



Airbus Group Innovations

# Unsupervised parameter estimation in computer experiments

Journées MAS, 28<sup>th</sup> August 2014

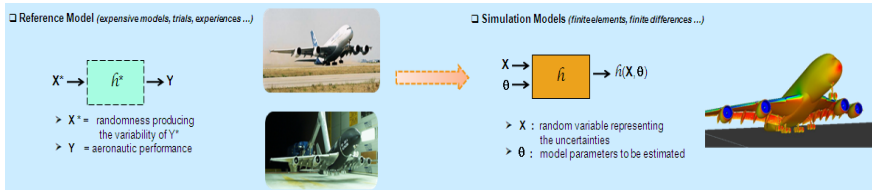
Nabil RACHDI, [nabil.rachdi@airbus.com](mailto:nabil.rachdi@airbus.com)

# Outline

- 1** Statistical Learning for Prediction with Computer Experiments
  - Introduction
  - Introductory examples
  - General Settings
  - Parameter Estimation
    - Estimator construction
  - Applications

# Context

- From Real life to Simulated life...

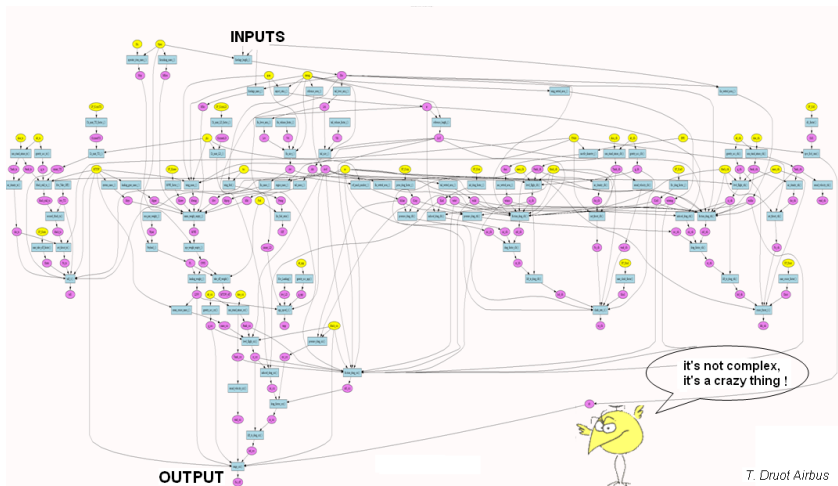


- $Y$  = Variable of Interest (**uncertain !**)
- $\rho^*$  = Quantity of Interest (*quantile, pdf, exceed. probability ...*)
- **Challenge :**

From ref. data  $Y_1, \dots, Y_n$  or  $(X_1^*, Y_1), \dots, (X_n^*, Y_n)$  (*n limited !*)

→ Choose  $h$  and  $\theta$  to predict  $\rho^*$  with simulation model(s)  $h$

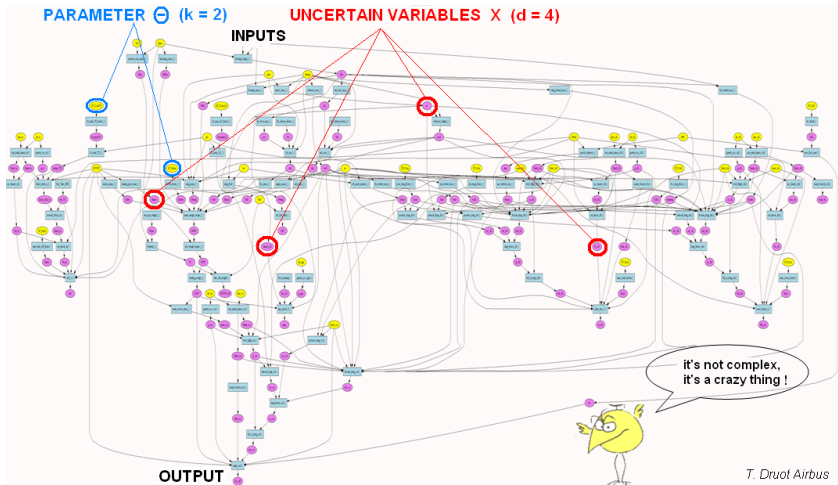
# Numerical Simulations under Uncertainties



