M-estimation in Complex Modeling

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Outline

1. Motivations and notations
2. Model Selection
3. Risk excess bound
4. Theorical Results
5. Examples

General framework

Variable of Interest: Y, density f, probability measure $\mathbb{Q}$ unknown

Feature: Density distribution, mean, threshold probability, quantile etc...

Experimental data: $\mathcal{Y}_n^{exp} = Y_1^{exp}, ..., Y_n^{exp}$ (*a priori* training data) supposed i.i.d from $\mathbb{Q}$

- Link to history
- Arise from experiments, complex codes etc...
- Small number
- Difficult to obtain

Simulation model: $h \in \mathcal{H} : (\mathbf{x}, \boldsymbol{\theta}) \in \mathcal{X} \times \Theta \mapsto y = h(\mathbf{x}, \boldsymbol{\theta})$
For a configuration $\mathbf{x}_0$, the model gives $y_0 = h(\mathbf{x}, \boldsymbol{\theta}_0) \Rightarrow$ Deterministic !!

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Simulated data: Consider that $\mathcal{X} \leftrightarrow (\mathcal{X}, \mathcal{B}, \mathbb{P}_X)$ i.e **x** (deterministic) $\leftrightarrow$ **X** (random).
For $m \geq 0$, let $\mathcal{Y}_m^{sim} = Y_1^{sim}, ..., Y_m^{sim}$ (depends on the model h and the parameter $\boldsymbol{\theta}$)

- $h \in \mathcal{H}$ (set of models), $\boldsymbol{\theta} \in \Theta$ (set of parameters)
- $Y_i^{sim} = h(X_i, \boldsymbol{\theta}), \quad i = 1, ..., m, \ X_i$ i.i.d random variables (distribution $\mathbb{P}_X$).
- $X \sqcup Y^{exp}$

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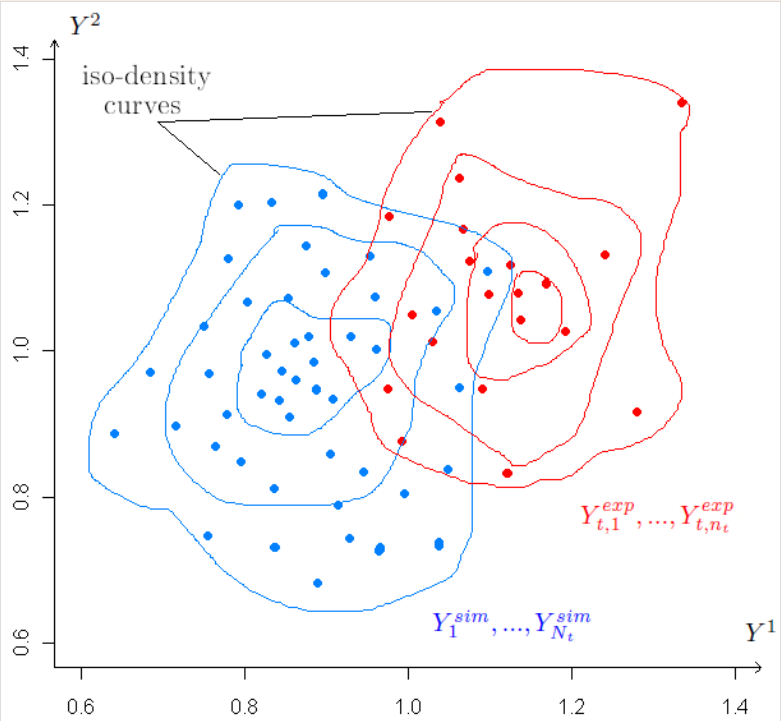
Goal: Use Simulated data to improve feature estimation of Y:

$\Rightarrow$ 1. Estimation procedure: choice of the model h, and parameter $\boldsymbol{\theta}$

$\Rightarrow$ 2. Study of a feature based on $(\widehat{Y}_1^{sim}, ..., \widehat{Y}_m^{sim})$ (*a posteriori* training data)
to compare with the feature based on $(Y_1^{exp}, ..., Y_n^{exp})$

Simulated data estimation

- Illustration of Experimental & Simulated Data: Example of a 2D-Performance $Y = (Y^1, Y^2)$



