A least square based method using sparse low-rank approximation for uncertainty propagation

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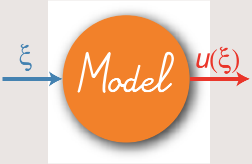
Uncertainty quantification using functional approaches

Stochastic/parametric models



Uncertainties represented by "simple" random variables $\xi = (\xi_1, \cdots, \xi_d) : \Theta \to \Xi$ defined on a probability space $(\Theta, \mathcal{B}, P)$.

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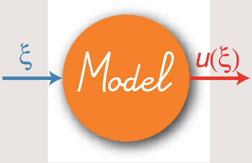

Uncertainties represented by "simple" random variables $\xi = (\xi_1, \cdots, \xi_d) : \Theta \to \Xi$ defined on a probability space $(\Theta, \mathcal{B}, P)$.

Ideal approach

Compute an accurate and explicit representation of $u(\xi)$ that allows fast evaluations of output quantities of interest, observables, or objective function.

$$u(\xi) \approx \sum_{i=1}^{P} u_i \phi_i(\xi), \quad \xi \in \Xi$$

where the $\phi_i(\xi)$ constitute a suitable basis (ex. Polynomial chaos)

Motivations

Issue

- Approximation of a high dimensional function $u(\xi)$, $\xi \in \Xi \subset \mathbb{R}^d$
- Use of classical deterministic solvers (black box)
  $\hookrightarrow$ Numerous solutions of deterministic problems: $O(\#\mathcal{I}_P)$

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Possibly fine deterministic models

$$dim(\mathcal{V}_N) \approx 10^6, 10^9, 10^{12} \ldots$$

Make inacceptable numerous evaluations of the model

Possibly high parametric dimensionality d

Many input parameters or stochastic processes with high spectral content

$$dim(\mathcal{S}_P) \approx 10, 10^{10}, 10^{100}, 10^{1000}, \ldots$$

$\rightarrow$ Need adapted representations for high dimensional functions

Motivations

Question

Can we compute low dimensional representations *a priori* ?

Outline

1. Non intrusive sparse approximation
2. Non intrusive sparse tensor methods
3. Numerical illustrations
   - Analytical model: checker-board function
   - Diffusion equation with multiple inclusions
   - Advection-Diffusion equation with random field
4. Conclusion

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Non intrusive sparse approximations

Aim

Compute an approximation of $u \in \mathcal{S}_P$

$$u(\xi) \approx \sum_{\alpha \in \mathcal{I}_P} u_\alpha \phi_\alpha(\xi)$$

using a few samples $\{u(y^k)\}_{k=1}^Q$

where $\{y_k\}_{k=1}^Q$ is a collection of sample points and the $u(y^k)$ are approximate solutions of deterministic problems

$$\mathcal{A}(u(y^k); y^k) = f(y^k)$$

Non intrusive sparse approximations

Least-squares in $\mathcal{S}_P = span\{\phi_i\}_{i=1}^P$

Approximation $v(\xi) = \sum_{i=1}^P v_i \phi_i(\xi)$ defined by

$$\boxed{\min_{v \in \mathcal{S}_P} \|u - v\|_Q^2} \quad \text{with} \quad \|u - v\|_Q^2 = \sum_{k=1}^{Q} |u(y^k) - v(y^k)|^2$$

or equivalently by

$$\boxed{\min_{\mathbf{v} \in \mathbb{R}^P} \|\mathbf{z} - \mathbf{\Phi v}\|_2^2} \quad \text{with } \mathbf{v} = (v_i)_i, \; \mathbf{\Phi} = (\phi_i(y^k))_{k,i}, \; \mathbf{z} = (u(y^1), \dots, u(y^Q))^T$$

Regularized least-square

$$\boxed{\min_{v \in \mathcal{S}_P} \|u - v\|_Q^2 + \lambda \mathcal{L}(v)} \quad \text{Choice of } \mathcal{L} \text{ ?}$$