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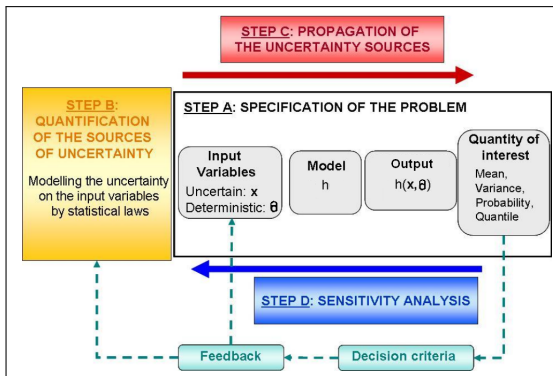
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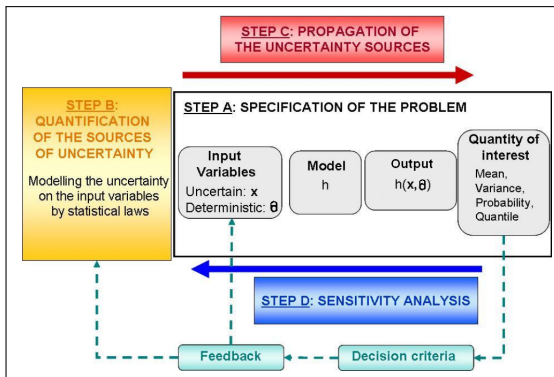
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# Methodology commonly adopted [de Rocquigny et al. (2008)]



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⇒ 2 kind of problems:

- **Inverse Problem:** identify the parameter  $\theta$  (mechanical, thermal...) from a set  $Y_1, \dots, Y_n$
- **Prediction Problem:** estimate  $\theta$  (tuning parameters, etc.) and simulate with  $h(\mathbf{X}, \hat{\theta})$  under  $\mathbf{X}$

## Questions ?

- **Inverse problem:** If the "real life" inputs  $X_i^*$ 's are not observed ? How to calibrate ?  
(e.g input code  $\neq$  experimental conditions etc...)



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(e.g input code  $\neq$  experimental conditions etc...)

In other words, for each simulation input  $\mathbf{X}_i$  we do not have the associated response  $Y_i$ , which may be referred to as **Unsupervised Learning**.

# Link with Statistical Learning

Classical learning areas (see Hastie et al [7], Massart [8])

- **Unsupervised learning:** We observe  $\mathbf{X}_1^*, \dots, \mathbf{X}_n^*$  i.i.d  $\mathbb{P}_{\mathbf{X}}^*$  (unknown) and we look for a probabilistic feature of  $P_{\mathbf{X}}^*$
- **Semi-supervised learning** With  $l < n$ , we observe  $(\mathbf{X}_i^*, \mathbf{Y}_i^*)_{i \leq l} + \mathbf{X}_{l+1}^*, \dots, \mathbf{X}_n^*$  and we look for a map  $g : \mathcal{X}^* \rightarrow \mathcal{Y}^*$
- **Supervised/inductive learning:** We observe  $(\mathbf{X}_1^*, \mathbf{Y}_1^*), \dots, (\mathbf{X}_n^*, \mathbf{Y}_n^*)$  and we look for a map  $g : \mathcal{X}^* \rightarrow \mathcal{Y}^*$

Our learning context

- If the  $\mathbf{X}_i^*$ 's are observed ?

