Predicted sensitivity for establishing well-posedness conditions in stochastic inversion problems

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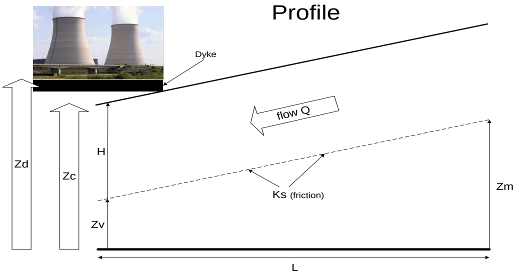
Some typical industrial problems of inversion at EDF (1/3)

Water management

Finding the value (or a relevant range of values) for the Strickler-Manning friction coefficient K_s

- for a given (penalized) water flow Q and a known river geometry
- using a hydraulic computer model involving fluid mechanics equations
- using observations of water level H



Some typical industrial problems of inversion at EDF (2/3)

Energy consumption management

Finding the value (or a relevant range of values) for the influent parameters of thermal models

- (albedo, thermal bridge factor, convective coefficient..)
- using measures of injected electric power

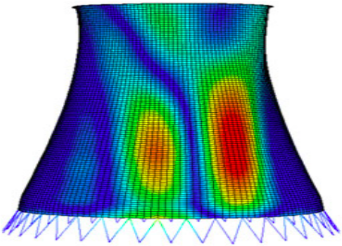
BESTLAB experimental measurement station (EDF Lab)

Some typical industrial problems of inversion at EDF (3/3)

Ageing management

Finding the value (or a relevant range of values) for the localization of crack primings that may appear on concrete cooling towers of nuclear plants

Most sensitive parts of a cooling tower [6]



General framework

Assume to have observations $\mathbf{y_n} = (y_i^*)_{i\in\{1,\dots,n\}}$ of Y^* such that

$$\begin{aligned} Y^* &= Y + \varepsilon, && (1) \\ Y &= g(X) && (2) \end{aligned}$$

where

- Y lives in a $q-$dimensional space
- X is a $p-$dimensional random variable of unknown distribution $\mathcal{F}$
- ε is a (experimental or/and process) "noise" with known distribution f_ϵ
- g is some deterministic function (computer model) from $\mathbb{R}^p$ to $\mathbb{R}^q$

Inversion (in a broad sense).

Inferring on $\mathcal{F}$ from the knowledge of $\mathbf{y_n}$ and f_ϵ

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Stochastic inversion

1. *Bayesian calibration* [8, 4] **[epistemic uncertainty framework]**
   - X random with prior $\pi \Rightarrow \mathcal{F} \equiv \pi(.|\mathbf{y_n}, f_\epsilon)$
   - posterior computation reached by MCMC

2. *Stochastic inversion* [3] **[random uncertainty framework]**
   - the form of $\mathcal{F}$ is fixed and does not "degenerate" to x_0 when $n \to \infty$
   - usually $\mathcal{F}$ is assumed to be a normal or mixture of normal distribution parameterized by θ (finite dimension)
   - frequentist inference on θ [3, 1]
   - Bayesian inference on θ [5]
     - mixture of random and epistemic uncertainties

Both approaches possibly involve meta-modelling if g is a **time consuming black box** [4, 5] (e.g., kriging, polynomial chaos...)

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Stochastic inversion: a typical Bayesian algorithm for posterior simulation

Assume $\mathcal{F}_\theta \equiv \mathcal{N}(\mu, \Gamma)$ with $\theta = (\mu, \Gamma)$

1. Reconstitute missing sample $X_{1,i+1}, \dots, X_{n,i+1}$ given $y_1^*, \dots, y_n^*$ and (μ_i, Γ_i)
2. Sample μ_{i+1} given Γ_i and $X_{1,i+1}, \dots, X_{n,i+1}$
3. Sample Γ_{i+1} given μ_{i+1} and $X_{1,i+1}, \dots, X_{n,i+1}$

Well-posedness conditions and identifiability in stochastic inversion problems

Hadamard's well-posedness : the solution $\hat{\mathcal{F}}$ should exist, be unique and be continuously dependent on observations according to a reasonable topology

