Certified goal-oriented error estimation, application to sensitivity analysis

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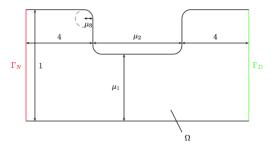






Venturi's example [Rozza and A.T., 2008, Janon et al., 2015]

Let
$$\mu = (\mu_1, \mu_2, \mu_3) \in \mathcal{P} = [0.25, 0.5] \times [2, 4] \times [0.1, 0.2]$$
, let $\Omega = \Omega(\mu)$ defined as:



Let us define the continuous state variable $u_e = u_e(\mu) \in X_e$ as:

$$\left\{ \begin{array}{l} \Delta u_e = 0 \text{ in } \Omega \\ u_e = 0 \text{ on } \Gamma_D \\ \frac{\partial u_e}{\partial n} = -1 \text{ on } \Gamma_N \\ \frac{\partial u_e}{\partial n} = 0 \text{ on } \partial \Omega \setminus (\Gamma_N \cup \Gamma_D) \end{array} \right.$$

with

$$X_e = \{ v \in H^1(\Omega) \text{ s.t. } v|_{\Gamma_D} = 0 \}.$$

Define the output of interest as:

$$s(\mu) = s(u_e(\mu)) = \int_{\Gamma_u} u_e(\mu).$$

We are interested in determining the respective influence of parameters μ_1, μ_2, μ_3 on $s(\mu)$.

The variational formulation for the Venturi's example is:

$$\int_{\Omega} \nabla u_{\mathsf{e}}.\nabla v = -\int_{\Gamma_{\mathsf{N}}} v, \ \forall \ v \in X_{\mathsf{e}}.$$

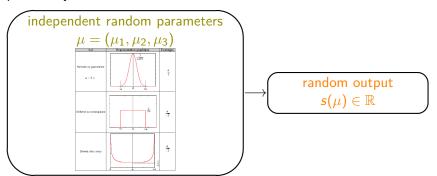
Let \mathcal{T} be a finite triangulation of Ω and $\mathbf{P}^1(\mathcal{T})$ the associated finite element subspace. The above problem is discretized as follows:

$$\int_{\Omega} \nabla u . \nabla v = - \int_{\Gamma_N} v, \ \forall \ v \in X,$$

where $X = \{v \in \mathbf{P}^1(\mathcal{T}) \text{ s.t. } v|_{\Gamma_d} = 0\}.$

Towards global sensitivity analysis:

Uncertainties on parameters μ_1, μ_2, μ_3 are modeled by independent probability distributions.



In the previous example, let μ be modeled by a random vector distributed uniformly on $\mathcal{P} = [0.25, 0.5] \times [2, 4] \times [0.1, 0.2]$.

Is the output of interest $s(\mu)$ more or less variable when setting one of the parameters μ_i , i=1,2,3 to a nominal value?

$$Var(s(\mu)|\mu_i = \mu_{i,0})$$
, how to choose $\mu_{i,0}? \Rightarrow \mathbb{E}[Var(s(\mu)|\mu_i)]$

Theorem (total variance)

$$Var(s(\mu)) = Var[\mathbb{E}(s(\mu)|\mu_i)] + \mathbb{E}[Var(s(\mu)|\mu_i)].$$

Definition (First-order Sobol' indices)

$$i = 1, 2, 3$$

$$0 \leq S_i = 1 - \frac{\mathbb{E}\left[\mathsf{Var}\left(s(\mu)|\mu_i\right)\right]}{\mathsf{Var}(s(\mu))} = \frac{\mathsf{Var}\left[\mathbb{E}\left(s(\mu)|\mu_i\right)\right]}{\mathsf{Var}(s(\mu))} \leq 1$$

A value close to 1 (resp. a small value) for the first-order Sobol' index S_i means that μ_i has many (resp. little) influence on $s(\mu)$.

Estimation procedure:

Monte Carlo based estimation procedures for Sobol' indices require many evaluations of the output of interest $s(\mu)$. It is possible to obtain confidence intervals.

What happens if the output $s(\mu)$ is costly to evaluate?