Data at disposal:

$$(\mathbf{X}_1^*, \mathbf{Y}_1^*), \dots, (\mathbf{X}_n^*, \mathbf{Y}_n^*) + (\mathbf{X}_1, h(\mathbf{X}_1, \theta)), \dots, (\mathbf{X}_m, h(\mathbf{X}_m, \theta)), \quad m \gg n$$

*The framework  $\mathbf{Y}_1^*, \dots, \mathbf{Y}_n^* + \mathbf{X}_1, \dots, \mathbf{X}_m$  may be seen between Supervised and Semi-supervised learning...*

- If the  $\mathbf{X}_i^*$ 's are NOT observed ?

Data at disposal:  $\mathbf{Y}_1^*, \dots, \mathbf{Y}_n^* + h(\mathbf{X}_1, \theta), \dots, h(\mathbf{X}_m, \theta), \quad m \gg n$

*The framework  $\mathbf{Y}_1^*, \dots, \mathbf{Y}_n^* + \mathbf{X}_1, \dots, \mathbf{X}_m$  may be seen between Unsupervised and Semi-supervised learning...*

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$$\mathbb{P}(h(\mathbf{X}, \hat{\theta}_{reg}) > s) \quad \text{or} \quad pdf_{h(\mathbf{X}, \hat{\theta}_{reg})} ?$$

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... "duality" between estimation procedure and target prediction ...

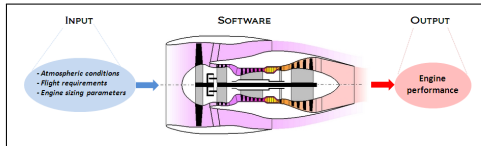
## Example 1: Inverse Problem

N. Rachdi, J-C. Fort, T. Klein [2]

### ■ Fuel Mass data:

Reference Fuel Masses [kg]							
7918	7671	7719	7839	7912	7963	7693	7815
7872	7679	8013	7935	7794	8045	7671	7985
7755	7658	7684	7658	7690	7700	7876	7769
8058	7710	7746	7698	7666	7749	7764	7667

### ■ Model (noisy simulator):



### ■ Goal: Identify $SFC(=\theta)$ (Specific Fuel Consumption) under uncertainties $X$

Rq: We do not have at disposal the inputs providing the Fuel Mass data

## Example 1: Inverse Problem

- **Idea:** Minimize the "distance" between the distribution of Fuel Mass reference data  $Y_i$  and the distribution of the noisy computer code  $h(\mathbf{X}, \theta)$  ( $\mathbf{X}$  = uncertainties,  $\theta$ =SFC)

- **Kullback-Leibler minimization:**

$$KL(f_1, f_2) = \int_{\mathcal{Y}} \log \left( \frac{f_1}{f_2} \right) f_1$$

Set  $f$  = density of  $Y$ ,  $f_{\theta}$  = density of  $h(\mathbf{X}, \theta)$

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- **2 Difficulties**

- $f$  is unknown  $\rightarrow$  replaced by  $f^n = \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}$
- $f_{\theta}$  intractable  $\rightarrow$  replaced by a **simulation density** (Kernel, projection, etc...)  $\left( f_{\theta}^m = \frac{1}{m} \sum_{j=1}^m K_{b_m}(\cdot - h(\mathbf{X}_j, \theta)), \quad \mathbf{X}_j \underset{i.i.d.}{\sim} P^{\mathbf{x}} \right)$



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- **Estimator**

$$\hat{\theta}_{KL} = \underset{\theta \in \Theta}{\text{Argmin}} KL(f^n, f_{\theta}^m) = \underset{\theta \in \Theta}{\text{Argmin}} -\frac{1}{n} \sum_{i=1}^n \log(f_{\theta}^m)(Y_i)$$

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- **Estimator**

**Remark:** This Estimator doesn't depend on the (unknown)  $\mathbf{X}_i$ 's providing the  $Y_i$ 's !

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$$\widehat{\text{SFC}} = \hat{\theta}_{KL}$$

## Example 2: Density prediction ( $\hat{f}_{MS}$ )

N. Rachdi, J-C. Fort, T. Klein [1]

Suppose that  $\mathbf{X}^* = \mathbf{X}$  and that  $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$  are available.

