New Sensitivity Indices based on contrasts

Goal Oriented Sensitivity Analysis (GOSA)

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Outline

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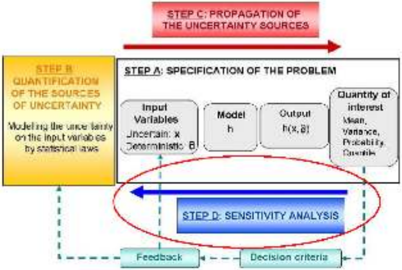
Motivations

- **Uncertainty Management for Flight Control**

- **Engineering methodology**



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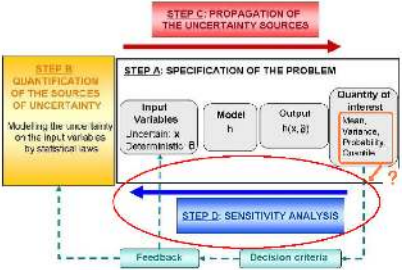

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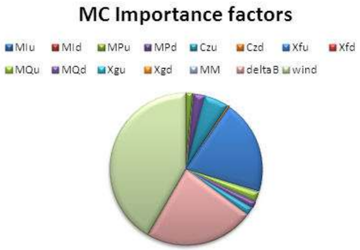
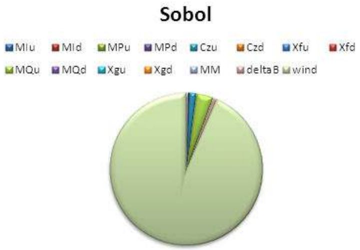
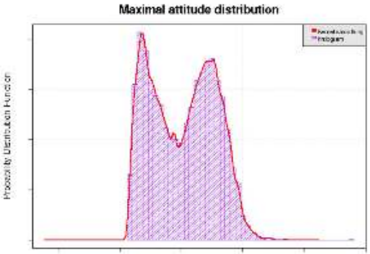
Motivations

Case of Maximal Attitude: various sensitivity measures ...







Motivations

How to explain such differences between sensitivity indicators in a single framework ?
How to define other indicators ?

Issues

- Gather the notion of sensitivity to the notion of quantity/feature of interest of Y
- Define generic sensitivity indices relatively to a feature of Y
- Study the importance ranking between these new indices and the Sobol ones: a variable X_k may have a negligible Sobol index (the lower for instance) and may have a significant importance for some other (contrast-based) index

Motivations

- In a model $Y = h(X_1, \dots, X_d)$ the global Sobol index quantify the influence of a random variable X_i on the output Y. This index is based on the variance (see *[Sobol, 1993]*[6], *[Saltelli et al., 2000]*[5]): in particular, the first order index compares the total variance of Y to the expected variance of the variable Y conditioned by X_i,

$$S_i = \frac{\mathrm{Var}(\mathbb{E}[Y|X_i])}{\mathrm{Var}(Y)}. \quad (1)$$

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$$S_i = \frac{\mathrm{Var}(\mathbb{E}[Y|X_i])}{\mathrm{Var}(Y)}. \tag{1}$$
- By the property of the conditional expectation it writes also
$$S_i = \frac{\mathrm{Var}(Y) - \mathbb{E}_{X_i}(\mathrm{Var}[Y|X_i])}{\mathrm{Var}\,Y}. \tag{2}$$
- Formula (1) is popular and very used by computer scientists

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- Formula (1) is popular and very used by computer scientists
- We propose to adopt formula (2) to extend Sobol indices

Key remarks

What is hidden in the expression $S_i = \frac{\text{Var}(Y) - \mathbb{E}_{\boldsymbol{X_i}}(\text{Var}[Y|X_i])}{\text{Var}Y}$ ...

- Notice that $\text{Var}(Y) = \min_\theta \mathbb{E}(Y-\theta)^2$ (min. reached at $\theta^* = \mathbb{E}Y$)
- Similarly, $\text{Var}[Y|X_i] = \min_\theta \mathbb{E}[(Y-\theta)^2|X_i]$ (min. reached at $\theta^* = \mathbb{E}[Y|X_i]$)

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$$S_i = \frac{\mathbb{E}(Y - \mathbb{E}Y)^2 - \mathbb{E}_{(X_i,Y)}(Y - \mathbb{E}[Y|X_i])^2}{\mathbb{E}(Y - \mathbb{E}Y)^2}$$

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- New general writing of Sobol index

$$S^i_\psi = \frac{\mathbb{E}\psi(Y;\mathbb{E}Y) - \mathbb{E}_{(X_i,Y)}\psi(Y;\mathbb{E}[Y|X_i])}{\mathbb{E}\psi(Y;\mathbb{E}Y)}$$

where for Sobol indices the function ψ is $(y;\theta) \mapsto (y-\theta)^2$

- we will call ψ a *contrast function* which depends on the considered feature of interest, it will play a crucial rule (see *[Rachdi et al., 2012]*[3], *[Fort et al., 2012]*[1])

What about changing contrast ? ...