It is then possible to approximate $s(\mu)$ by $\widetilde{s}(\mu) = s(\widetilde{u}(\mu))$ with $\widetilde{u}(\mu)$ an approximation of the state variable $u(\mu)$.

What about confidence intervals in that case?

The approximation error $|s(\mu) - \tilde{s}(\mu)|$ has to be taken into account in their construction [Janon et al., 2014b, Janon et al., 2014a].

A nonlinear toy example

Nonviscous Burgers' equation:

we are looking for u = u(t, x) satisfying:

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial (u^2)}{\partial x} = 0\\ u(t, x = 0) = 1 \ \forall t\\ u(t = 0, x) = \cos^2(\alpha x) + \beta x \end{cases}$$

where the parameter vector $\mu = (\alpha, \beta)$ belongs to $[0,1] \times [0,1]$.

Discretization upwind scheme: we look for $(u_i^n)_{i,n}$ so that:

$$\begin{cases} \frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{1}{2} \frac{(u_i^{n+1})^2 - (u_{i-1}^{n+1})^2}{\Delta x} = 0 & \forall i \ge 1 \\ u_0^n = 1 & \forall n \\ u_i^0 = \cos^2(\alpha i \Delta x) + \beta i \Delta x & \forall i \end{cases}$$

with N_t the number of timesteps, N_x the number of space points, $\Delta t = 1/N_t$ and $\Delta x = 1/N_x$.

A linear toy example with nonlinear outputs

The linear transport equation

Let us define $u_e = u_e(t, x)$ solution of the following equation for all $(t, x) \in (0, 1) \times (0, 1)$:

$$\begin{cases} \frac{\partial u_e}{\partial t}(t,x) + \mu \frac{\partial u_e}{\partial x}(t,x) = \sin(x) \exp(-x) \\ u_e(t=0,x) = x(1-x) \quad \forall x \in [0,1] \\ u_e(t,x=0) = 0 \quad \forall t \in [0,1] \end{cases}$$

We consider: $\mu \sim \mathcal{U}([0.5, 1])$.

Discretization: let us consider $u=(u_i^n)_{i=0,\dots,N_x;n=0,\dots,N_t}$ with $\forall i,\ u_i^0=i\Delta_x(1-i\Delta_x),\ \forall n,\ u_0^n=0$ and the first-order upwind scheme implicit relation

$$\forall i, n \ \frac{u_{i+1}^{n+1} - u_{i+1}^n}{\Delta_t} + \mu \frac{u_{i+1}^{n+1} - u_{i}^{n+1}}{\Delta_x} = \sin(i\Delta_x) \exp(-i\Delta_x).$$

A linear toy example with nonlinear outputs

Full dimension: the space-time vector u is of dimension $\mathcal{N} = (N_x + 1)(N_t + 1)$.

Nonlinear outputs:

- Square output: $s(\mu) = \left(u_{N_x}^{N_t}\right)^2$
- Exponential output: $s(\mu) = \exp\left(u_{N_x}^{N_t}\right)$
- ullet Triple exponential output: $s(\mu) = \exp\left(3u_{N_x}^{N_t}\right)$

Outline of the talk

I- Problem statement in the linear context

II- Goal oriented probabilistic error bound

III- A first numerical example

IV- Extension to nonlinear models

V- From nonlinear models to nonlinear outputs

I- Problem statement

Let \mathcal{P} be the parameter space. For any $\mu \in \mathcal{P}$, let $u(\mu)$ be the solution of the linear system:

$$A(\mu)u(\mu)=f(\mu),$$

with $A(\mu)$ $(f(\mu))$ a known $\mathcal{N} \times \mathcal{N}$ matrix $(\mathcal{N} \times 1 \text{ vector})$.

The linear output of interest is defined as: $s(\mu) = \ell^{\top} u(\mu)$.

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Dimension reduction: let \widetilde{X} be a subspace of X of dimension $n << \mathcal{N}$. Let Z be the $\mathcal{N} \times n$ matrix whose columns are the components of a (reduced) basis of \widetilde{X} in the canonical basis of X.