- No regularization ($\lambda = 0$): requires $Q \gg P$ for well-posedness and avoid overfitting

Non intrusive sparse approximations

Ideal sparse regression

For a given precision ϵ, ideal sparse regression problem:

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{z}-\mathbf{\Phi}\mathbf{v}\|_2^2 \quad \text{subject to} \quad \|\mathbf{v}\|_0 \leq m} \quad \text{with } \|\mathbf{v}\|_0 = \#\{i; v_i \neq 0\}$$

[Blatman and Sudret 2011, Doostan and Owhadi 2011, Mathelin 2012, Najm 2012]

Approximate sparse regression (Lasso or Basis Pursuit)

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{z}-\mathbf{\Phi}\mathbf{v}\|_2^2 \quad \text{subject to} \quad \|\mathbf{v}\|_1 \leq \delta} \quad \text{with } \|\mathbf{v}\|_1 = \sum_{i=1}^{P} |v_i|$$

which for some $\lambda(\delta)$ is equivalent to

$$\boxed{\min_{\mathbf{v}\in\mathbb{R}^P} \|\mathbf{z}-\mathbf{\Phi}\mathbf{v}\|_2^2 + \lambda\|\mathbf{v}\|_1}$$

Issues

- Algorithms limited to approximation spaces with low dimension P
- Selection of good bases ?

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Strategies for high dimensional approximation

Instead of evaluating the coefficients of an expansion in a given approximation basis, function u is approximated in suitable low-rank tensor subsets

Nonlinear approximation using tensor approximation methods

- Exploit the tensor structure of function space

$$\mathcal{S}_P = \mathcal{S}^1_{P_1} \otimes \ldots \otimes \mathcal{S}^d_{P_d}$$

- Choose suitable low rank tensor subsets $\mathcal{M}$

$$\mathcal{M} = \left\{ v = F_{\mathcal{M}}(\mathbf{p}^{(1)}, \ldots, \mathbf{p}^{(d)}); \mathbf{p}^{(k)} \in \mathbb{R}^{P_k} \right\}$$

- Rank-one tensors

$$\mathcal{R}_1 = \left\{ w(y) = \langle \phi(y), \mathbf{w}^{(1)} \otimes \ldots \otimes \mathbf{w}^{(d)} \rangle; \mathbf{w}^{(k)} \in \mathbb{R}^{P_k} \right\}$$

with $\boxed{dim(\mathcal{R}_1) = \sum_{k=1}^{d} P_k}$

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- sparse Rank-one tensors

$$\mathcal{R}_1^{\gamma} = \left\{ w(y) = \langle \phi(y), \mathbf{w}^{(1)} \otimes \ldots \otimes \mathbf{w}^{(d)} \rangle; \mathbf{w}^{(k)} \in \mathbb{R}^{P_k}, \|\mathbf{w}^{(k)}\|_1 \leq \gamma_k \right\},$$

Non intrusive sparse tensor approximations

[Chevreuil, Lebrun, Nouy, Rai, *A least-squares method for sparse low rank approximation of multivariate functions*, arXiv:1305.0030, 2013]

Adaptive sparse tensor approximation

- Greedy construction of a basis $\{w_i\}_{i=1}^m$ selected in a tensor subset $\mathcal{R}_1^{\gamma^i}$
- Compute $u_m = \sum_{i=1}^m \alpha_i w_i$ using regularized least-squares

Algorithm

Let $u_0 = 0$. For $m \geq 1$,

- Compute a sparse rank one correction $w_m \in \mathcal{R}_1^{\gamma}$ by solving

$$\min_{w \in \mathcal{R}_1^{\gamma}} \|u - u_{m-1} - w\|_Q^2$$

  Computed using alternating minimization on the parameters of $\mathcal{R}_1^{\gamma}$.
- Set $U_m = span\{w_i\}_{i=1}^m$ (reduced approximation space)
- Compute $u_m = \sum_{i=1}^m \alpha_i w_i \in U_m$ using sparse regularization

$$\min_{\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_m)\in\mathbb{R}^m} \|u - \sum_{i=1}^m \alpha_i w_i\|_Q^2 + \lambda' \|\boldsymbol{\alpha}\|_1$$