**Goal:** Estimate the pdf of  $Y$  from a computer code  $h(\mathbf{X}, \theta)$  where  $\mathbf{X} \sim P^{\mathbf{x}}$

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*Other Estimation Procedures...*

- **Mean-Squares minimization (version 2)**

$$\hat{\theta}_M = \underset{\theta \in \Theta}{\text{Argmin}} \frac{1}{n} \sum_{i=1}^n \left( Y_i - \frac{1}{m} \sum_{j=1}^m h(\mathbf{X}_j, \theta) \right)^2$$

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Rq : This version of mean squares minimizes the distance between the "expectations", whereas the previous estimator  $\hat{\theta}_{MS}$  minimizes the distance between "conditional expectations".



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Question ?

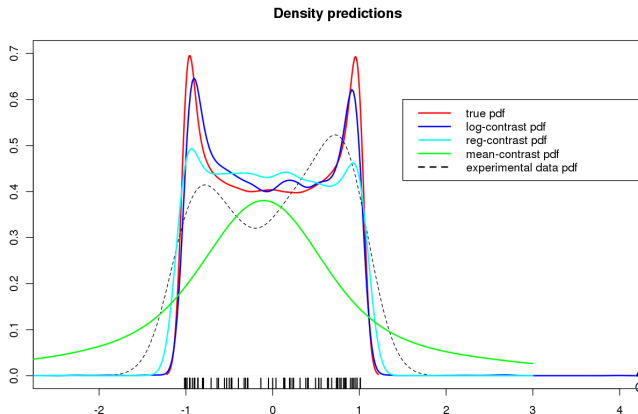
What is the "best" estimator of the density  $f$  of  $Y$ ,

$\hat{f}_{MS}$ ,  $\hat{f}_M$  or  $\hat{f}_{KL}$  ?

## Toy application

- ▶  $Y = \sin(X^*) + 0.01 \varepsilon$ ,  $X^*, \varepsilon \sim \mathcal{N}(0, 1)$  independents
- ▶  $h(X, \theta) = \theta_1 + \theta_2 X + \theta_3 X^3$ ,  $X \sim P^x = \mathcal{N}(0, 1)$
- ▶  $n = 50$  and  $m = 10^3$

true pdf,  $\hat{f}_{MS}$ ,  $\hat{f}_M$ ,  $\hat{f}_{KL}$



## Issues

- **Inverse problem:**  
Formalize Stochastic Inverse Problems in a Statistical Learning framework
- **Prediction problem:**  
Define "adapted" estimation procedures (learning algorithms) for a computer code based prediction

# General Framework

- **Reference data** : set  $\mathbf{X}^* = \mathbf{X}$  (i.e " phenomenon causes = code inputs ")

$$Z_1 = (\mathbf{X}_1, Y_1), \dots, Z_n = (\mathbf{X}_n, Y_n)$$

with (**unknown**) dist.  $Q^z$  and denote by  $Q$  the marginal dist. of  $Y$   
 $\rightarrow \mathbf{X}_1, \dots, \mathbf{X}_n$  **may be unobserved**