Let $\widetilde{u}(\mu)$, e.g., be the $n \times 1$ vector solution of:

$$(Z^{\top}A(\mu)Z)\widetilde{u}(\mu) = Z^{\top}f(\mu).$$

Define the approximated output as:

$$\widetilde{s}(\mu) = \ell^{\top} Z \widetilde{u}(\mu) \approx \ell^{\top} u(\mu) = s(\mu).$$

I- Problem statement

Under some (more or less technical) hypotheses on $A(\mu)$ and on the norm $\|\cdot\|$ (say, Euclidean norm), the reduced basis comes with an error bound $\epsilon^u(\mu)$:

$$\forall \mu \in \mathcal{P}, \|\mathbf{u}(\mu) - Z\widetilde{\mathbf{u}}(\mu)\| \leq \epsilon^{\mathbf{u}}(\mu)$$

which can be computed *efficiently* (i.e., with the order of complexity of the computation of $\widetilde{u}(\mu)$).

Question: Can we deduce from it an error bound $\epsilon(\mu)$ on s:

$$\forall \mu \in \mathcal{P}, \ |\mathbf{s}(\mu) - \widetilde{\mathbf{s}}(\mu)| \le \epsilon(\mu)$$

which can be explicitly and efficiently computed?

Answer: Yes, as the "Lipschitz bound" holds:

$$\forall \mu \in \mathcal{P}, |s(\mu) - \widetilde{s}(\mu)| \leq L\epsilon^{u}(\mu), \text{ with } L = \sup_{\|u\| = 1} \ell^{\top} v.$$

We aim at improving this "Lipschitz" bound.

By **efficiently computable**, one means that the computation may be divided in two phases:

an *offline* phase during which quantities not depending on μ are computed, this phase can be relatively costly;

an *online* phase during which quantities depending on μ are computed, this phase has to be efficient.

Indeed, let c_{off} (resp. c_{on}) be the cost of the offline (resp. online) phase. If one wants to estimate all first-order Sobol' indices, one needs to evaluate 2N times the model, with N the size of the Monte Carlo sample. Thus the cost is $c_{off} + 2N \times c_{on}$.

Starting point:

Usually, the bound $\epsilon^u(\mu)$ on $||u(\mu) - \widetilde{u}(\mu)||$ is based on the **residual** and its **norm**:

$$r(\mu) = A(\mu)Z\widetilde{u}(\mu) - f(\mu) \in X.$$

We also want to exploit that the (say, Euclidean) scalar products of the residual, $\langle r(\mu), \phi \rangle$, are efficiently computable $\forall \phi \in X$, in the usual setting of reduced basis for affinely parametrized PDE. Let $\{\phi_i\}_{i=1,\dots,\mathcal{N}}$ be an orthonormal basis of X (to be chosen later). We have:

$$\widetilde{s}(\mu) - s(\mu) = \sum_{i>1} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle,$$

where $w(\mu)$ is the solution of the so-called **adjoint** (or **dual**) problem:

$$w(\mu) = A(\mu)^{-\top} \ell.$$

Let $K \in \mathbb{N}^*$. We have:

$$|\widetilde{s}(\mu) - s(\mu)| \leq \left| \sum_{i=1}^K \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle \right| + \left| \sum_{i>K} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle \right|.$$

Consider first

$$au_1(\mu) := \left| \sum_{i=1}^K \underbrace{\langle w(\mu), \phi_i \rangle}_{ ext{to bound}} \overbrace{\langle r(\mu), \phi_i
angle}^{ ext{computable}} \right|$$

We compute (once for all the values of μ):

$$\beta_i^{min} = \min_{\mu \in \mathcal{P}} D_i(\mu), \quad \beta_i^{max} = \max_{\mu \in \mathcal{P}} D_i(\mu),$$

where: $D_i(\mu) = \langle w(\mu), \phi_i \rangle$, (2K optimization problems on \mathcal{P}).