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Algorithm

Let $u_0 = 0$. For $m \geq 1$,

- Compute a sparse rank one correction $w_m \in \mathcal{R}_1^{\gamma}$ by solving

$$\min_{\mathbf{w}^{(1)} \in \mathbb{R}^{P_1}, \ldots, \mathbf{w}^{(d)} \in \mathbb{R}^{P_d}} \|u - u_{m-1} - \langle \boldsymbol{\phi}, \mathbf{w}^{(1)} \otimes \ldots \otimes \mathbf{w}^{(d)} \rangle\|_Q^2 + \sum_{k=1}^{d} \lambda_k \|\mathbf{w}^{(k)}\|_1$$

  Computed using Alternating regularized Least Squares (with Lasso modified LARS alg.)
- Set $U_m = span\{w_i\}_{i=1}^m$ (reduced approximation space)
- Compute $u_m = \sum_{i=1}^m \alpha_i w_i \in U_m$ using sparse regularization

$$\min_{\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_m) \in \mathbb{R}^m} \|u - \sum_{i=1}^m \alpha_i w_i\|_Q^2 + \lambda' \|\boldsymbol{\alpha}\|_1$$

Global sensitivity analysis

Expectation

- Mean

$$\mathbb{E}[u(\boldsymbol{\xi})] = \sum_{i=1}^{m} \alpha_i \prod_{k=1}^{d} \mathbb{E}[w_i^{(k)}(\xi_k)]$$

- Conditional Expectation

$$\mathbb{E}[u(\boldsymbol{\xi})|\xi_j] = \sum_{i=1}^{m} w_i^{(j)}(\xi_j) \left(\alpha_i \prod_{\substack{k=1 \\ k \neq j}} \mathbb{E}[u_i^{(k)}(\xi_k)] \right)$$

Sobol indices

- First order Sobol index S_j for a random variable ξ_j

$$S_j = \frac{\mathbb{V}(\mathbb{E}[u(\boldsymbol{\xi})|\xi_j])}{\mathbb{V}(u(\boldsymbol{\xi}))}$$

- Closed sensitivity indices for a group of random variables

$$S_K^C = \sum_{J \subset K} S_J = \frac{\mathbb{V}(E[u(\boldsymbol{\xi})|\xi_K)}{\mathbb{V}(u(\boldsymbol{\xi}))}$$

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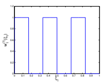
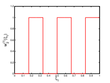
Analytical model: checker-board function

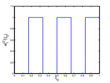
Rank-2 function: $u(\xi_1, \xi_2) = \sum_{i=1}^{2} w_i^{(1)}(\xi_1) w_i^{(2)}(\xi_2)$



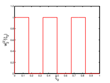
(a) $w_1^{(1)}(\xi_1)$



(b) $w_2^{(1)}(\xi_1)$

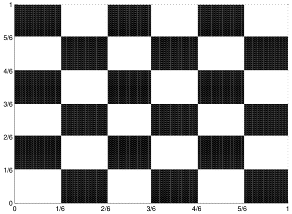


(c) $w_1^{(2)}(\xi_2)$



(d) $w_2^{(2)}(\xi_2)$

with $\xi_i \in U(0,1)$. $\Xi = (0,1)^2$.