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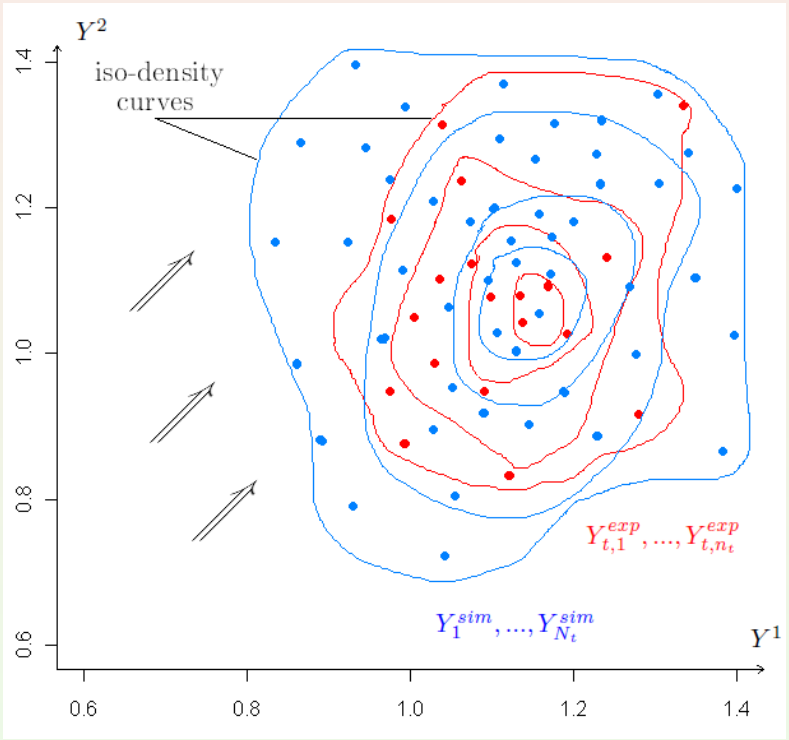


- Choice of $h \in \mathcal{H}$ and $\boldsymbol{\theta} \in \Theta$? $\Rightarrow$ driven by the feature considered

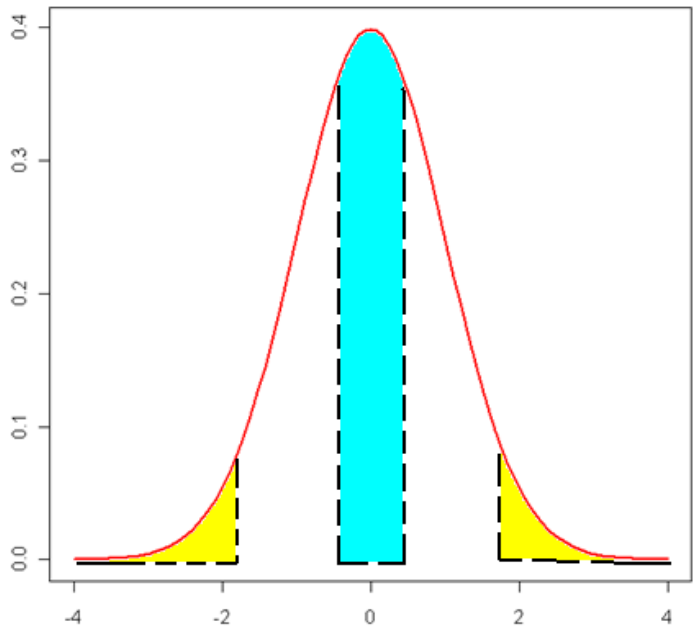
Definition: Feature

Let $\mathcal{P}$ be the set of all probability measures, $\mathbb{D}$ a metric space, we define a **feature** as a function

$$\begin{array}{rccc} \rho : & \mathcal{P} & \longrightarrow & \mathbb{D} \\ & \mu & \longmapsto & \rho(\mu). \end{array}$$

Some feature:

- $\rho(\mu) = \mathbb{E}_{W\sim\mu}(W)$ (mean), q_W^α (α-quantile) $\Rightarrow \mathbb{D} = \mathbb{R}$
- $\rho(\mu) = \mathbb{P}(W > s) \quad \Rightarrow \mathbb{D} = [0, 1]$
- $\rho(\mu) = f_\mu \quad \Rightarrow \mathbb{D} = \{\textit{set of distributions}\}$
- etc ...



Choice of $(h, \boldsymbol{\theta})$ for a Feature ρ

In our framework:

- the model

$$\mathbb{P}_X \xrightarrow{(h,\boldsymbol{\theta})} \mathbb{P}_{h,\boldsymbol{\theta}} \xrightarrow{\text{feature } \rho} \rho(\mathbb{P}_{h,\boldsymbol{\theta}}) := \rho_h(\boldsymbol{\theta})$$

  Important Remark: the feature $\rho_h(\boldsymbol{\theta})$ can be unreachable $\rightarrow$ we say that h is complex

- denote the "true" feature by $\rho(\mathbb{Q}) := \rho^*$
- For fix $h \in \mathcal{H}$, choice of $\boldsymbol{\theta}$

$$\boldsymbol{\theta}_0 = \underset{\Theta}{\text{Argmin}}\, \mathcal{D}(\rho_h(\boldsymbol{\theta}), \rho^*)$$

  with $\mathcal{D}$ *a measure of distance* $\mathbb{D} \times \mathbb{D}$.

- We use the form:

$$M(h, \boldsymbol{\theta}) = \int \gamma_{h,\boldsymbol{\theta}}(y)\, \mathbb{Q}(dy)$$

  where the function $\gamma_{h,\boldsymbol{\theta}}$ is called contrast of $(h, \boldsymbol{\theta})$.
  We have

$$\gamma_{h,\boldsymbol{\theta}} = \Psi\left(\rho_h(\boldsymbol{\theta})\right)$$

  with Ψ some operator on $\mathbb{D}$.

