Reduced basis metamodels for sensitivity analysis

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Journées du GDR MASCOT-NUM, 21 mars 2012

Context: Global sensitivity analysis

- **Input parameters:** $\mu = (\mu_1, \ldots, \mu_p)$ independent random variables of known distribution.
- **Quantity of interest:** $Y = f(\mu)$.
- For $i = 1, \ldots, p$, we consider the i^{th} **Sobol index**:

$$S_i = \frac{\mathbf{Var}\left(\mathbf{E}(Y|\mu_i)\right)}{\mathbf{Var}\, Y}$$

- This index quantifies, on a scale from 0 to 1, the fraction of variance in Y explained by uncertainty on μ_i.

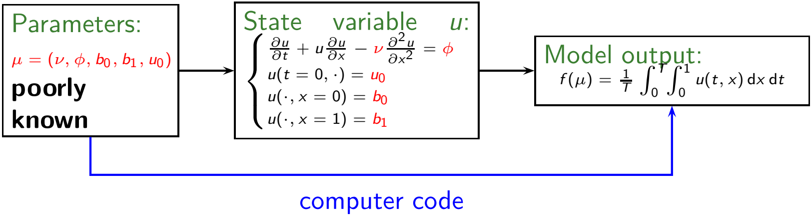
Context: Model with uncertain parameters

- **For us:**

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

where $u(\mu)$ satisfies a μ-parametrized PDE (boundary/boundary-initial value problem).

- **Example:**



Context: Monte-Carlo estimation

- In general, S_i can not be analytically computed.
- It has to be **estimated**, using a sample of outputs.
- Monte-Carlo: $\{\mu^k\}$ and $\{\mu'^k\}$: are two N-sized samples of μ's distribution;

$$\widehat{S}_i = \frac{\frac{1}{N}\sum_{k=1}^N y_k y'_k - \left(\frac{1}{N}\sum_{k=1}^N y_k\right)\left(\frac{1}{N}\sum_{k=1}^N y'_k\right)}{\frac{1}{N}\sum_{k=1}^N (y_k)^2 - \left(\frac{1}{N}\sum_{k=1}^N y_k\right)^2}$$

with $y_k = f(\mu^k), \;\; y'_k = f(\mu_1'^k, \mu_2'^k, \dots, \mu_{i-1}'^k, \mu_i^k, \mu_{i+1}'^k, \dots, \mu_p'^k)$

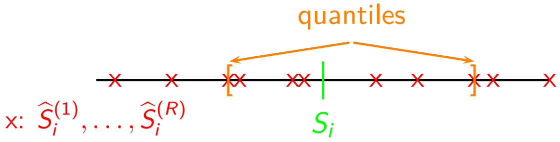
- This requires $2N$ code calls $\rightarrow$ the use of a **metamodel** (surrogate model, response surface, emulator...) is justified.
- We aim at **quantifying** the total estimation error, caused by:
  - the Monte-Carlo estimation;
  - the replacement of the original model by the metamodel.

Outline

- Monte-Carlo error quantification
- Metamodel: reduced basis method
- Combined confidence intervals
- Simulation parameters choice
- Numerical results

Monte-Carlo error
"Standard" approach

- $\widehat{S}_i = \widehat{S}_i(\mathcal{E})$ where $\mathcal{E} = \left(\{\mu^k\}, \{\mu'^k\}\right)$ are iid. random samples of μ's distribution.
- To quantify the error between $\widehat{S}_i$ and S_i, we compute $\widehat{S}_i(\mathcal{E})$ for several independent samples $\mathcal{E}^{(1)}, \dots, \mathcal{E}^{(R)}$.
- We hence get a sample of replications $\mathcal{R} = \{\widehat{S}_i^{(1)}, \dots, \widehat{S}_i^{(R)}\}$ of $\widehat{S}_i$.



- We deduce an (approximate) confidence interval of chosen level.