- **Model** :  $\{\mathbf{x} \in \mathcal{X} \mapsto h(\mathbf{x}, \boldsymbol{\theta}) \in \mathcal{Y}, \boldsymbol{\theta} \in \Theta\}$ 
  - mathematical model :  $h(\mathbf{x}, \boldsymbol{\theta}) = \sum_{l=1}^{l=q} \phi(\mathbf{x}) \boldsymbol{\theta}$  etc ...
  - physical/simulation model :  $h(\mathbf{x}, \boldsymbol{\theta})$  is the result of a computer code
- **Uncertainty** : Equip  $\mathcal{X}$  with a prob. measure  $P^x : \mathbf{X} \in (\mathcal{X}, P^x)$ 
  - stochastic codes, Monte-Carlo codes, uncertain variables etc...
- **Stochastic Output**:  $h(\mathbf{X}, \boldsymbol{\theta})$  supposed known through input/output simulations
  - for instance  $\mathbf{x} \mapsto h(\mathbf{x}, \boldsymbol{\theta})$  is has an analytical form but too complicated to compute the distribution  $h(\mathbf{X}, \boldsymbol{\theta})$
  - or  $\mathbf{x} \mapsto h(\mathbf{x}, \boldsymbol{\theta})$  is an input/output simulation code

# From Loss function to Contrast function

- **Loss function:** Given an action set  $\mathcal{A}$  and an output set  $\mathcal{Y}$  (for us  $\mathcal{A} = \mathcal{Y}$ )

$$\begin{aligned} \ell : \mathcal{Y} \times \mathcal{Y} &\longrightarrow \mathbb{R} \\ (a, y) &\longmapsto \ell(a, y) \end{aligned}$$

→ here think  $a \in \mathcal{A}$  as:  $a = h(\mathbf{x}, \theta)$

→ ex: the square loss writes  $\ell(h(\mathbf{x}, \theta), y) = (h(\mathbf{x}, \theta) - y)^2$

- **Towards Contrast functions:** For instance in the case of the square loss, we define the associated "contrast" function as

$$\ell(h(\mathbf{x}, \theta), y) = (h(\mathbf{x}, \theta) - y)^2 = \Psi(h(\cdot, \theta), (\mathbf{x}, y))$$

- **Definition:** Denote by  $\mathcal{F}$  some feature space, a contrast  $\Psi$  is defined as

$$\begin{aligned} \Psi : \mathcal{F} &\longrightarrow L_1(\mathcal{Q}^2) \\ \rho &\longmapsto \Psi(\rho, \cdot) : (\mathbf{x}, y) \in \mathcal{X} \times \mathcal{Y} \longmapsto \Psi(\rho, (\mathbf{x}, y)) \end{aligned}$$

In the example before, if we consider  $\mathcal{F} = \{\rho : \mathcal{X} \rightarrow \mathcal{Y}, \|\rho\|_{L_2(\rho^x)} < \infty\}$ , we may define  $F = \{\rho_\theta : \mathbf{x} \mapsto h(\mathbf{x}, \theta), \theta \in \Theta\} \subset \mathcal{F}$ .

We will call  $F$  as (computer code based) **Model**



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The contrast function **emphasizes** the **quantity of interest** in  $\mathcal{F}$  involved

# Notion of Risk

- **Risk with Loss function:**

$$\mathcal{R}(f) = \mathbb{E}[\ell(f(X), Y)] \underset{\text{e.g.}}{=} \mathbb{E}(f(X) - Y)^2$$

- **Risk with Contrast function,  $\Psi$ -Risk :**

$$\mathcal{R}_{\Psi}(\rho) := \mathbb{E} \Psi(\rho, (\mathbf{X}, Y))$$

- **Target :**

$$\rho^* = \underset{\rho \in \mathcal{F}}{\text{Argmin}} \mathcal{R}_{\Psi}(\rho) \quad \text{if it exists}$$

- **Interpretation:**

In Computer Experiments framework, the "target" defined before will be the "quantity of interest" (Qol) depending on the contrast considered

## Examples of contrasts and associated Qol

(Abuse of notation: we will write  $\Psi(\rho, y)$  a contrast function which does not depend on the joint data  $(\mathbf{x}, y)$ )

- $\mathcal{F} = \{\rho : \mathcal{X} \rightarrow \mathcal{Y}, \|\rho\|_{L_2(P^{\mathbf{x}})} < \infty\}$