- **Example of contrasts:**

  If the feature is the density
  - $\gamma_{h,\boldsymbol{\theta}}(y) = -\ln\left(\rho_h(\boldsymbol{\theta})\right)(y) \quad \Rightarrow \quad M(h,\boldsymbol{\theta}) = K(\rho^*, \rho_h(\boldsymbol{\theta}))$
  - $\gamma_{h,\boldsymbol{\theta}}(y) = ||\rho_h(\boldsymbol{\theta})||_2^2 - 2\rho_h(\boldsymbol{\theta})(y) \quad \Rightarrow \quad M(h,\boldsymbol{\theta}) = ||\rho^* - \rho_h(\boldsymbol{\theta})||_2^2.$
  - etc...

  The same for mean, quantile, threshold probability etc...

- **Criterion to minimize:**

$$M(h,\boldsymbol{\theta}) = \int \gamma_{h,\boldsymbol{\theta}}(y)\, \mathbb{Q}(dy)$$

- Assume that $(h^*, \boldsymbol{\theta}^*)$ is the unique minimum of $M(\cdot,\cdot)$

- **Difficulties:**
  - The measure $\mathbb{Q}$ is unknown (Classical !)
  - For complex models h, the feature $\rho_h(\boldsymbol{\theta})$ is unreachable so the contrast too $(\gamma_{h,\boldsymbol{\theta}} = \Psi\left(\rho_h(\boldsymbol{\theta})\right))$.

$$M(h,\boldsymbol{\theta}) = \int \gamma_{h,\boldsymbol{\theta}}(y)\,\mathbb{Q}(dy)$$

- **Alternative: Use of Experimental & Simulated data**
  - Replace $\mathbb{Q}$ by its empirical version $\mathbb{Q}_n$ (depends on n-Experimental data $\mathcal{Y}_n^{exp}$)
    We have
    $$M_n(h,\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \gamma_{h,\boldsymbol{\theta}}(Y_i^{exp})$$
  - Since $\gamma_{h,\boldsymbol{\theta}}^m = \Psi\left(\rho_h^m(\boldsymbol{\theta})\right)$, replace the feature $\rho_h(\boldsymbol{\theta})$ by an estimator $\rho_h^m(\boldsymbol{\theta})$ (depends on m-Simulated data $\mathcal{Y}_m^{sim}$).

▷ Pakes and Pollard (1989) studied estimators minimizing an approximation $\widetilde{M}_n(h,\boldsymbol{\theta}) \sim M_n(h,\boldsymbol{\theta})$ (Optimization Estimators).

▷ They prove $\sqrt{n}$-consistency and give limit theorems

▷ The conditions are given on the (approximated) criterion $\widetilde{M}_n(h,\boldsymbol{\theta})$

▶ We want conditions on the simulation (quantification) and on the feature (regularity)

- **Criterion to minimize in practice:**

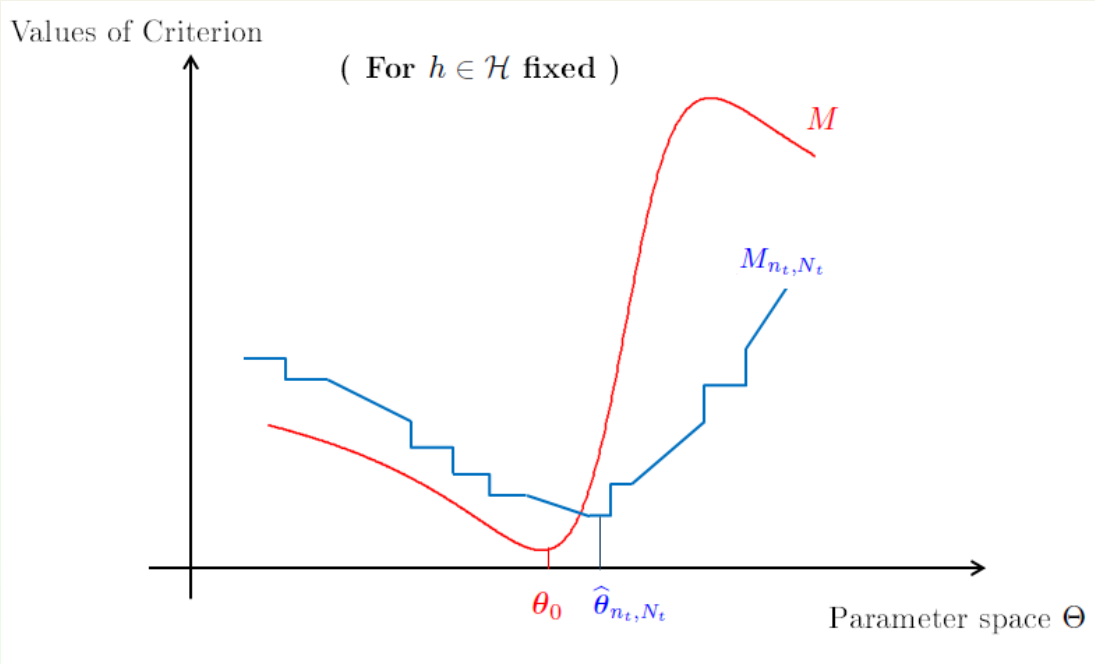
$$M_{n,m}(h,\boldsymbol{\theta}) := \frac{1}{n}\sum_{i=1}^{n} \gamma^{m}_{h,\boldsymbol{\theta}}(Y_i^{exp})$$