- g linear or linearizable, ie. $\exists$ a linear operator H_g such that

$$Y^* \simeq H_g X + \varepsilon'$$

$\Rightarrow$ a low value of the *condition number* [2]

$$\kappa(H_g) = \|H_g^{-1}\| \cdot \|H_g\| \; = \; \frac{|\lambda_{\max}|}{|\lambda_{\min}|} \; \geq \; 1$$

for $\|\cdot\| = L^2$ norm and H_g symmetric

identifiability : in similar situations (g linear or close to linearity) [3]

- H_g must be injective ($\text{rank}(H) = p$)
- dimension requirement: $p \leq nq$

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A new well-posedness principle

Predictive sensitivity analysis principle

- Independently of the availability of $\mathbf{y}^*$, imagine that the problem is solved and $\mathcal{F}$ is known
- Any sensitivity study, for instance based on Sobol' indices [7], should highlight that the main source of uncertainty, explaining the variations of Y^*, is X and not ε

- Property often "checked" a posteriori in practice
- Should be thought as a prior constraint for the inversion problem
- Could improve prior elicitation of θ in a Bayesian framework
- Could improve the (usually stochastic) search for θ in a wide parameter space (e.g., *covariance matrices space*)

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Two possible definitions

Definition

Let (S_X, S_ε) be the first-order Sobol indices quantifying the uncertainty on Y^* explained by X and ε, respectively. The stochastic inversion problem is said to be well-posed in Sobol' sense if

$$S_X \quad > \quad S_\varepsilon. \tag{3}$$

Definition

Denote $\mathcal{E}(X)$ the entropy of X. The stochastic inversion problem is said to be well-posed in the entropic sense if

$$\mathcal{E}(\mathbb{E}(Y^* \mid X)) \quad > \quad \mathcal{E}(\mathbb{E}(Y^* \mid \varepsilon)). \tag{4}$$

Many others can be made, based on usual sensitivity analysis criteria ...

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Example 1

Assume the simple linear model:

$$Y^* = a^T X + \varepsilon \tag{5}$$

with

- $X \in \mathbb{R}^p \sim \mathcal{F} \equiv \mathcal{N}(\mu, \Gamma)$ where $\theta = (\mu, \Gamma)$
- $a \in \mathbb{R}^p$
- $\varepsilon \in \mathbb{R}^p \sim \mathcal{N}(0, \sigma^2 I_p)$

Proposition

The stochastic inversion problem is well-posed in Sobol' and entropic sense if and only if

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Example 1 (inversion)

In a Bayesian framework, assuming

$$X \quad \sim \quad \mathcal{N}(\mu, (k-1)\sigma^2) \quad \text{(missing observations)}$$

with μ, σ^2 known and the following Jeffreys-type prior

$$k \sim \frac{1}{k}$$

Adding of not adding the prior constraint gives two different posterior distributions :

$$k | \ldots \quad \sim \quad \mathcal{IG}\left(n/2, \sum_{i=1}^{n} (y_i^* - a\mu)^2/(2\sigma^2)\right)$$

and (most reliably)

$$k | \ldots \quad \sim \quad \mathcal{IG}\left(n/2, \sum_{i=1}^{n} (y_i^* - a\mu)^2/(2\sigma^2)\right) \mathbb{1}_{\{k>1+1/a^2\}}$$

Example 2

- Assume that g is differentiable in the neighborhood of $\mathbb{E}(X) := (\mathbb{E}(X_1), \ldots, \mathbb{E}(X_p))$
- Assume $X \sim \mathcal{N}(\mu, \Gamma)$, $\varepsilon \in \mathbb{R}^p \sim \mathcal{N}(0, \sigma^2 I_p)$
- Denote $Dg_{\mathbb{E}(X)} := \left(\frac{\partial g}{\partial x_1}(\mathbb{E}(X_1)), \ldots \frac{\partial g}{\partial x_p}(\mathbb{E}(X_p)) \right)$.