**regression-contrast:**  $\Psi(\rho, (\mathbf{x}, y)) = (y - \rho(\mathbf{x}))^2 \rightarrow \rho^*(\cdot) = \mathbb{E}(Y|\mathbf{X} = \cdot)$

- $\mathcal{F} = \mathbb{R}$

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## Examples of contrasts and associated Qol

(Abuse of notation: we will write  $\Psi(\rho, y)$  a contrast function which does not depend on the joint data  $(\mathbf{x}, y)$ )

- $\mathcal{F} = \{\rho : \mathcal{X} \rightarrow \mathcal{Y}, \|\rho\|_{L_2(P^{\mathbf{X}})} < \infty\}$

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- **In practice** we define a model  $F \subset \mathcal{F}$  based on a code  $h(\mathbf{X}, \theta)$  where  $\mathbf{X} \sim P^{\mathbf{X}}$

$$F = \{\rho_\theta : \mathbf{x} \mapsto h(\mathbf{x}, \theta), \theta \in \Theta\} \subset \{\rho : \mathcal{X} \rightarrow \mathcal{Y}\}$$

$$F = \{\rho_\theta = \text{pdf of } h(\mathbf{X}, \theta), \theta \in \Theta\} \subset \{\text{density functions on } \mathcal{Y}\}$$

Etc.

$$F = \{\rho(\theta), \theta \in \Theta\}$$

# Empirical Risk Minimisation

Given a set  $Y_1, \dots, Y_n$  and a simulation code  $h(\mathbf{X}, \theta)$ , with  $\mathbf{X} \sim P^x$ .

Consider a contrast  $\Psi : \mathcal{F} \rightarrow L_1(Q)$  (i.e contrasts only the data  $y$ ) and a Model  $F = \{\rho(\theta), \theta \in \Theta\} \subset \mathcal{F}$  provided by the simulation code

- **Goal:** estimate the parameter

$$\theta_{\Psi}^* = \underset{\theta \in \Theta}{\operatorname{Argmin}} \mathcal{R}_{\Psi}(\theta) = \underset{\theta \in \Theta}{\operatorname{Argmin}} \mathbb{E} \Psi(\rho(\theta), Y)$$

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$$\mathbb{E} \Psi(\rho(\theta), Y) \quad \Rightarrow \quad \frac{1}{n} \sum_{i=1}^n \Psi(\rho^m(\theta), Y_i)$$

where  $\rho^m(\theta)$  is a kernel estimate of  $\rho(\theta)$

$$\rho^m(\theta) = \frac{1}{m} \sum_{j=1}^m \kappa(h(\mathbf{X}_j, \theta)), \quad \mathbf{X}_j \underset{i.i.d}{\sim} P^x.$$

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Example:  $\mathcal{F} = \text{"means"}$ ,  $\kappa(y) = y$

$\mathcal{F} = \text{"densities"}$ ,  $\kappa(y)(\cdot) = \frac{1}{\sqrt{2\pi}b} \exp((y - \cdot)^2 / 2b^2)$

etc...



# Ψ-Estimator

## ■ Generic Ψ-estimator:

$$\hat{\theta}_{\Psi} = \underset{\theta \in \Theta}{\operatorname{Argmin}} \sum_{i=1}^n \Psi(\rho^m(\theta), Y_i)$$

## ■ Examples:

▶ mean-contrast  $\Psi_{mean}$ ,  $\hat{\theta}_{mean} = \underset{\theta \in \Theta}{\operatorname{Argmin}} \sum_{i=1}^n \left( \sum_{j=1}^m (Y_i - h(\mathbf{X}_j, \theta)) \right)^2$

▶ log-contrast  $\Psi_{\log}$ ,  $\hat{\theta}_{\log} = \underset{\theta \in \Theta}{\operatorname{Argmin}} - \sum_{i=1}^n \log \left( \sum_{j=1}^m K_b(Y_i - h(\mathbf{X}_j, \theta)) \right)$