Monte-Carlo error
Bootstrap approach

- **Problem:** the R replications of $\widehat{S}_i$ require $2N \times R$ evaluations of f.
- In the bootstrap approach:
  - we draw a couple of samples:
  $$\mathcal{E} = \left(\{\mu^k\}_{k=1,\dots,N}, \{\mu'^k\}_{k=1,\dots,N}\right)$$
  - for $r = 1, \dots, R$, we compute the r^{th} replication $\widehat{S}_i^{(r)}$ on the *bootstrap resample* couple:
  $$\mathcal{E}^{(r)} = \left(\{\mu^k\}_{k \in L_r}, \{\mu'^k\}_{k \in L_r}\right)$$
  where L_r is a list *list* sampled with replacement from $\{1, \dots, N\}$;
  - The replication set is then used as before.
- These R replications can be computed using the $2N$ evaluations of f on the points of $\mathcal{E}$.

Monte-Carlo error
Asymptotic approach

- We have a *central limit theorem:*

$$\sqrt{N}(\widehat{S}_i - S_i) \underset{N\to\infty}{\overset{\mathcal{L}}{\to}} \mathcal{N}\left(0, \sigma_S^2\right),$$

where

$$\sigma_S^2 = \frac{\mathbf{Var}\left((Y - \mathbf{E}(Y))\left[(Y' - \mathbf{E}(Y)) - S_i(Y - \mathbf{E}(Y))\right]\right)}{(\mathbf{Var}\, Y)^2},$$

for: $Y' = f(\mu'_1, \mu'_2, \ldots, \mu'_{i-1}, \mu_i, \mu'_{i+1}, \ldots, \mu'_p)$, (μ, μ') iid. μ-distributed variables.

- The asymptotic variance σ_S^2 can be "naturally" estimated, which leads to an asymptotic confidence interval:

$$\left]\widehat{S}_i \mp \frac{\widehat{\sigma}_S}{\sqrt{N}}\right[$$

Metamodel choice

- **Non intrusive metamodels:** we have at hand an input-output sample $\{(\mu^1, f(\mu^1)), \ldots, (\mu^n, f(\mu^n))\}$
  - Kriging/RKHS interpolation, Non-intrusive polynomial chaos decomposition.

- **Intrusive metamodels:** we work on the equations satisfied by the state variable(s).
  - Polynomial chaos decomposition, Reduced basis metamodels.
  - *Con:* we have to know and be able to analyze this equation.
  - *Pros:*
    - More efficiency is expected.
    - We can expect to have a certified error bound between metamodel output and original output.

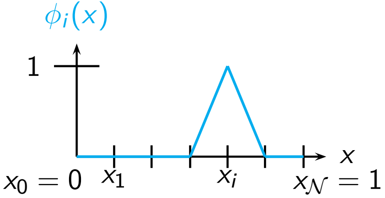
- We now focus on reduced basis methods.

Reduced basis introduction
Classical finite element resolution

- Let our unknown $u : [0;1] \to \mathbb{R}$ be such that:

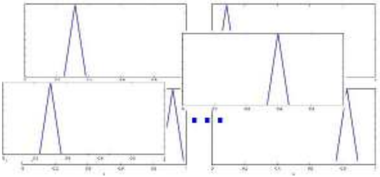
$$\begin{cases} -\mu_1 u'' + \mu_2 u = 1 \\ u(0) = u(1) = 0 \end{cases} \quad \text{ie.} \quad \begin{cases} \mu_1 \int_0^1 u'v' + \mu_2 \int_0^1 uv = \int_0^1 v \quad \forall v \quad (*) \\ u(0) = u(1) = 0 \end{cases}$$

- **Numerical resolution:**
  - we look for u as a linear combination of $\mathcal{N}$ basis functions: $u = \sum_{i=1}^{\mathcal{N}-1} u_i \phi_i$ satisfying $(*)$ for $v = \phi_1, \ldots, \phi_{\mathcal{N}-1}$.
  - We obtain a linear system whose unknowns are the u_i's.