- **Estimator of** $\theta_0(h) = \text{Argmin}_{\boldsymbol{\theta}\in\Theta}\ M(h,\boldsymbol{\theta})$

$$\widehat{\boldsymbol{\theta}}_{n,m}(h) = \underset{\boldsymbol{\theta}\in\Theta}{\text{Argmin}}\ M_{n,m}(h,\boldsymbol{\theta})\,.$$

First question: Consistency

$$\widehat{\boldsymbol{\theta}}_{n,m}(h) \underset{\substack{n\to+\infty\\ m\to+\infty}}{\longrightarrow} \boldsymbol{\theta}_0(h)\,?$$



Source of errors

Proposition: Model Error Upper Bound

We prove

$$\underbrace{M(h,\widehat{\boldsymbol{\theta}}_{n,m}(h)) - M(h^*,\boldsymbol{\theta}^*)}_{\text{risk excess of } (h,\,\widehat{\boldsymbol{\theta}}_{n,m}(h))} \lesssim \frac{1}{\sqrt{n}}||\,\mathbb{G}_n\gamma^m_{h,.}\,||_\Theta + ||\mathcal{E}^m_h||_\Theta + \Delta_h$$

- **Variance terms (random terms):**
  - $\frac{1}{\sqrt{n}}||\,\mathbb{G}_n\gamma^m_{h,.}\,||_\Theta = \sup_{\boldsymbol{\theta}\in\Theta}\left|\frac{1}{n}\sum_{i=1}^{n}\left(\gamma^m_{h,\boldsymbol{\theta}}(Y_i^{exp}) - \mathbb{E}_Y(\gamma^m_{h,\boldsymbol{\theta}}(Y))\right)\right|$ (deviation)

    $\Rightarrow$ *Estimation Error of Statistical Data* $\quad(\mathbb{G}_n := \sqrt{n}(\mathbb{Q}_n - \mathbb{Q}))$
  - $||\mathcal{E}^m_h||_\Theta = \sup_{\boldsymbol{\theta}\in\Theta}||\,\gamma^m_{h,\boldsymbol{\theta}} - \gamma_{h,\boldsymbol{\theta}}\,||_{1,\mathbb{Q}}$, with $||g||_{1,\mathbb{Q}} = \int_{\mathbb{R}}|g(y)|\,\mathbb{Q}(dy)$

    $\Rightarrow$ *Simulation Error*
- **Bias term :**
  - $\Delta_h = M(h,\boldsymbol{\theta}_0(h)) - M(h^*,\boldsymbol{\theta}^*)$

    $\Rightarrow$ *Approximation Error of the model h*

Link with classical methods

Classical Inequality

Recall $M(h,\theta) = \int \gamma_{h,\theta}(y)\,\mathbb{Q}(dy)$, we have

$$M(h,\widehat{\theta}_n(h)) - M(h^*,\theta^*) \leq \frac{1}{\sqrt{n}} || \,\mathbb{G}_n\gamma_{h,.}\,||_\Theta + \Delta_h$$

- **For no complex models:** (Statistical models, simplified models etc...)

  $\Rightarrow$ the feature $\rho_h(\theta)$ is reachable $\Rightarrow$ Simulation is useless

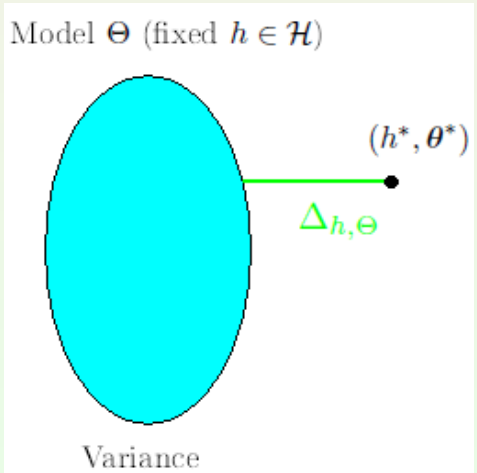
Advantages

- Well studied
- Maximum Likelihood, Regression etc...

Drawback

- Δ_h can be large (due to simplification of h)

  Trade-off Bias-Variance



OUR GOAL: Extend the theory to physical models

Theorical result

- **Recall:**

  model h + parameter $\boldsymbol{\theta} \Rightarrow$ Feature $\rho_h(\boldsymbol{\theta}) \Rightarrow$ Contrast $\gamma_{h,\boldsymbol{\theta}}$

  In our framework:

  model h + parameter $\boldsymbol{\theta} \Rightarrow$ Feature $\rho_h^m(\boldsymbol{\theta}) \Rightarrow$ Contrast $\gamma_{h,\boldsymbol{\theta}}^m$

- **Inequality:**

$$M(h, \widehat{\boldsymbol{\theta}}_{n,m}(h)) - M(h^*, \boldsymbol{\theta}^*) \lesssim \frac{1}{\sqrt{n}} || \mathbb{G}_n \gamma_{h,.}^m ||_\Theta + ||\mathcal{E}_h^m||_\Theta + \Delta_h$$