Birth of new indices ?...

- **We will define ψ-indices as**

  QoI = Quantity of Interest and $QoI|X_i$ = Conditional Quantity of Interest

$$S^i_{\psi} = \frac{\mathbb{E}\psi(Y; QoI) - \mathbb{E}_{(X_i,Y)}\psi(Y; QoI|X_i)}{\mathbb{E}\psi(Y; QoI)}$$

  where ψ is the (a) contrast adapted to the Quantity of Interest

Theoretical definition: ψ-index

Assumption

Let ψ be some contrast, assume that

$$\mathbb{E} \min_{\theta} \psi(Y;\theta) \in \mathbb{R}.$$

All the contrasts presented before satisfy this Assumption since $\min_\theta \psi(y;\theta) = 0$.

Definition: ψ-index

Let $\Psi(\theta) = \mathbb{E}\psi(Y;\theta)$ be a contrast associated to a feature of Y, $\theta^* = \operatorname{Argmin}_{\theta} \Psi(\theta)$.

The ψ-index of the variable $Y = h(X_1, \ldots, X_d)$ w.r.t the contrast ψ and the variable X_k is defined as

$$S_\psi^k = \frac{\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}_{(X_k,Y)}\psi(Y;\theta_k(X_k))}{\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}\min_\theta \psi(Y;\theta)}$$

where $\theta_k(x) = \operatorname{Argmin}_{\theta} \mathbb{E}(\psi(Y;\theta)|X_k = x)$ is the feature of interest of Y conditionally to $X_k = x$

do not solve minimisation problems to compute θ^* and $\theta_k(x)$!
"just" compute the features if known ... (see Simulation section)

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Comments on ψ-index

Lemma

The ψ-index S_ψ^k is non negative.

Proof: comes from the fact that for any random variable ξ and any function g

$$\mathbb{E} \min_\theta g(\theta, \xi) \leq \min_\theta \mathbb{E} g(\theta, \xi) \,.$$

- If Y does not depends on X_k, then $S_\psi^k = 0$. Moreover, assuming that the variables $(X_1, \dots, X_d)$ are independent, if $Y = h(X_k)$ then $S_\psi^k = 1$ and the other indices $S_\psi^l, l \neq k$ are 0
- we have that
$$S_\psi^k \in [0, 1] \,.$$
- These basic properties were expected from a reasonable sensitivity index.

Outline

Notion of Contrast Function

- **Goal:** Define formal indices adapted to a feature of interest of Y
- **Idea: to characterize a feature of Y by a contrast function** (see *[Rachdi, 2011]* [2])

"a feature of interest of Y *induces (defines)* a contrast function which *induces (defines)* an adapted sensitivity index"

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Example of the "mean feature":

$$\theta^* = \mathbb{E}Y \Rightarrow \mathbb{E}Y = \text{Argmin}_{\theta\in\Theta}\,\mathbb{E}(Y-\theta)^2 \Rightarrow \psi : (y;\theta) \mapsto (y-\theta)^2$$

$$\Rightarrow S^i_\psi = \frac{\mathbb{E}\psi(Y;\mathbb{E}Y) - \mathbb{E}_{(X_i,Y)}\psi(Y;\mathbb{E}[Y|X_i])}{\mathbb{E}\psi(Y;\mathbb{E}Y)} = \frac{\text{Var}(Y) - \mathbb{E}(\text{Var}[Y|X_i])}{\text{Var}\,Y}$$

that is "the mean feature" $\Rightarrow$ 1st order Sobol index

- **Feature of Interest formalization:**

a feature of interest is viewed as a minimizer of contrast

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Other contrast functions ?