Reduced basis metamodel: Principle

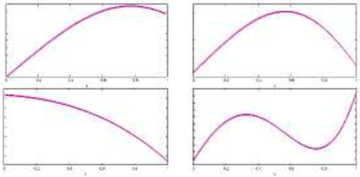
Classical code: u is searched in a large dimension space, **not specifically tailored** for the problem.



$$u(\mu) = \sum_{i=1}^{\mathcal{N}-1} u_i(\mu)\phi_i$$

unknowns

Metamodel: $\tilde{u}$ is searched in a smaller dimension space, **adapted** to the problem.



$$\tilde{u}(\mu) = \sum_{i=1}^{n} \tilde{u}_i(\mu)\zeta_i$$

unknowns

model-dependent; to find

Typically, for a 1D problem: $\mathcal{N} \simeq 100$, $n \simeq 10$.

Reduced basis: Offline and online phases

- Offline phase:
  - Choose a reduced basis $\{\zeta_1, \ldots, \zeta_n\}$.
  - Preassemble the parameter-independent parts of the equation.
- Online phase:
  - Assemble and solve the $n \times n$ linear system.

Reduced basis: Generalizations

- More generally, the reduced basis method can be applied to PDEs under variational form:

$$a(u(\mu), v; \mu) = b(v) \;\; \forall v \in X$$

  where X is a functional space, b is a linear form, and $a(\cdot, \cdot; \mu)$ is a bilinear form satisfying:

$$a(w, v; \mu) = \sum_{q=1}^{Q} \Theta_q(\mu) a_q(w, v) \quad (*)$$

  where Θ_q are functions, and a_q bilinear forms.
- It can also be generalized (under some hypotheses, and at a certain cost), to time-dependent problems, nonlinear problems, and those who can not exactly be cast under form $(*)$.

Reduced basis choice
Proper orthogonal decomposition (POD)

- We are looking for an *orthonormal* basis $\zeta_1, \dots, \zeta_n$ which minimizes:
$$\int_\mu ||u(\mu) - \Pi_{\zeta_1,\dots,\zeta_n} u(\mu)||^2 \, \mathrm{d}\mu$$
where $\Pi_{\zeta_1,\dots,\zeta_n}$ is an orthogonal projector on $\mathrm{Vect}\{\zeta_1, \dots, \zeta_n\}$.
- In practice, the integral is replaced by a discrete sum:
$$\sum_{\mu \in \Xi} ||u(\mu) - \Pi_{\zeta_1,\dots,\zeta_n} u(\mu)||^2$$
where Ξ is a finite sample of μ's distribution.
- We get a constrained minimization problem, which can be solved by computing $u(\mu)$ for all $\mu \in \Xi$ and the resolution of an eigenvalue problem of size $\#\Xi$.

Error bound

- Under coercivity hypotheses, we can get an upper bound of the error between $u(\mu)$ and $\widetilde{u}(\mu)$.
- This bound is explicitly computable with an offline/online efficient procedure.
- We can deduce a bound $\epsilon(\mu)$ on the output error:

$$\left| f(\mu) - \widetilde{f}(\mu) \right| \leq \epsilon(\mu) \quad \forall \mu$$

Back to Sobol indices' estimation

- We wish to take into account:
  - sampling error
  - and metamodel error
- The estimator is a function of sampled model outputs:

$$\widehat{S}_i = \Psi\left(\{y_k\}_{k=1,\ldots,N}, \{y'_k\}_{k=1,\ldots,N}\right)$$

- We have, for all k: $y_k \in [\widetilde{y}_k - \epsilon_k; \widetilde{y}_k + \epsilon_k]$ where $\widetilde{y}_k = \widetilde{f}(\mu_k), \epsilon_k = \epsilon(\mu_k)$; and so with $'$s.
- For:

$$\widehat{S}_i^m = \min_{\substack{y_k \in [\widetilde{y}_k - \epsilon_k; \widetilde{y}_k + \epsilon_k], \\ y'_k \in [\widetilde{y}'_k - \epsilon'_k; \widetilde{y}'_k + \epsilon'_k]}} \Psi\left(\{y_k\}_{k=1,\ldots,N}, \{y'_k\}_{k=1,\ldots,N}\right)$$

$$\widehat{S}_i^M = \max_{\substack{y_k \in [\widetilde{y}_k - \epsilon_k; \widetilde{y}_k + \epsilon_k], \\ y'_k \in [\widetilde{y}'_k - \epsilon'_k; \widetilde{y}'_k + \epsilon'_k]}} \Psi\left(\{y_k\}_{k=1,\ldots,N}, \{y'_k\}_{k=1,\ldots,N}\right)$$