- **Key point:** Let the class of functions

$$\Gamma_h^m := \{\gamma_{h,\boldsymbol{\theta}}^m, \boldsymbol{\theta} \in \Theta\} = \{\Psi(\rho_h^m(\boldsymbol{\theta})), \boldsymbol{\theta} \in \Theta\}$$

  - the class is random (simulated data)
  - the class changes with m

- **Important Remark:** $|| \mathbb{G}_n \gamma_{h,.}^m ||_\Theta = || \mathbb{G}_n ||_{\Gamma_h^m}$

  Main difficulty : Prove the tightness of the random variable sequence $\left(|| \mathbb{G}_n ||_{\Gamma_h^m} \right)_{n,m}$

Definition: $L_2(\mathbb{Q})$ Bracketing numbers and Entropy with bracketing

▷ Let $\mathcal{G}$ be a class of functions. Given two functions l, u, the bracket $[l, u]$ is the set of all functions g with $l \leq g \leq u$. An ε-bracket is a bracket $[l, u]$ with $||u - l||_{2,\mathbb{Q}} < \varepsilon$. The bracketing number $N_{[]}(\varepsilon, \mathcal{G}, L_2(\mathbb{Q}))$ is the minimum number of ϵ-brackets needed to cover the class of functions $\mathcal{G}$.

▷ The entropy with bracketing is the logarithm of the bracketing number.

Definition: $L_2(\mathbb{Q})$ Bracketing integral

The bracketing integral is defined as

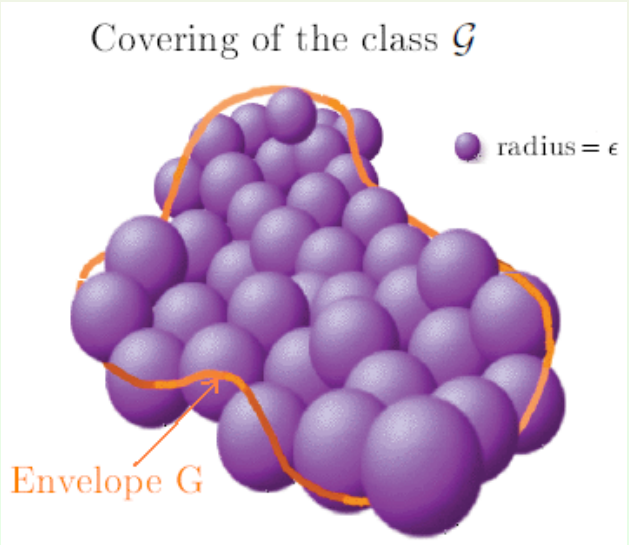
$$J_{[]}(\delta, \mathcal{G}, L_2(\mathbb{Q})) := \int_0^{\delta} \sqrt{\log N_{[]}(\varepsilon, \mathcal{G}, L_2(\mathbb{Q}))} d\varepsilon \,.$$

References:

v d Vaart & Wellner (1996) *Weak Convergence and Empirical Processes*

v d Vaart (1998) *Asymptotics Statistics*

S van de Geer (2000) *Empirical Processes in M-estimation*



Particular classes

- Recall that $\mathbb{G}_n := \sqrt{n}(\mathbb{Q}_n - \mathbb{Q})$

Definition: Glivenko-Cantelli classes

A class of function $\mathcal{G}$ is $(\mathbb{Q})$-Glivenko-Cantelli if

$$\frac{1}{\sqrt{n}} || \mathbb{G}_n ||_{\mathcal{G}} \xrightarrow[p.s]{} 0 \,.$$

Definition: Donsker classes

A class of function $\mathcal{G}$ is $(\mathbb{Q})$-Donsker if

$$\mathbb{G}_n \rightsquigarrow \mathbb{G} \quad in \quad l^{\infty}(\mathcal{G})$$

Theorems

1. If for all $\varepsilon > 0$, $N_{[]}(\varepsilon, \mathcal{G}, L_1(\mathbb{Q})) < \infty$ then $\mathcal{G}$ is Glivenko-Cantelli.
2. If $J_{[]}(1, \mathcal{G}, L_2(\mathbb{Q})) < \infty$ then $\mathcal{G}$ is Donsker.

- The class Γ_h^m is random and changes with m. We need more results.

Our Results

- Theorical study of the Γ_h^m-indexed empirical $\mathbb{G}_n = \sqrt{n}(\mathbb{Q}_n - \mathbb{Q})$ process

Consistency

We prove that $\widehat{\boldsymbol{\theta}}_{n,m} \underset{\substack{n\to+\infty \\ m\to+\infty}}{\longrightarrow} \boldsymbol{\theta}_0$, under some conditions in terms of :

- Model Complexity *(Bracketing Numbers)* (model h + feature regularity)
- Simulation Speed *(Size of Simulated Data set, m)*
- Control of Simulated contrasts *(Modified Lindeberg conditions)*

