mu(\delta_{X_{t+h}}) - \mu(P_0), \mu(\delta_{X_t}) - \mu(P_0) \right\rangle_{\mathcal{H}} \right| .$$

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Lemma - dependent case

When $X_1, \dots, X_n$ are identically distributed from P_0,

$$\mathbb{E}\left[\mathbb{D}_K\left(\hat{P}_n, P^0 \right) \right] \leq \frac{1}{n} \left[1 + \sum_{h=1}^{n} \varrho_h \right]$$

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Theorem - dependent case

When $(X_1, \dots, X_n, \dots)$ is a stationary process with marginal distribution P_0

$$\mathbb{E}\left[\mathbb{D}_K\left(P_{\hat{\theta}_n^{MMD}}, P_0\right)\right] \leq \inf_{\theta\in\Theta} \mathbb{D}_K(P_\theta, P_0) + \frac{2 + 2\sum_{h=1}^{n} \varrho_h}{\sqrt{n}}.$$

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2. we also have a bound in probability, based on Rio's version of Hoeffding's inequality ; it requires more assumptions.

An example : auto-regressive processes

Proposition

Assume that X_t takes values in $\mathbb{R}^d$ and that $K(x,y) = F(\|x-y\|)$ where F is an L-Lipschitz function. Assume that

$$X_{t+1} = AX_t + \varepsilon_{t+1}$$

where the (ε_t) are i.i.d with $\mathbb{E}\|\varepsilon_0\| < \infty$, and A is a matrix with $\|A\| = \sup_{\|x\|=1} \|Ax\| < 1$.

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Then

$$\varrho_t \leq \|A\|^t \frac{2L\mathbb{E}\|\varepsilon_0\|}{1-\|A\|} \text{ and } \Sigma = \sum_{t=1}^{\infty} \varrho_t = \frac{2\|A\|L\mathbb{E}\|\varepsilon_0\|}{(1-\|A\|)^2}.$$

A non-mixing process with $\Sigma < +\infty$

Example : consider $X_0 \sim \mathcal{U}([0,1])$, η_t i.i.d $\mathcal{B}e(1/2)$ and

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More generally, we prove the following result :

Proposition

Under some (non-restrictive) assumption on the kernel K,

$$\varrho_t \leq c_K . \beta_t \text{ (the } \beta\text{-mixing coef.)}$$

Thank you !