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Examples of Contrast Functions

Recall that a generic contrast writes $\Psi(\theta) = \mathbb{E}\psi(Y;\theta)$ and $\theta^* = \text{Argmin}_\theta \Psi(\theta)$

$\Rrightarrow$ feature of interest θ^* $\longleftrightarrow$ contrast function Ψ $\Lleftarrow$

- **Central parameters:**
  - The mean $\theta^* = \mathbb{E}Y$: $\Psi(\theta) = \mathbb{E}|Y-\theta|^2$.
  - The median (in $\mathbb{R}$) $\theta^* = q_{0.5}(Y)$: $\Psi(\theta) = \frac{1}{2}\mathbb{E}|Y-\theta|$.
- **An excess probability :** $\theta^* = \mathbb{P}(Y \geq t)$, $\Psi(\theta) = \mathbb{E}|\mathbf{1}_{Y\geq t} - \theta|^2$.
- **All the probability tail:** $\theta^* = \int_{t_0}^{\infty} \mathbb{P}(Y \geq t)dt$, $\Psi(\theta) = \mathbb{E}\int_{t_0}^{\infty} |\mathbf{1}_{Y\geq t} - \theta(t)|^2 dt$.
- **The α-quantile :** $\theta^* = q_\alpha(Y)$, $\Psi(\theta) = \mathbb{E}(Y-\theta)(\alpha - \mathbf{1}_{Y\leq\theta})$.
- **Quantile tail:** $\theta^* = \int_{\alpha_0}^{1} q_\alpha(Y)d\alpha$, $\Psi(\theta) = \mathbb{E}\int_{\alpha_0}^{1}(Y-\theta(\alpha))(\alpha - \mathbf{1}_{Y\leq\theta(\alpha)})d\alpha$.
- **The probability density function** $\theta^* = pdf(Y)$ (infinite dimensional parameter)
  - Using the kernel method, with $K_r(y) = \frac{1}{r}K(\frac{y}{r})$, $r > 0$

$$\Psi(\theta) = \mathbb{E}\int_{-\infty}^{+\infty} (K_r(Y-t) - \theta(t))^2 dt \quad \text{or } L^2 \text{ basis, etc.}$$

- **Etc.**

One easily checks that all these contrasts achieve their minimal value at θ^*

Illustration: feature of interest as minimizer of contrast

Consider the trivial case $Y \sim \mathcal{N}(0,1)$

- **mean-contrast:** $\Psi : \theta \mapsto \mathbb{E}|Y-\theta|^2 = \theta^2 + 1$

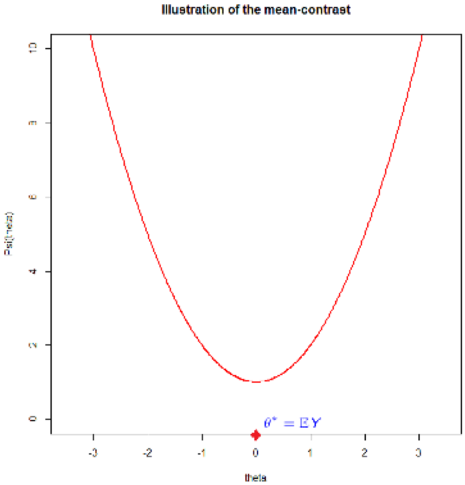

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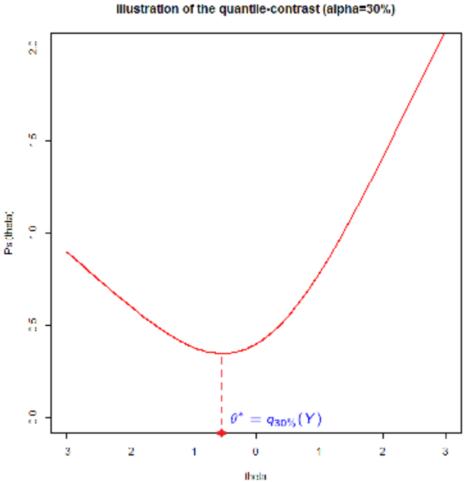
Illustration: feature of interest as minimizer of contrast

Consider the trivial case $Y \sim \mathcal{N}(0,1)$

- α-**quantile-contrast:** $\Psi : \theta \mapsto \mathbb{E}(Y-\theta)(\alpha - 1_{Y \leq \theta}),\ \alpha = 0.3$