Limiting Distribution

1. It exists $r_{n,m} \geq 0$ such that $r_{n,m}(\widehat{\boldsymbol{\theta}}_{n,m} - \boldsymbol{\theta}_0) = \boldsymbol{O}_{\mathbb{P}}(1)$
2. Under some conditions on the model h and on the feature ρ, we can define $m_n := \inf\{m \geq 0,\ r_{n,m} \gtrsim n^{\frac{1}{2}-\varepsilon_n}\}$, where $\varepsilon_n > 0$ is a nonincreasing sequence.
3. Under some conditions,
$$\widehat{\boldsymbol{\theta}}_{n,m} - \boldsymbol{\theta}_0 \rightsquigarrow \mathcal{N}(0, \Sigma)$$

- In some applications, for $n = 30$ we have $m_n \sim 10000$

Example of the *Range* study

Phenomenon : $Y = Range$ (distance an aircraft can travel), feature = density distribution

- ***A priori* training data :** Experimental data, $n = 20$, $\mathcal{Y}_n^{exp} = Y_1^{exp}, ..., Y_n^{exp}$

  (obtained from complex model h^* supposed to be the "true")

- **Additional knowledge :** Simulated data, $m = 3000$, $\mathcal{Y}_m^{sim} = Y_1^{sim}, ..., Y_m^{sim}$ from

$$h(X, \theta) = \frac{F\,V}{C_s}\frac{1}{\theta_1}\log\left(\frac{1}{1-\theta_2}\right)$$

  - Uncertain Inputs $X = (F, V, C_s)^T$
  - Parameters $\boldsymbol{\theta} = (\theta_1, \theta_2) \in \Theta$

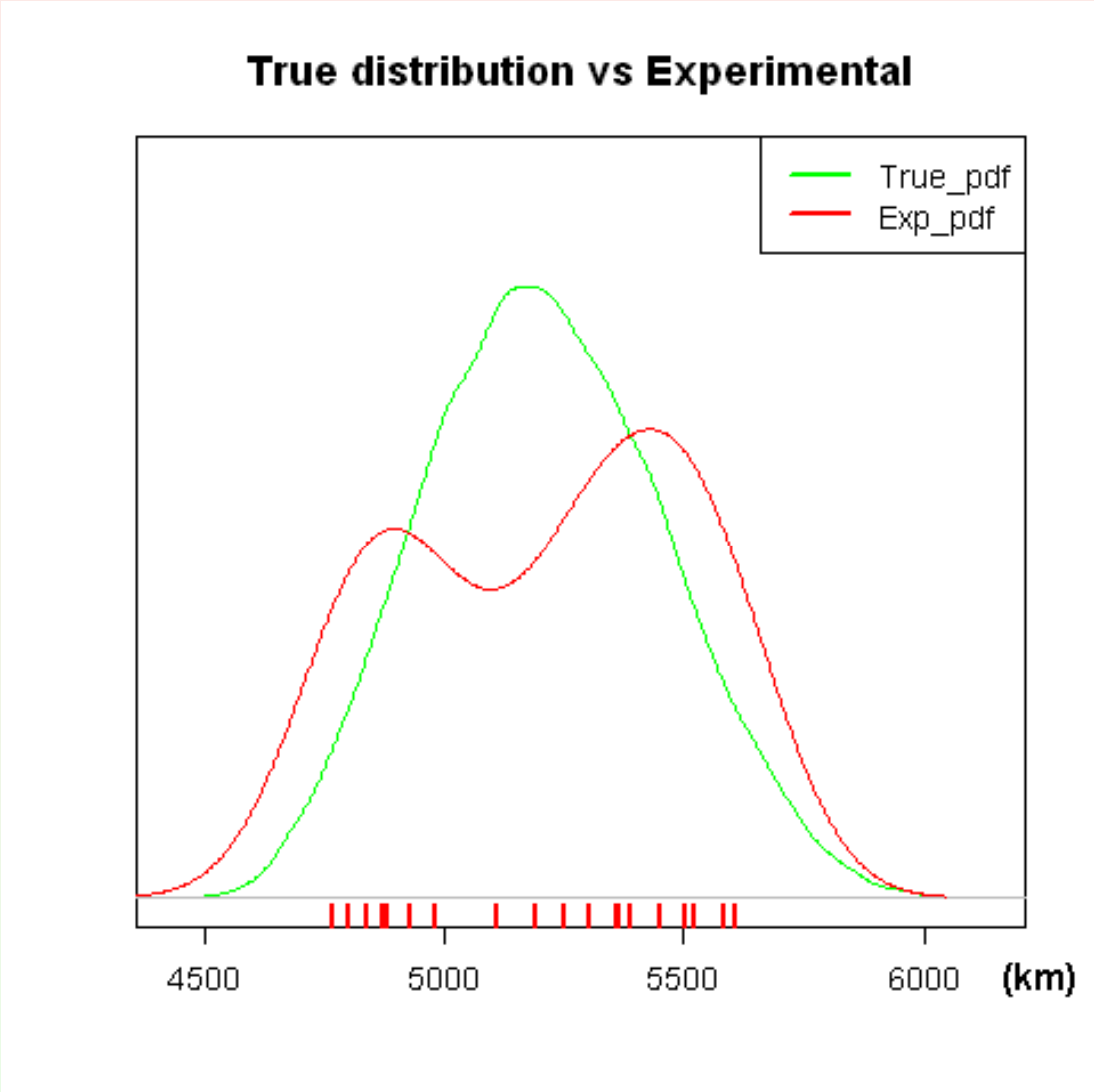
- **Choice of θ ?** $\quad \theta_0(h) = \underset{\boldsymbol{\theta}\in\Theta}{\text{Argmin}} \int_{\mathbb{R}} \gamma_{h,\boldsymbol{\theta}}(y)\, f(y)\, dy$