Let

$$\beta_{i}^{up}(\mu) = \begin{cases} \beta_{i}^{max} & \text{if } \langle r(\mu), \phi_{i} \rangle > 0 \\ \beta_{i}^{min} & \text{else,} \end{cases} \quad \beta_{i}^{low}(\mu) = \begin{cases} \beta_{i}^{min} & \text{if } \langle r(\mu), \phi_{i} \rangle > 0 \\ \beta_{i}^{max} & \text{else.} \end{cases}$$

We then have:

$$|\tau_1(\mu)| \leq \max\left(\left|\sum_{i=1}^K \langle r(\mu), \phi_i \rangle \beta_i^{low}(\mu)\right|, \left|\sum_{i=1}^K \langle r(\mu), \phi_i \rangle \beta_i^{up}(\mu)\right|\right) =: T_1(\mu).$$

We then have:

$$| au_1(\mu)| \leq \max\left(\left|\sum_{i=1}^K \langle r(\mu), \phi_i \rangle \beta_i^{low}(\mu)\right|, \left|\sum_{i=1}^K \langle r(\mu), \phi_i \rangle \beta_i^{up}(\mu)\right|\right) =: T_1(\mu).$$

Let now $\tau_2(\mu) = |\sum_{i>K} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle|.$

This term is not efficiently computable. We assume that μ is a random vector on \mathcal{P} , with known distribution. Let us control $T_2 = \mathbb{E}_{\mu} \left[\tau_2(\mu) \right]$ by:

$$\frac{1}{2}\mathbb{E}_{\mu}\left(\sum_{i>K}\langle w(\mu),\phi_i\rangle^2 + \sum_{i>K}\langle r(\mu),\phi_i\rangle^2\right) = \sum_{i>K}\langle G\phi_i,\phi_i\rangle$$

where G is the positive, self-adjoint operator defined by:

$$\forall \phi \in X, \ \ G\phi = \frac{1}{2}\mathbb{E}_{\mu}\left(\langle r(\mu), \phi \rangle r(\mu) + \langle w(\mu), \phi \rangle w(\mu)\right).$$

Recall that:

$$T_2 \leq \sum_{i>K} \langle G\phi_i, \phi_i \rangle.$$

Let $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_{\mathcal{N}} \geq 0$ be the eigenvalues of G, and ϕ_i^G be a unitary eigenvector of G with respect to λ_i . The term $\sum_{i>\mathcal{K}} \langle G\phi_i, \phi_i \rangle$ is minimized for $\phi_i = \phi_i^G \ \forall i>\mathcal{K}$.

With this choice for the orthonormal basis $\{\phi_1, \dots, \phi_{\mathcal{N}}\}$, we get the following *a priori* bound:

$$T_2 \leq \sum_{i>K} \lambda_i^2$$
.

In [Janon et al., 2015] is described a way of estimating the ϕ_i^G with a cost independent of the dimension \mathcal{N} of X.

Probabilistic error bound: one accepts the risk of the bound for $|s(\mu) - \tilde{s}(\mu)|$ being violated for a set of parameters having "small" probability measure.

Theorem ([Janon et al., 2015])

Let
$$\alpha \in (0,1)$$
, $\mathbb{P}_{\mu}\left(|s(\mu) - \widetilde{s}(\mu)| > T_1(\mu) + \frac{T_2}{\alpha}\right) < \alpha$.

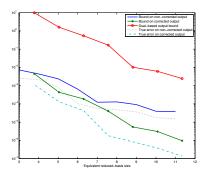
Idea of proof: The main ingredient is Markov Inequality. \Box

In practice, we use a Monte Carlo estimation of T_2 (once for all the values of μ).

III- A first numerical example

Venturi's example with $s(\mu) = \int_{\Gamma_N} u(\mu)$, $\mathcal{P} = [0.25, 0.5] \times [2, 4] \times [0.1, 0.2]$.