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Higher order ψ-indices

Higher order ψ-index

The indices S_ψ^k can be generalized to higher order indices, for $I \subset \{1, ..., d\}$ and denoting by $\mathbf{X}_I = (X_i)_{i \in I}$, we define

$$S_\psi^I = \frac{\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}_{(\mathbf{X}_I, Y)}\psi(Y;\theta_I(\mathbf{X}_I))}{\mathbb{E}_Y\psi(Y;\theta^*)} \qquad (3)$$

where $\theta_I(\mathbf{X}_I)$ is the feature associated to the contrast ψ of the random variable $Y|\mathbf{X}_I$

(In what follows we deal with first order indices)

ψ-Indices Simulation: basic Monte-Carlo approach

Assume that $\mathbb{E}\min_\theta \psi(Y;\theta) = 0$ (it is the case for all presented contrasts), let's estimate

$$S_\psi^k = \frac{\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}_{(X_k,Y)}\psi(Y;\theta_k(X_k))}{\mathbb{E}_Y\psi(Y;\theta^*)} \tag{4}$$

1. Generate $X_1^j, \ldots, X_p^j$ and compute the $Y^j = h(X_1^j, \ldots, X_p^j)$, for $j = 1, \ldots, n_1$. Then compute $\widehat{\theta^*}$ and replace in (4) the expectations $\mathbb{E}_{(X_k,Y)}$ and $\mathbb{E}_Y$ by their empirical versions.
2. Generate $X_1'^j, \ldots, X_p'^j$ for $j = 1, \ldots, n_2$ (independent from the previous set) and compute the $Y'^j = h(X_1'^j, \ldots, X_p'^j)$. Then, from the sample $Y_k'^j(x) = h(X_1'^j, \ldots, X_{k-1}'^j, x, X_{k+1}'^j, \ldots, X_p'^j)$, $j = 1, \ldots, n_2$, compute the function $x \mapsto \widehat{\theta}_k(x)$.
3. Compute the Monte-Carlo estimator

$$\widehat{S}_\psi^k = \frac{\frac{1}{n_1}\sum_{j=1}^{n_1}\left(\psi(Y^j;\widehat{\theta}^*) - \psi(Y^j;\widehat{\theta}_k(X_k^j))\right)}{\frac{1}{n_1}\sum_{j=1}^{n_1}\psi(Y^j;\widehat{\theta}^*)} \tag{5}$$

ψ-Indices Simulation: Sobol indices

We retrieve the basic Monte-Carlo estimator of the 1st order Sobol index

- considering the mean-contrast $\psi(y;\theta) = (y-\theta)^2$ and $n_1 = n_2 = N$ we have that

$$\widehat{\theta}^* = \frac{1}{N}\sum_{l=1}^{N} Y^l \quad \text{and} \quad \widehat{\theta}_k(X_k^j) = \frac{1}{N}\sum_{l=1}^{N} Y_k'^{\,l}(X_k^j)\,.$$

- it is easy to check that the index $\widehat{S}_\psi^k$ in (5) is the well known Monte-Carlo estimator of the first order Sobol index, see [4]:

$$\widehat{S}_\psi^k = \frac{\overline{\mathbf{Y}\mathbf{Y}_k'} - \overline{\mathbf{Y}}\,\overline{\mathbf{Y}_k'}}{\overline{\mathbf{Y}^2} - \overline{\mathbf{Y}}^2},$$

where $\mathbf{Y} = (Y^1, \ldots, Y^N)$ and $\mathbf{Y}_k' = (Y_k'^{\,1}(X_k^1), \ldots, Y_k'^{\,N}(X_k^N))$ and for any vector $\mathbf{u} = (u_1, \ldots, u_N)$

$$\overline{\mathbf{u}} = \frac{1}{N}\sum_{j=1}^{N} u_j\,.$$

Outline

Toy example

Let $Y = X_1 - X_2$, with $X_1, X_2 \sim Exp(1)$ independent

- It is clear that first order Sobol indices are

$$S^1_{Sob} = S^2_{Sob} = 1/2$$

- Sobol indices $\leftrightarrow$ mean-contrast indices ... what about using other contrasts ?