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The stochastic inversion problem is well-posed in Sobol' sense if and only if

$$Dg_{\mathbb{E}(X)}^T \Gamma Dg_{\mathbb{E}(X)} \quad > \quad \sigma^2.$$

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Being more general: well-posedness in Fisher's sense

Sobol' well-posedness is limited to reflect how input uncertainty from X or ε is transmitted to the observed output Y^*

Ubiquitous to describe how information is transmitted: quantities of information (as entropy) $\Leftrightarrow$ measures of eliminated uncertainty

A parametric measure of information seems appropriate to be used for defining well-posedness $\Leftrightarrow$ most usual = Fisher information

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General principle (1/2)

Denote by $I_{g(X)}(\theta)$ and $I_{Y^*}(\theta)$ the Fisher information carried respectively by $g(X)$ and Y^* about θ

(a) Since the impact of ε is to degrade information, then it is **expected** / **desired** that

$$I_{g(X)}(\theta) \quad > \quad I_{Y^*}(\theta)$$

where $A > B$, for two squared matrices A and B, means that $A - B$ is a positive-definite matrix

$\Rightarrow$ always true for Gaussian linear problems

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General principle (2/2)

(b) Most of information on θ in Y^* is transmitted from $g(X)$

$\Rightarrow$ The difference

$$I_{g(X)}(\theta) - I_{Y^*}(\theta) \;=\; \text{measure of the information loss because of the noise } \varepsilon$$

should not be greater than a fraction $(1 - 1/c)I_{g(X)}(\theta)$ where $c > 1$

It follows that the prior constraint is

$$I_{g(X)}(\theta) > I_{Y^*}(\theta) > \frac{1}{c} I_{g(X)}(\theta)$$

An intuitive value for c is 2.... but further arguments can be used to assess another value for c

An argument to give a value to c (1/3)

Consider Gaussian linear problems such that $g : x \mapsto Hx$ and

- $X \in \mathbb{R}^p \sim \mathcal{N}(\mu, \Gamma)$, where $\Gamma = \tau^2 I_p$
- $\varepsilon \in \mathbb{R}^q \sim \mathcal{N}(0, \Sigma)$

Proposition

Assume HH^T and Σ commute. A sufficient condition for Fisher's well-posedness is

$$\left(\sqrt{c} - \frac{\max\limits_{1 \le i \le q} \left(\lambda_i^{HH^T} \right)}{\min\limits_{1 \le i \le q} \left(\lambda_i^{HH^T} \right)} \right) \tau^2 \quad \ge \quad \frac{\max\limits_{1 \le i \le q} \left(\lambda_i^{\Sigma} \right)}{\min\limits_{1 \le i \le q} \left(\lambda_i^{HH^T} \right)}.$$

where

- $\{\lambda_i^Z\}_{1 \le i \le q}$ = eigenvalues of Z

An argument to give a value to c (2/3)

Denote $\Psi := \Sigma^{-1/2} H H^T \Sigma^{-1/2}$

Theorem

A sufficient condition for Fisher's well-posedness is

$$(\sqrt{c}-1)\tau^2 > \frac{1}{\min\limits_{1\leq i\leq q}\{\lambda_i^\Psi\}}$$

A necessary condition for Fisher's well-posedness is

$$\sqrt{c} > 1 + \frac{1}{\tau^2 \max\limits_{1\leq i\leq q}\{\lambda_i^\Psi\}}$$

An argument to give a value to c (3/3)

Link with Sobol' / entropy.

- $\tau^2 \max_{1 \leq i \leq q} \{\lambda_i^\Psi\}$ can be interpreted as the signal over noise ratio for the model to invert
- Reasonable to expect $\tau^2 \max_{1 \leq i \leq q} \{\lambda_i^\Psi\} \geq 1$
$$\Rightarrow \sqrt{c} \geq 2 \Rightarrow c \geq 4$$
- If $c = 4$ and $q = 1$ the sufficient condition is strictly equivalent to Sobol' / entropic conditions

Remark. The sufficient condition can be easily extended when $\Gamma \neq \tau^2 I_p$