"Effective dimension: 24"

Approximation of u in $\mathcal{S}^1_{P_1} \otimes \mathcal{S}^2_{P_2}$

Piecewise polynomials of degree p defined on a uniform partition of Ξ_k of s intervals:

$$\boxed{\mathcal{S}^k_{P_k} = \mathbb{P}_{p,s}}$$

Analytical model: checker-board function

- **Performance of the method for sparse low rank approximation**
  - $Q = 200$ samples
  - Optimal rank-m_{op} selected using 3-fold cross validation
  - Relative error ε estimated with Monte Carlo simulations

Comparison of different regularizations within Alternated Least Squares

	OLS		ℓ_2		ℓ_1	
Approximation space	ε	m_{op}	ε	m_{op}	ε	m_{op}
$\mathcal{R}_m(\mathbb{P}_{2,3} \otimes \mathbb{P}_{2,3})$, $P = 9^2$	0.527	2	0.508	2	0.507	2
$\mathcal{R}_m(\mathbb{P}_{2,6} \otimes \mathbb{P}_{2,6})$, $P = 18^2$	0.664	2	0.061	8	$2.41\,10^{-13}$	2
$\mathcal{R}_m(\mathbb{P}_{2,12} \otimes \mathbb{P}_{2,12})$, $P = 36^2$	-	-	0.566	4	$1.50\,10^{-12}$	3
$\mathcal{R}_m(\mathbb{P}_{10,6} \otimes \mathbb{P}_{10,6})$, $P = 66^2$	-	-	0.855	10	$7.88\,10^{-13}$	2

With few samples:

- ℓ_1-regularization detects sparsity and gives accurate results
- Rank 2 is retrieved

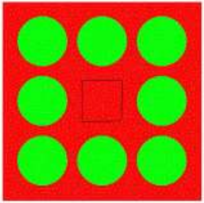
Diffusion equation with multiple inclusions

$$\begin{cases} -\nabla \cdot (\kappa \nabla u) = I_D(x) \quad on \quad \Omega = (0,1) \times (0,1) \\ u = 0 \quad on \quad \partial\Omega \end{cases}$$

with

$$\kappa(x,\xi) = \begin{cases} 1 & \textit{if } x \in \Omega_0 \\ 1 + 0.1\xi_i & \textit{if } x \in \Omega_i, \; i = 1...8 \end{cases}$$

with $\xi_i \in U(-1,1)$. $\Xi = (-1,1)^8$.



Approximation of a Quantity of Interest $I(u)$ in $\mathcal{S}_P \subset L^2_\mu(\Xi)$

$$I(u)(\xi) = \int_D u(x,\xi)dx, \quad D = (0.4, 0.6) \times (0.4, 0.6)$$

Polynomials of degree p: $\boxed{\mathcal{S}^k_{P_k} = \mathbb{P}_p}$

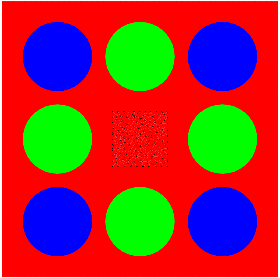
Diffusion equation with multiple inclusions

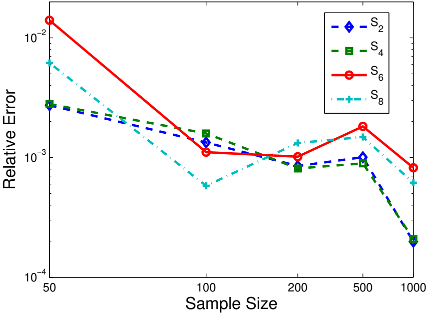
- **Influence of tensor format**
  - Optimal rank-m_{op} selected using 3-fold cross validation
  - Relative error ε $(\times 10^5)$ estimated with Monte Carlo simulations

Effect of variables regrouping w.r.t. the number of samples and to the approximation space