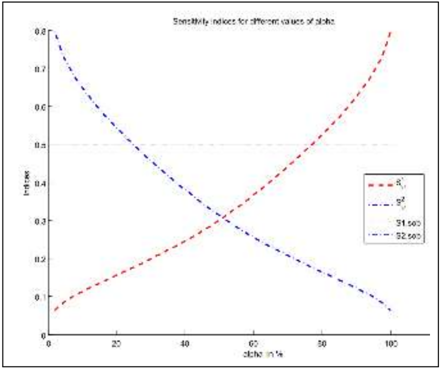
Toy example

Let $Y = X_1 - X_2$, with $X_1, X_2 \sim Exp(1)$ independent

- **feature of interest:** the α-quantile $q_Y(\alpha)$ of Y
- **associated contrast:**

$$\Psi_\alpha(\theta) = \mathbb{E}(Y - \theta)(\alpha - \mathbf{1}_{Y \leq \theta}),$$

- **indices computation:** (computed analytically)



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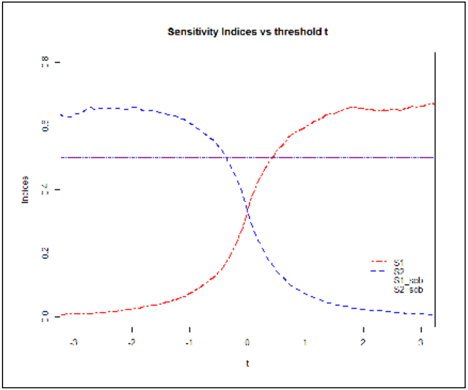
Toy example

Let $Y = X_1 - X_2$, with $X_1, X_2 \sim Exp(1)$ independent

- **feature of interest:** the exceeding probability $\mathbb{P}(Y \geq t)$
- **associated contrast:**

$$\Psi_t(\theta) = \mathbb{E}|\mathbf{1}_{Y \geq t} - \theta|^2 ,$$

- **indices computation:** (simulated by Monte-Carlo methods)

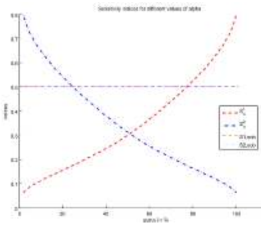


Toy example

Let $Y = X_1 - X_2$, with $X_1, X_2 \sim Exp(1)$ independent

- **Remark:** the threshold-contrast $\Psi_t(\theta) = \mathbb{E}|\mathbf{1}_{Y \geq t} - \theta|^2$ induces Sobol indices of the random variable $Z_t = \mathbf{1}_{Y \geq t}$ (which is a well known fact)
- **Contrast comparison:** t-threshold-contrast and α-quantile-contrast bring the same information since

$$\mathbb{P}(Y > t) \leq \alpha \iff q_\alpha(Y) \leq t$$



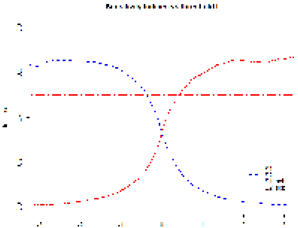
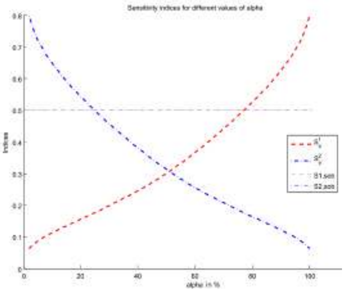


Figure : α-quantile contrast & t-threshold contrast

Toy example

Let $Y = X_1 - X_2$, with $X_1, X_2 \sim Exp(1)$ independent

- **Comparison with Sobol index:**



- **Remark:**
  - First order Sobol indices are insensitive to the quantile level α and (equivalently) the threshold t (Sobol indices $\leftrightarrow$ mean-contrast !)
  - We retrieve the Sobol ranking at the level $\alpha = 0.5$ for the quantile-contrast or equivalently at a threshold $t = 0$ ("the middle") for the threshold-contrast.

Outline

Ishigami function

- **Ishigami function:** Consider $Y = \sin(\xi_1) + 7\,\sin(\xi_2)^2 + 0.1\,\xi_3^4\,\sin(\xi_1)$, where $\xi_1, \xi_1 \sim \mathcal{U}(-\pi, \pi)$ are independent