We choose: $\mathcal{N}=525$, the reduced basis is a POD computed from a snapshot of size 80, K=20, $\#\Xi=200$, the risk level $\alpha=0.0001$



III- A first numerical example

Results for first-order sensitivity analysis:

input parameter	$\left[\widehat{S}_{i}^{m};\widehat{S}_{i}^{M}\right]$	$\left[\widehat{S}_{i,\alpha_{as}/2}^{m};\widehat{S}_{i,1-\alpha_{as}/2}^{M}\right]$
μ_1	[0.530352;0.530933]	[0.48132; 0.5791]
μ_2	[0.451537;0.452099]	[0.397962;0.51139]
μ_3	[0.00300247;0.0036825]	[-0.0575764;0.0729923]

Table: Certification via bootstrap : size of the Monte Carlo sample 1000, bootstrap B=500, reduced basis size m=10, confidence level 0.95.

IV- Extension to nonlinear models

[Janon et al., 2016b] Problem statement: $\mathcal{M}: \mathcal{P} \times X \to Y$, $\mathcal{M}(\mu, u(\mu)) = 0$.

One wants to achieve Formula

$$\widetilde{s}(\mu) - s(\mu) = \sum_{i>1} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle,$$

where $w(\mu)$ is the solution of the so-called **adjoint** (or **dual**) problem, one wants to define an operator

$$\mathcal{M}^*: \mathcal{P} \times X \times X \times Y \to X$$
,

linear in the last variable, such that the following identity holds:

$$\forall \mu \in \mathcal{P}, \forall x_1, x_2 \in X, \forall y \in Y,$$
$$\langle x_1 - x_2, \mathcal{M}^*(\mu, x_1, x_2, y) \rangle = \langle \mathcal{M}(\mu, x_1) - \mathcal{M}(\mu, x_2), y \rangle.$$

IV- Extension to nonlinear models

Assume that $\mathcal{M}: \mathcal{P} \times X \to Y$ is C^1 with respect to x, $\forall x \in X$. Let $d \mathcal{M}(\mu, x): X \to Y$ the derivative of \mathcal{M} in $x \in X$, $d \mathcal{M}(\mu, x)^*: Y \to X$ the (linear) adjoint of $d \mathcal{M}(\mu, x)$.

Adapting the ideas developed for goal-oriented adaptive FEM, we first define the *finite difference adjoint* operator of $\mathcal M$ by

$$\mathcal{M}^{\star}(\mu, x_1, x_2, y) = \int_0^1 d\mathcal{M}^{\star}(\mu, x_2 + s(x_1 - x_2))(y) ds$$
.

What assumptions on the nonlinearity and on the dependence in the parameter ? main issue: computation of all the scalar products $\langle r(\mu), \phi_i \rangle$ $(i=1,\ldots,K)$ at a low cost, ideally independent from \mathcal{N} .

$$\{y_1,\ldots,y_{\mathcal{S}}\}\ (\textit{resp.}\{x_1,\ldots,x_{\mathcal{N}}\})$$
 orthonormal basis of Y ($\textit{resp.}\ X$).

$$\mathcal{M}: \mathcal{P} \times X \to Y, \quad \mathcal{M}\left(\mu, \sum_{i=1}^{\mathcal{N}} v_i x_i\right) = \sum_{j=1}^{\mathcal{S}} m_j(\mu, v_1, \dots, v_{\mathcal{N}}) y_j$$

- affine parameter dependence

$$m_j(\mu, v_1, \ldots, v_{\mathcal{N}}) = \sum_{k=0}^{T_j} Q_{k,j}(v_1, \ldots, v_{\mathcal{N}}) h_k(\mu)$$

- polynomial nonlinearity

$$Q_{k,j}(v_1,\ldots,v) = \sum_{\alpha=(\alpha_1,\ldots,\alpha_N)\in I_{j,k}} q_{j,k,\alpha} \prod_{l\in V_\alpha} v_l^{\alpha_l}$$

Then, it is possible to compute all the scalar products $\langle r(\mu), \phi_i \rangle$ (i = 1, ..., K) with an offline/online procedure whose online phase has a cost independent from the full dimension \mathcal{N} .