Approximation	Q=50				Q=100			
	ℓ_2		ℓ_1		ℓ_2		ℓ_1	
	ε	m_{op}	ε	m_{op}	ε	m_{op}	ε	m_{op}
$\mathcal{R}_m(\mathbb{P}_2^{(1)} \otimes \ldots \otimes \mathbb{P}_2^{(1)})$	2.68	8	2.78	1	2.36	10	2.66	1
$\mathcal{R}_m(\mathbb{P}_2^{(4)} \otimes \mathbb{P}_2^{(4)})$	1.83	2	1.72	1	0.91	2	0.88	3
$\mathcal{R}_m(\mathbb{P}_3^{(1)} \otimes \ldots \otimes \mathbb{P}_3^{(1)})$	2.85	6	2.79	2	2.81	10	2.67	2
$\mathcal{R}_m(\mathbb{P}_3^{(4)} \otimes \mathbb{P}_3^{(4)})$	1250	1	18.3	2	15.54	3	1.05	2
$\mathcal{R}_m(\mathbb{P}_5^{(1)} \otimes \ldots \otimes \mathbb{P}_5^{(1)})$	12.40	3	4.42	2	3.11	9	2.97	1
$\mathcal{R}_m(\mathbb{P}_5^{(4)} \otimes \mathbb{P}_5^{(4)})$	-	-	-	-	-	-	24.5	1

Sobol Sensitivity Indices





Sobol indices of diffusion coefficient in Ω_i

Illustration: advection-diffusion equation with random field

Stationary advection diffusion reaction stochastic equation

$$-\nabla \cdot (\mu(x,\xi)\nabla u) + c \cdot \nabla u + \kappa u = I_{\Omega_1}$$

$$+ \text{ homogeneous BCs}$$

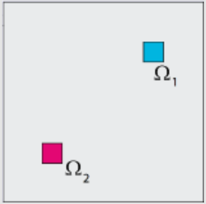
- random diffusion field

$$\mu(x,\xi) = \mu_0 + \sum_{i=1}^{100} \sqrt{\sigma_i}\mu_i(x)\xi_i$$

- approximation space

$$\mathcal{V}_N \otimes \underbrace{\mathbb{P}_3(\Xi_1) \otimes \ldots \otimes \mathbb{P}_3(\Xi_{100})}_{\mathcal{S}_P}$$

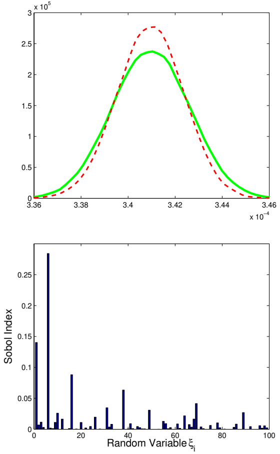
Problem and QoI



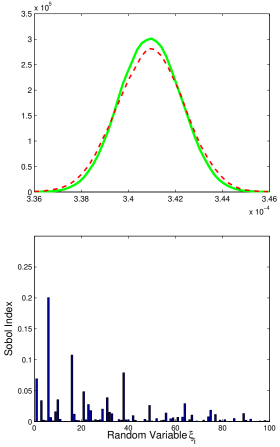
$$I(\xi) = \int_{\Omega_2} u(x,\xi)dx$$

Advection-diffusion equation with random field

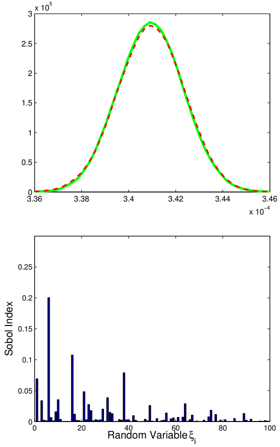
Probability density function and Sensitivity analysis



Q=100



Q=200



Q=1000

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Conclusion

Least-squares method for sparse low rank approximation of high dimensional functions

- A non intrusive method
- Detects and exploits low-rank and sparsity
- A mean to circumvent the curse of dimensionality

Some challenges

- New formats for low rank tensor approximation
- Adaptive search of optimal tensor formats

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[Chevreuil, Lebrun, Nouy, Rai, *A least-squares method for sparse low rank approximation of multivariate functions*, arXiv:1305.0030, 2013]