Tensor approximation methods based on regression for parametric uncertainty propagation

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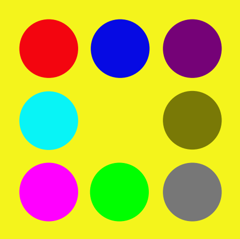
Uncertainty quantification using functional approaches

Example of model problem

$$-\nabla.(\kappa \nabla u) = f \quad \text{on} \quad \Omega$$
$$\kappa \nabla u \cdot n = 0 \quad \text{on} \quad \Gamma_N$$
$$u = 0 \quad \text{on} \quad \Gamma_D$$

Possible uncertainties on:

- the forcing term: f
- the behavior: κ



- Uncertainties represented by "simple" random variables $\xi : \Theta \rightarrow \Xi$ defined on a probability space $(\Theta, \mathcal{B}, P)$.
- Functional representation of any $\sigma(\xi)$-measurable random variable $\eta(\theta)$

$$\eta(\theta) \equiv \eta(\xi(\theta))$$

- Approximation theory for the approximation of functionals

$$\eta(\xi) \approx \sum \eta_\alpha \psi_\alpha(\xi), \quad \xi \in \Xi$$

Uncertainty quantification using functional approaches

Stochastic/parametric models

$$u : \xi \in \Xi \mapsto u(\xi) \in \mathcal{V} \quad \text{such that} \quad \mathcal{A}(u(\xi);\xi) = f(\xi)$$

- Propagation: $P_\xi \longrightarrow \mathcal{O}(u)$
- Optimization or identification: $\mathcal{O}(u) \longrightarrow \xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow \xi_2$
- Probabilistic inverse problem: $\mathcal{O}(u) \longrightarrow P_\xi$ or $\{\mathcal{O}(u), P_{\xi_1}\} \longrightarrow P_{\xi_2}$

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Ideal approach

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

Construction of approximation spaces

$$u \in L^p_\mu(\Xi; \mathcal{V}) = \mathcal{V} \otimes \mathcal{S}$$

Tensorization of predefined bases

$$u(\xi) \approx \sum_{i=1}^{N} \sum_{\alpha \in \mathcal{I}_P} u_{i,\alpha} \varphi_i \psi_\alpha(\xi) \in \mathcal{V}_N \otimes \mathcal{S}_P$$

with given approximation spaces

$$\mathcal{V}_N = span\{\varphi_i\}_{i=1}^{N}$$

$$\mathcal{S}_P = span\{\psi_\alpha(\xi) = \psi^1_{\alpha_1}(\xi_1) \dots \psi^d_{\alpha_d}(\xi_d); \alpha \in \mathcal{I}_P\}$$

- Pre-defined index set $\mathcal{I}_P$

$$\left\{\alpha \in \mathbb{N}^d; |\alpha|_\infty \leq r\right\} \supset \left\{\alpha \in \mathbb{N}^d; |\alpha|_1 \leq r\right\} \supset \left\{\alpha \in \mathbb{N}^d; |\alpha|_q \leq r\right\},\ 0 < q < 1$$

- Choice of $\mathcal{I}_P$ based on *a priori* analysis

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

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

Make inacceptable numerous evaluations of the model problems

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Possibly high parametric dimensionality

Many input parameters or stochastic processes with high spectral content

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

$\longrightarrow$ Need adapted representations for high dimensional functions

Motivations

Low effective dimensionality

In most problems,

- although we have initial high dimensional objet u
- its dimensionality is effectively low

Question

Can we compute suitable low dimensional approximation spaces *a priori* ?

Outline

Outline

Non intrusive sparse approximations

Aim

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

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

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

Regression in $\mathcal{S}_P = span\{\psi_i\}_{i=1}^P$

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

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

Regularized regression

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

- 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:

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

Blatman2011, Doostan2011, Mathelin2012, Najm2012

Approximate sparse regression (Basis Pursuit Denoising)

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

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

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

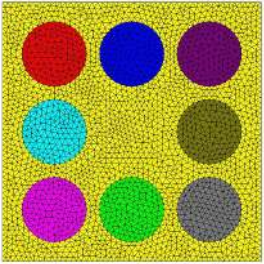
Illustration: diffusion problem with multiple inclusions

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

with

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

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



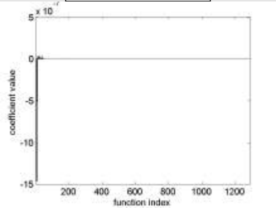
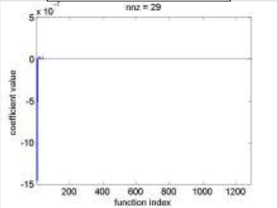
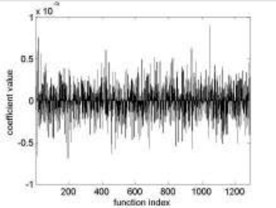
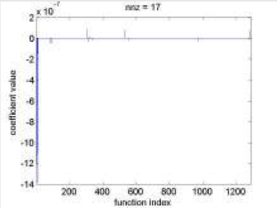
Approximation of a Quantity of Interest $I(u)$ in $\mathcal{S}_P \subset L^2_\mu(\Xi)$

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

$$\boxed{\mathcal{S}_P = \mathbb{P}_4(\Xi), \quad dim(\mathcal{S}_P) = 1286}$$

Illustration: diffusion problem with multiple inclusions

$I(\xi) \approx \sum_{\alpha} I_{\alpha}\psi_{\alpha}(\xi)$: coefficients $\{I_{\alpha}\}$ obtained by regression

	Least-square	ℓ_1-regularization
$Q = 2000$		
$Q = 50$		

Non intrusive sparse approximations

Issues

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

Outline

Strategies for high dimensional approximation

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 tensor subsets $\mathcal{M}$, e.g.

$$\mathcal{M} = \left\{ \sum_{i=1}^{m} \phi_i^1 \otimes \ldots \otimes \phi_i^d ; \phi_i^k \in \mathcal{S}^k_{P_k} \right\},$$

with $\boxed{dim(\mathcal{M}) = O(d)}$.