  We have:

$$\widehat{S}_i^m \leq \widehat{S}_i \leq \widehat{S}_i^M$$

Back to Sobol indices' estimation

- We have:

$$\widehat{S}_i^m \leq \widehat{S}_i \leq \widehat{S}_i^M$$

bounds that are functions of metamodel output and metamodel output bound

- Bootstrap on $\widehat{S}_i^m$ and $\widehat{S}_i^M$
  $\rightarrow$ *combined* confidence intervals taking into account:
  - sampling error
  - and metamodel error

Optimal parameters choice
Context

We have two simulation parameters:

- **Reduced basis size:** $n \in \mathbb{N}^*$
  Increase n decreases metamodel error and increases computation time.

- **Sample size:** $N \in \mathbb{N}^*$
  Increase N decreases sampling error and increases comp. time.

$\rightarrow$ We look for an "optimal" combination of n and N.

Optimal parameters choice
Errors and computation time model

- **Computation time** is proportional to:
  - N (we do $2N$ metamodel output evaluations)
  - and n^3 (metamodel cost is dominated by a $n \times n$ linear system solve)

- We suppose that **combined confidence interval width** is the sum of:
  - a term $\frac{s_\alpha}{\sqrt{N}}$, where $s_\alpha > 0$;
  - a term $\frac{C}{a^n}$, where $C > 0$ and $a > 1$.

Optimal parameters choice
Errors and computation time model

- The optimal n^* and N^* are given by the argmin of $N \times n^3$, constrained by:

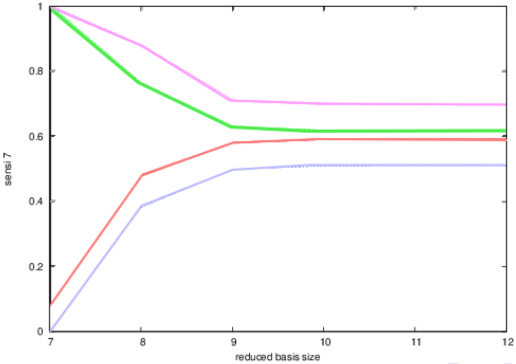
$$\frac{s_\alpha}{\sqrt{N}} + \frac{C}{a^n} = P$$

  where $P > 0$ is the desired width for the combined confidence interval.

- In practice:
  - we estimate s_α, C and a by regressing combined CI widths for some values of n and N;
  - we solve for n^* and N^*.

Numerical results

- **Benchmark PDE:** viscous, time-dependent, 1D Burgers equation.
- **Parameters:** viscosity, Fourier coefficients of boundary and initial values.
- Confidence interval for a Sobol index, for different reduced bases sizes and fixed sample sizes:



Reduction in computation times

- **Comparison with classical code-based estimation:**
  factor 5 to 6 in computation time, with equal certified precision.
- **Comparison with a non-intrusive metamodelling approach:**
  more precise result, obtained in **shorter time**.
- **We took full advantage from:**
  - **model properties**
  - **theoretical work** required to design the metamodel code and the error bound

Conclusion

- Uncertainty quantification and sensitivity analysis require a large number of code calls.
- Using a metamodel can lessen the required amount of computation, at the expense of some approximation.
- We have an approach to precisely quantify this approximation, in order to:
  - guarantee the obtained numerical estimation
  - choose in an optimal way the estimation parameters
- **Perspectives:**
  - apply the methodology on different models;
  - improve reduced basis choice by taking the temporal structure and/or the quantity of interest.