Linearizable models

We could assume that

$$g(x) = g(x_0) + J_g(x_0)\,(x - x_0) + o(\| x - x_0 \|)$$

where $J_g(x_0)$ denotes the Jacobian matrix of g in x_0

Under the assumption of a negligible linearization error, the linearization turns out to consider

$$Y^*_{x_0} = H_{x_0} X + \varepsilon. \tag{6}$$

where $H_{x_0} := J_g(x_0)$ and $Y^*_{x_0} := Y^* - g(x_0) + H_{x_0} x_0$. Former propositions can be easily adapted

Warning

Main drawbacks of the linearization method

- the approximation error is assumed to be negligible and is not really taken into account
- the choice of the linearization point
  - may induce large variations in the value of the Fisher information
  - previous conditions can be not fully respected with high probability

Choosing the linearization point

1. Choosing the best point as the one for which the associated linearized model preserves the maximum amount of information about θ

$$\max_{x_{\mathbf{0}} \in \mathbb{R}^p} \left\{ I_{g(x_{\mathbf{0}})+H_{x_{\mathbf{0}}}(X-x_{\mathbf{0}})}(\theta) \right\}$$

(too costly)

2. Choosing the approximate linear, well-posed model as the closest to the nonlinear model in the mean-square error sense

$$\min_{\substack{H \in \mathbb{R}^{q \times p} \\ u \in \mathbb{R}^q}} \left\{ \mathbb{E} \parallel Y^* - (HX + u) \parallel^2 \right\} \ s.t. \ I_{Y^*}(\theta) > \frac{1}{c} I_{HX+u}(\theta)$$

it does not longer require the differentiability of g

A third approach

Denote $\tilde{Y}$ the best linear approximation of Y in distributional sense, where $H \in \mathbb{R}^{q \times p}$ and $u \in \mathbb{R}^q$

The optimization problem to solve is the following one

$$H^* = \underset{H \in \mathbb{R}^{q,p}}{\operatorname{argmin}} \; D_{KL}(q, p_H)$$

where

- $D_{\mathrm{KL}}(P \| Q)$ is the Kullback-Leibler divergence
- q denotes the distribution of the random variable $g(X)$ and p_H the distribution of HX

Proposition

The best linear, well-posed approximation of Y is given by

$$Y = HX + \varepsilon, \quad s.t \quad H\Gamma H^T = \mathbb{E}_{g(X)}(xx^T)$$

and

$$(\sqrt{c} - 1) \min_{1 \le i \le q} \left\{ \lambda_i^{\Gamma} \right\} > \frac{1}{\min_{1 \le i \le q} \left\{ \lambda_i^{\Psi} \right\}},$$

where $\Psi := \Sigma^{-1/2} H H^T \Sigma^{-1/2}$

Main (temporary) conclusions

Our postulate

- Previously to use real observations, sensitivity analysis is a way of understanding what can be a “well-posed" problem
- Any (or many) sensitivity indice(s) has an interpretation in Hadamard's sense (and conversely)
- This interpretation can be used to produce useful prior constraints in inversion problems

Hadamard's condition is mainly qualitative: the condition number should be "close" to 1

Rule of thumb in practice : $\kappa(H_g) = 10^k$ with k the number of lost digits of accuracy

This new formalization of well-posedness is more suitable to sensitivity analysts

Linear or linearized models usually offer less contrast than nonlinear models ⇒ a prior constraint for linear models should be “approximately" respected too for nonlinear models

Work in progress

How to apply in practice? Monte Carlo-based computation + design of experiments

Modifying the way of sampling candidate covariance matrices in assessment procedures (typically, Monte Carlo Markov Chains) on the examples listed above: $\Rightarrow$ faster convergence

The restriction of the covariance matrix space due to inserting this new condition of well-posedness is likely to determine new invariance prior measures (Jeffreys-type) on Γ with good posterior coverage properties

Useful for conducting objective Bayesian stochastic inversion

Going from Sobol' to recently generalized indices (e.g. HSIC insides [Da Veiga 2015]): $\Rightarrow$ Building better interpretation of what is a well-posed inversion problem

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