$$\gamma_{h,\boldsymbol{\theta}} = -\ln(f_{h,\boldsymbol{\theta}}) \quad f_{h,\boldsymbol{\theta}} \leftrightarrow f_{h,\boldsymbol{\theta}}^m\,(Kernel) \quad f \leftrightarrow \frac{1}{n}\sum_{i=1}^{n} \delta_{Y_i^{exp}}$$

$$\widehat{\boldsymbol{\theta}}_{n,m}(h) = \underset{\boldsymbol{\theta}\in\Theta}{\text{Argmin}} -\frac{1}{n}\sum_{i=1}^{n} \ln\left(\frac{1}{m}\sum_{j=1}^{m} K_{h_m}(Y_i^{exp} - Y_j^{sim})\right)$$

- ***A posteriori* training data :** $(Y_1^{exp}, ..., Y_n^{exp}, \widehat{Y}_1^{sim}, ..., \widehat{Y}_m^{sim}) \longrightarrow n + m = 3020!$

- Feature with *a priori* (Experimental) and *a posteriori* (Experimental + Simulated) training data



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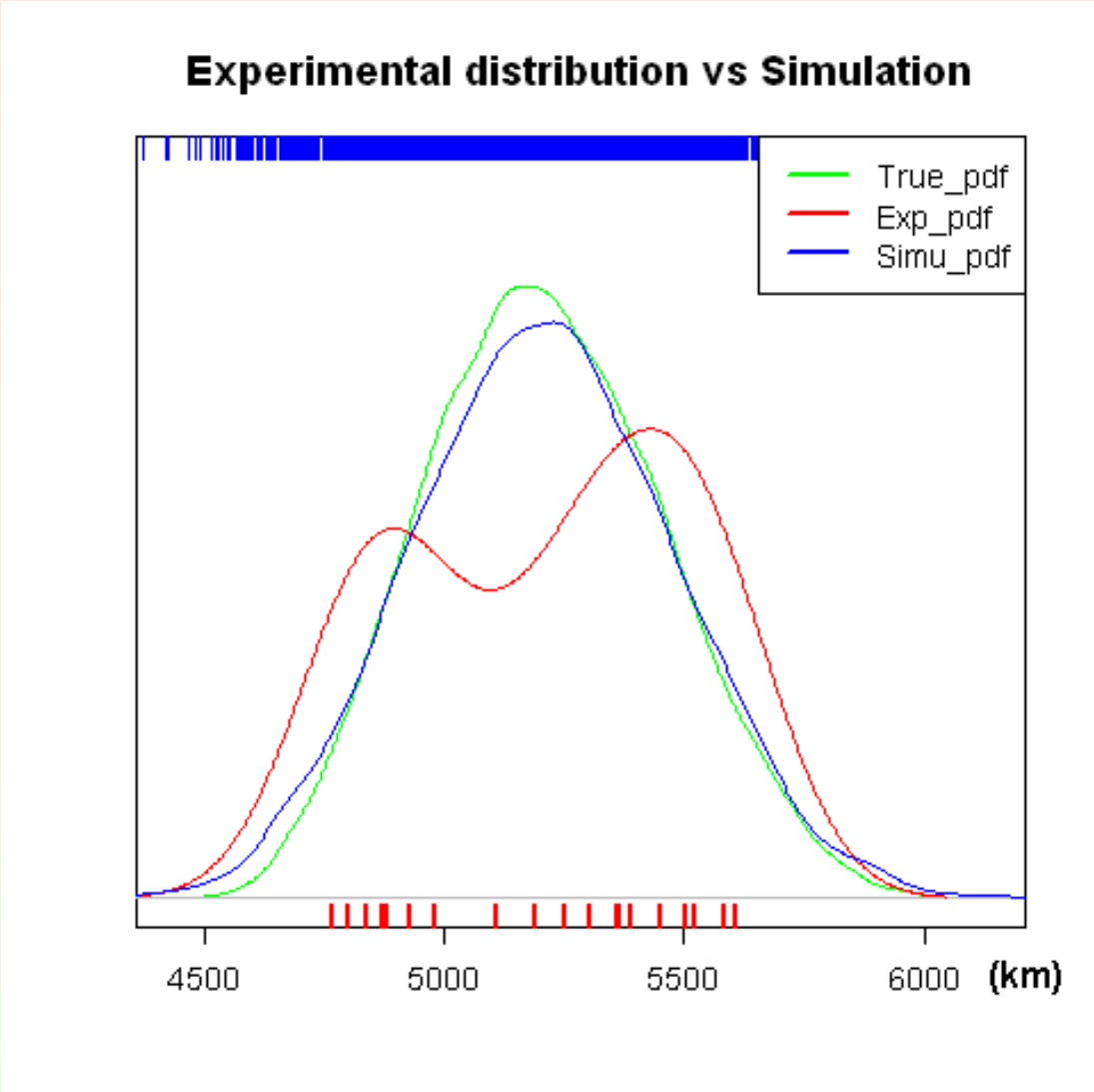