▶  $L_2$ -contrast  $\Psi_{L_2}$

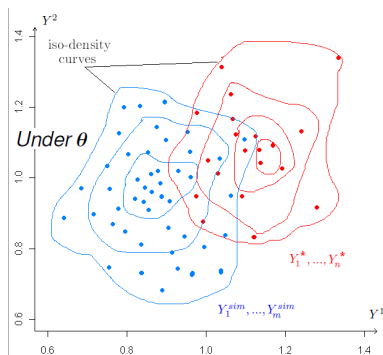
$$\hat{\theta}_{L_2} = \underset{\theta \in \Theta}{\operatorname{Argmin}} \left\{ \left\| \sum_{j=1}^m K_b(\cdot - h(\mathbf{X}_j, \theta)) \right\|_2^2 - \frac{2m}{n} \sum_{i=1}^n \sum_{j=1}^m K_b(Y_i - h(\mathbf{X}_j, \theta)) \right\}$$

▶ Etc...

# Contrast minimization: "the way of minimizing"

$$\hat{\theta}_{\psi} \xrightarrow{\text{plug}} \mathbf{X} \mapsto h(\mathbf{X}, \hat{\theta}_{\psi}), \mathbf{X} \sim P^{\mathbf{X}}$$

- In blue: Simulated data
- In red: Reference data

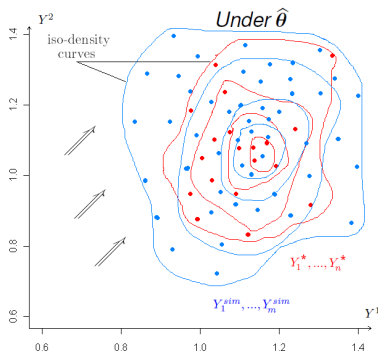


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Depending on the contrast used ...



# Results

N. Rachdi, J-C. Fort and T. Klein, *Risk bounds for new M-estimation problems*, ESAIM : Probability & Statistics, Volume 17 (2013), p. 740–766

## Consistency Results

Under regularity and tightness conditions, in probability

$$\widehat{\theta}_{\Psi}^{n,m} \xrightarrow[n,m \rightarrow \infty]{} \theta_{\Psi}^* = \underset{\theta \in \Theta}{\operatorname{Argmin}} \mathbb{E} \Psi(\rho(\theta), Y)$$

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Central Limit Theorem in progress ...

## Back to the questions in Introduction ...

- **Inverse problem:** If the  $\mathbf{X}_i^*$ 's are not observed ? How to calibrate ?  
(e.g input code  $\neq$  experimental conditions etc...)
- **Prediction problem:** even if they are observed, should we always use regression models for predicting some quantity of interest ?
- for instance, what is the meaning of

$$\mathbb{P}(h(\mathbf{X}, \hat{\boldsymbol{\theta}}_{reg}) > s) \quad \text{or} \quad pdf_{h(\mathbf{X}, \hat{\boldsymbol{\theta}}_{reg})} ?$$

where  $\hat{\boldsymbol{\theta}}_{reg}$  is the mean-squares estimator of the model  $Y_i = h(\mathbf{X}^i, \theta) + \varepsilon_i$

... "*duality*" between estimation procedure and target prediction

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... "*duality*" between estimation procedure and target prediction

Now, we have tools to study that questions ...

## Back to the inductive example

- From  $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$  and a computer code  $h(\mathbf{X}, \theta)$ , we built the density predictions  $\hat{f}_{MS}, \hat{f}_M, \hat{f}_{KL}$



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- We used 3 contrasts ( $\Psi_{reg}$ ,  $\Psi_{mean}$  and  $\Psi_{pdf}$ ) for parameter estimation

$$Y = \sin(X) + 0.01\varepsilon, \quad (X, \varepsilon \sim \mathcal{N}(0, 1) \text{ iid})$$