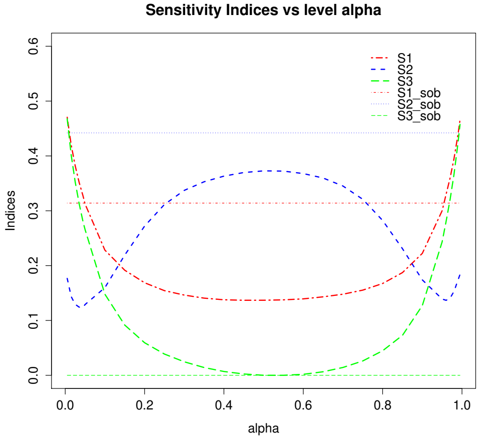
- **2 different ψ-indices :**
  - **mean-contrast:** $\Psi_{mean}(\theta) = \mathbb{E}|Y - \theta|^2 \rightarrow$ 1st order Sobol indices that are

    $$S^1_{Sob} = 0.3139, \quad S^2_{Sob} = 0.4424 \quad \text{and} \quad S^3_{Sob} = 0\,.$$

  - **quantile-contrast:** $\Psi_\alpha(\theta) = \mathbb{E}(Y - \theta)(\alpha - \mathbf{1}_{Y \leq \theta})$

    $\rightarrow$ let's compute the indices S^1_α, S^2_α and S^3_α

Results



- S^3_{Sob} is always equals to 0 whereas S^3_α is highly significative for extreme values of α... which is intuitive !
  It shows clearly the importance of taking into account the goal of the study when measuring the impact of the input variables.
- the importance ranking is different from the Sobol one for $\alpha \gtrsim 85\%$ and $\alpha \lesssim 15\%$

Conclusions & Perspectives

- We have introduced new indices of influence of an input random variable
- It allows to handle many cases that are not directly related to a mean/variance criterion
- Sobol indices are viewed as a particular case related to the mean-contrast
- This work is a first step toward a generalized theory of (goal oriented) sensitivity analysis

Thank you for your attention !

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Outline

Notion of Contrast Function

Definition: Contrast Function

Let Θ be some generic set and Q be some probability measure on a space $\mathcal{Y}$. A (Θ, Q)-**contrast function**, or simply **contrast function**, is defined as any function ψ

$$\begin{aligned} \psi : \Theta &\longrightarrow L_1(Q) \\ \theta &\longmapsto \psi(\cdot;\theta) : y \in \mathcal{Y} \longmapsto \psi(y;\theta), \end{aligned} \quad (6)$$

such that

$$\theta^* = \underset{\theta \in \Theta}{\mathrm{Argmin}}\, \mathbb{E}_{Y \sim Q}\, \psi(Y;\theta) \quad (7)$$

is *unique*. The function $\Psi : \theta \mapsto \mathbb{E}_{Y \sim Q}\, \psi(Y;\theta)$ is the **average contrast function**, or abusively contrast function if there is no ambiguity.

Comments on ψ-index

Let us retrieve the first order Sobol index:

- **trend of interest:** compute sensitivity carried by "the mean": $\theta^* = \mathbb{E}Y$
- **associated contrast:** it induces the mean-contrast
  $\mathbb{E}Y = \text{Argmin}_\theta \, \mathbb{E}(Y-\theta)^2 \Rightarrow \psi : (y;\theta) \mapsto (y-\theta)^2$
- **conditional feature of interest:** $\theta_k(x) = \mathbb{E}(Y|X_k = x)$
  with the contrast characterization $= \text{Argmin}_\theta \, \mathbb{E}(Y-\theta)^2 | X_k = x)$
- We compute

$$\begin{aligned}
\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}_{(X_k,Y)}\psi(Y;\theta_k(X_k)) &= \mathbb{E}(Y-\mathbb{E}Y)^2 - \mathbb{E}_{(X_k,Y)}(Y-\mathbb{E}(Y|X_k))^2 \\
&= \text{Var}(Y) - \mathbb{E}_{X_k}\mathbb{E}\left[(Y-\mathbb{E}(Y|X_k))^2|X_k\right] \\
&= \text{Var}(Y) - \mathbb{E}_{X_k}\text{Var}(Y|X_k) \\
&= \text{Var}(\mathbb{E}(Y|X_k))
\end{aligned}$$

  and

$$\mathbb{E}\psi(Y;\theta^*) - \mathbb{E}\min_\theta \psi(Y;\theta) = \text{Var}(Y) - 0 = \text{Var}(Y)\,.$$

- Finally, we obtain the following ψ-index

$$S_\psi^k = \frac{\text{Var}(\mathbb{E}(Y|X_k))}{\text{Var}(Y)}\,,$$

  which is exactly the first order Sobol index.