[Nouy2010, Doostan2010, Khoromskij2010, Ballani2010]...

Non intrusive sparse tensor approximations

with P. Rai, A. Nouy, J. Sen Gupta

Adaptive sparse tensor approximation

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

Algorithm

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

- Compute a correction $w_m \in \mathcal{M}$ defined by

$$w_m \in \arg\min_{w \in \mathcal{M}} \|u - u_{m-1} - w\|_Q^2$$

  Computed using alternating minimization on the parameters of $\mathcal{M}$.

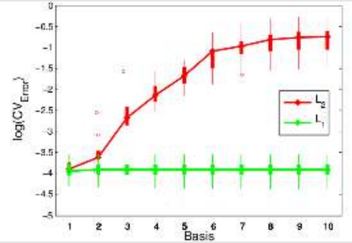
- Set $U_m = span\{w_i\}_{i=1}^m$ (reduced approximation space)
- Compute $u_m = \sum_{i=1}^m c_i w_i \in U_m$ using sparse regularization

$$\min_{\mathbf{c} \in \mathbb{R}^m} \|u - \sum_{i=1}^m c_i w_i\|_Q^2 + \lambda \|\mathbf{c}\|_s$$

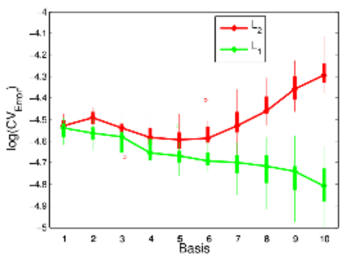
Illustration: diffusion problem with multiple inclusions

Error with ℓ_1 and ℓ_2 regularized update

$Q = 56$



$Q = 1000$



Error estimated using cross validation

Error with ℓ_1-regularized update for different sample sizes.

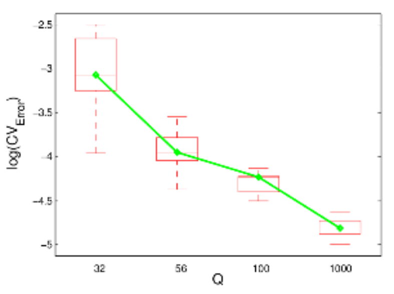
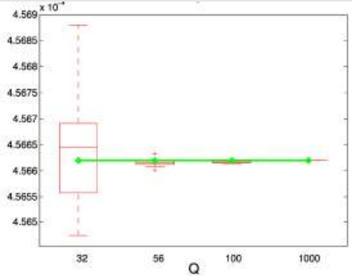


Illustration: diffusion problem with multiple inclusions

Mean



Standard deviation

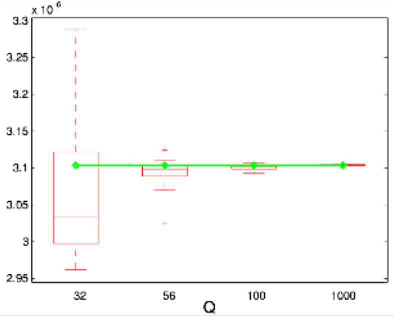


Illustration: advection-diffusion equation with random field

Stationary advection diffusion reaction stochastic equation

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

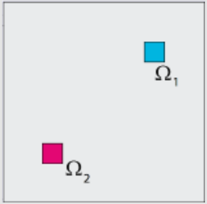
- random diffusion field

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

- approximation space

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

Problem and QoI

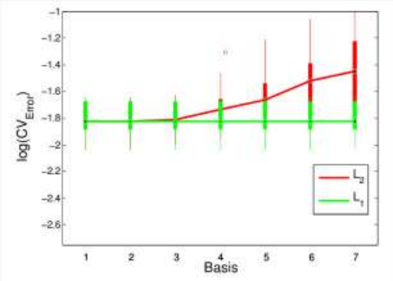


$$I(\xi) = \int_{\Omega_2} u(x,\xi)dx$$

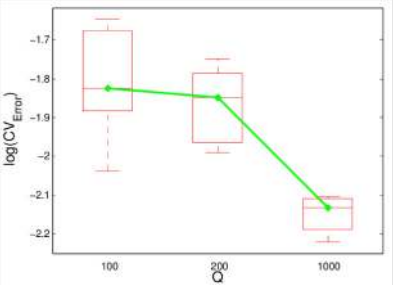
Illustration: advection-diffusion equation with random field

Error computed by cross-validation

Error of ℓ_1 and ℓ_2-regularized updates for sample size $Q = 100$



Error with ℓ_1-regularized update for different sample sizes



Conclusion

Tensor based and regression sparse approximation methods

- A non intrusive method
- A mean to circumvent the curse of dimensionality

Some challenges

- Strategy for random fields
- Robust non intrusive constructions of tensor approximations for irregular functions
- Adaptive search of optimal tensor formats

Thank you for your attention