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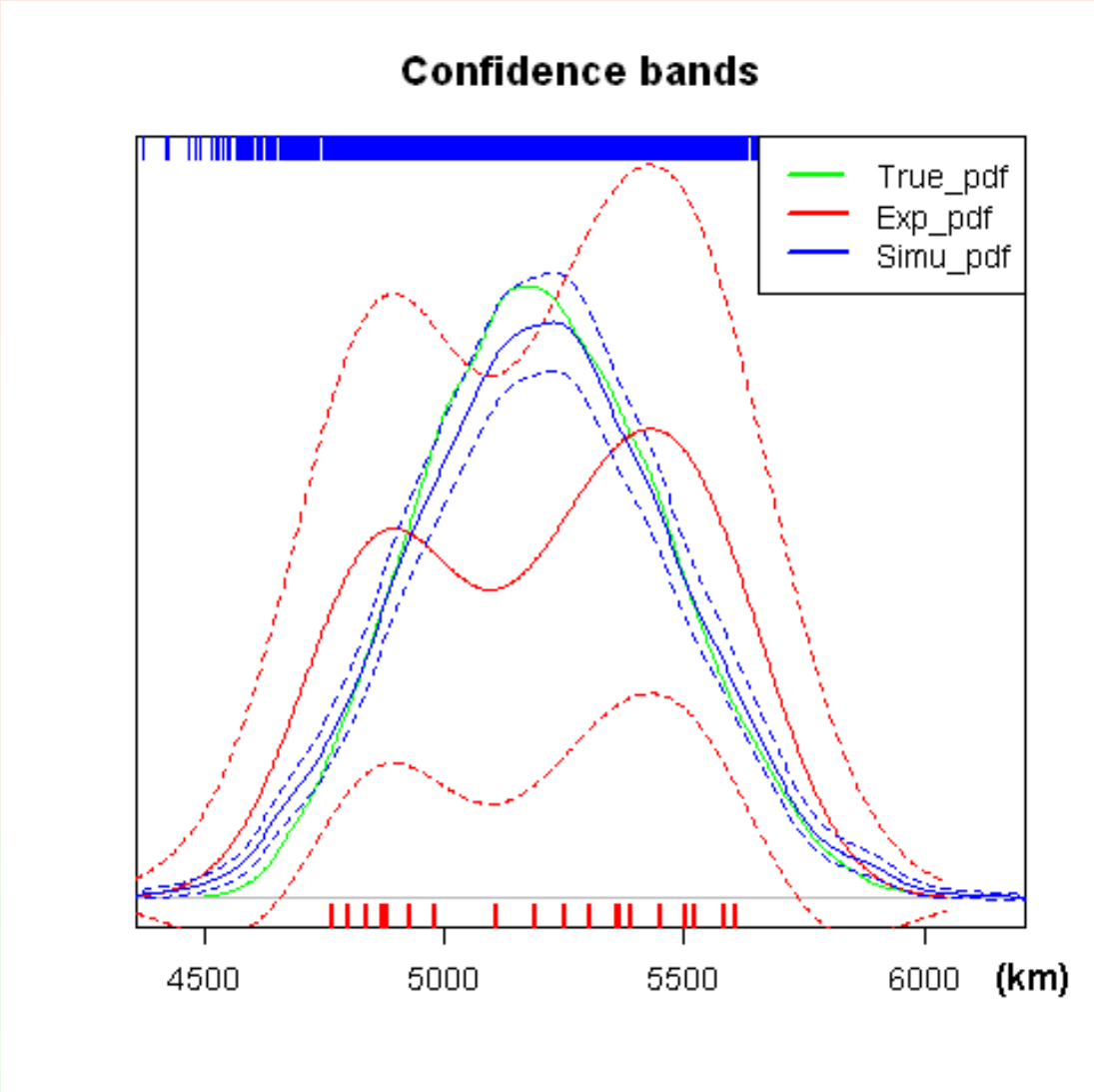

Work in progress

- **Non parametric estimation improvement:**
  - Let φ be a non parametric estimator of the feature ρ

$$\begin{array}{rcl} \varphi : \{\textit{set of samples}\} & \longrightarrow & \mathbb{D} \\ \Lambda & \longmapsto & \varphi(\Lambda). \end{array}$$

  - We note $\varphi_n = \varphi(\mathcal{Y}_n^{exp})$ and $\varphi_m = \varphi(\mathcal{Y}_m^{sim})$, and we consider the aggregate estimator

$$\varphi_{n,m} = \alpha \cdot \varphi_n + (1 - \alpha) \cdot \varphi_m$$

    with $0 < \alpha < 1$.
  - Estimation of $\alpha \longrightarrow$ Simulate or not to simulate ?
  - Asymptotic properties

Thank you for your attention !