IV- Extension to nonlinear models

Non-viscous Burgers' example: [Janon et al., 2016b]

Parameter	Description	Usual range
N _x	Number of points in x	10 - 80
N _t	Number of time steps	10 - 20
N _{test}	Monte-Carlo sample size	100
N _{snap}	Size of the POD training sample set	70
N_{ϕ}	Index K for the estimation of T_1 using basis ϕ_G	8
N _{basis}	Size of the POD basis	3 – 10
Δt	Time step	$\Delta t = 1/N_t$
Δχ	Space step	$\Delta x = 1/N_x$

Table: Table of experiment description and numerical setup.

Speed up ratios:

$$r_1 = rac{ ext{full pb computing time}}{ ext{online computing time}}$$

$$r_2 = \frac{K \times \text{full pb computing time}}{\text{offline} + K \times \text{online computing time}}$$

with K = 1000.

IV- Extension to nonlinear models

Experiment label	N _t	N _x	N _{test}	$N_{\rm snap}$	N_{ϕ}
t10 × x40	10	40	100	70	8
t20 × x40	20	40	200	150	12
t10 × x80	10	80	100	70	8
t20 × x80	20	80	200	150	12

Table: Table of experiment description and numerical setup.

Experiment name	(a) t10 × x40	(b) t20 × ×40	(c) t10 × ×80	(d) t20 × ×80
full pb computing time	47.1	354.1	178.5	24160
online computing time	13.6	41.6	21.1	35.79
offline computing time	426.4	2535	1236	112370
speed-up ratio r ₁	3.5	8.5	8.45	675
speed-up ratio r ₂	3.4	8	8	163

Table: Table of costs, for a size of the truncated POD equal to 8.

V- From nonlinear models to nonlinear outputs

[Janon et al., 2016b] Find $v(\mu)$ such that $\mathcal{H}(\mu, v(\mu)) = 0$ where $\mathcal{H}: \mathcal{P} \times X \to Y$ is a (not necessarily linear with respect to the second argument) function, and consider the following output:

$$S(\mu) = f(v(\mu))$$

where f is a (not necessarily linear) function from Y to \mathbb{R} .

Let

$$u(\mu) = \begin{pmatrix} v(\mu) \\ S(\mu) \end{pmatrix} = \begin{pmatrix} \overline{u}(\mu) \\ \underline{u}(\mu) \end{pmatrix} \in X \times \mathbb{R}.$$

We then define $\mathcal{M}: \mathcal{P} \times (X \times \mathbb{R}) \to Y$ by:

$$\mathcal{M}(\mu, u(\mu)) = \begin{pmatrix} \mathcal{H}(\mu, \overline{u}(\mu)) \\ f(\overline{u}(\mu)) - \underline{u}(\mu) \end{pmatrix},$$

and consider the following linear output:

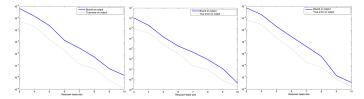
$$s(\mu) = S(\mu) = \underline{u}(\mu) = \langle \ell, u(\mu) \rangle \text{ with } \ell = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \in X \times \mathbb{R}.$$

V- From nonlinear models to nonlinear outputs

Let us come back to the linear transport example.

Numerical tuning: size of the POD snapshot 70, number of vectors $\hat{\phi}_i^{\mathcal{G}}$ $N_{\phi}=20$, risk level $\alpha=0.0001$.

The error bounds are averaged on a sample of 200 random parameter values, for the three different output cases: square, exponential and triple exponential.



Comparison between the mean error bound and the true error, for different reduced basis sizes, in the square (top left), the exponential (top right) and the triple exponential (down) output case.

Conclusion, perspectives

Conclusion

- we obtained a goal-oriented probabilistic error estimation for linear/nonlinear problems and linear/nonlinear outputs,
- this bound can be computed efficiently in an offline/online procedure,
- we applied such bounds to provide confidence intervals for sensitivity indices,
- during the talk I provided illustrations on toy examples.

Conclusion, perspectives

Generalizations, perspectives

- application to more complex models, see e.g., in [Janon et al., 2016a], an application to the sensitivity analysis for a flow control problem with linearized Shallow water equation,
- combination with EIM for non affinely parametrized PDE,
- what happens if one considers sensitivity indices which are not based on variance?
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Thanks for your attention