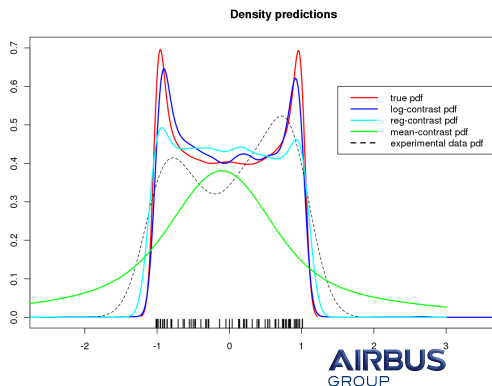
→ **Quantity of Interest:** pdf( $Y$ )

→ **model:**  $h(x, \theta) = \theta_1 + \theta_2 x + \theta_3 x^3$

→ **data:**  $n = 50$   $((X_i, Y_i))$ ,  $m = 10^3$   $(X_j)$

→ **output simulations** under  $X_j \sim P^x = \mathcal{N}(0, 1)$  using

- $h(\cdot, \hat{\theta}_{pdf})$  (blue)
- $h(\cdot, \hat{\theta}_{reg})$  (cyan)
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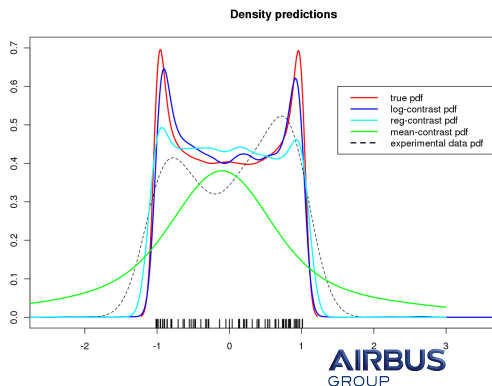
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## Other example: Conditional expectation

- $Y = \sin(X) + \varepsilon$ ,  $X, \varepsilon \sim \mathcal{N}(0, 1)$  independents
- $h(X, \theta) = \theta_1 + \theta_2 X + \theta_3 X^3$ ,  $X \sim P^x = \mathcal{N}(0, 1)$
- $n = 50$  ( $(X_i, Y_i)$ ) and  $m = 10^3$  ( $X_j$ )

**Qol:**  $\rho^* = \mathbb{E}(Y/X = \cdot) (= \sin(\cdot))$   
-->  $\Psi^* = \Psi_{reg}$  ("adapted" contrast)

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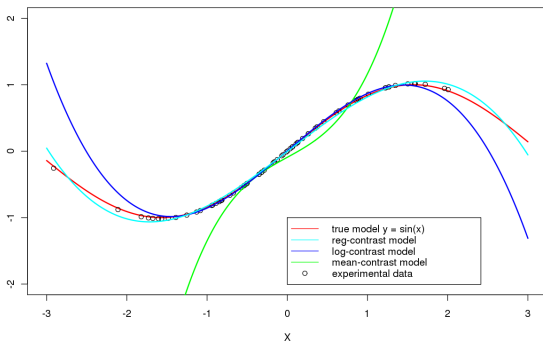
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Qol:  $\rho^* = \mathbb{E}(Y/X = \cdot) (= \sin(\cdot))$   
 $\rightarrow \Psi^* = \Psi_{reg}$  ("adapted" contrast)

■ consider 3  $\Psi$ -estimators:  $\hat{\theta}_{\Psi^*}$ ,  $\hat{\theta}_{\Psi_{\log}}$  and  $\hat{\theta}_{\Psi_{mean}}$

	$\theta_{\Psi}$	$\mathcal{R}_{\Psi^*}(\theta_{\Psi})$
$\Psi = \Psi^*$	(-0.0049, 0.9259, -0.1048)	0.064
$\Psi = \Psi_{\log}$	(0.0057, 1.025, -0.163)	0.36
$\Psi = \Psi_{mean}$	(-0.0924, 0.6607, 0.5965)	6.18

Model Predictions



**Thank you for your attention !**

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