Constrained and Adapted Representations for UQ.

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Constrained Representations: Objective

In many applications physical constraints require that uncertain parameters are positive, such as the permeability field in flow problems or reaction rates in chemical kinetics. Therefore it is necessary to choose PDF's with support containing only non-negative values. Even though the Wiener chaos expansions of such PDF's maintain this property, truncated PC expansions, in principle do not, leading to instabilities. We circumvent this obstacle by

- **projecting on the positive cone of random variables in finite chaos decomposition,**
- **solving a modified problem that avoids instabilities.**

Constrained Representations: Mathematical formulation

Constrained representation is a fixed point of $G(y) = \sum_{i=1}^{n} \mathbb{E}_\xi[\chi_{A(y)}\Psi_i]\Psi_i$.

Let $(\Omega, \mathcal{F}, P)$ be a probability space and H a Gaussian Hilbert space on $(\Omega, \mathcal{F}, P)$. Denote $\mathcal{P}_n(H)^+$ the set of positive random variable with order n chaos decomposition, $\mathcal{P}_n(H)^+ := \{y \in \mathcal{P}_n(H) : y(\omega) \geq 0 \forall \omega \in \Omega\}$.
Given $y \in \mathcal{P}_n(H)$,

$$y(\xi) = \sum_{i=0}^{n} c_i \Psi_i(\xi)\,, \quad c_i = \int_\Omega y(\xi(\omega))\Psi_i(\xi(\omega))dP(\omega) = \mathbb{E}_P[y\Psi_i],$$

then the projection of y on $\mathcal{P}_n(H)^+$ is given by

$$\tilde{y}(\xi) = \sum_{i=0}^{n} \tilde{c}_i \Psi_i(\xi)\,, \quad \tilde{c}_i = \lim_{k\to\infty} \tilde{c}_i^{(k)} \quad \tilde{c}_i^{(k)} = \mathbb{E}[\chi_{A(\tilde{y})}\tilde{y}^{(k-1)}\Psi_i],\ k = 1, 2, \ldots$$

where $\tilde{y}^{(k)}(\xi) = \sum_{i=0}^{n} \tilde{c}_i^{(k)}\Psi_i(\xi)$, $\tilde{y}^{(0)} = y \quad A(\tilde{y}^{(k)}) := \{\omega \in \Omega : \tilde{y}^{(k)}(\omega) \geq 0\}$, $\{\Psi_i\}$ are Hermite polynomials.

Constrained Representations: Algorithmic formulation

Iterative scheme:
Given the random variable y, construct random variables $\tilde{y}^{(k)}, k = 1, \ldots$ by:
$\tilde{y}^{(0)} = y$, for k=1,2…

- Generate a set of samples $\{\xi_q^{(k)}\}_{q=1}^{N}$ from the standard normal distribution ($\xi \sim \mathcal{N}(0,1)$),
- Construct $\tilde{y}^{(k)}(\xi) = \sum_{i=0}^{n} \tilde{c}_i^{(k)}\Psi_i(\xi)$

$$\tilde{c}_i^k = \frac{1}{N}\sum_{q=1}^{N} \max\{0, \tilde{y}^{(k-1)}(\xi_q^{(k)})\}\Psi_i(\xi_q^{(k)})$$

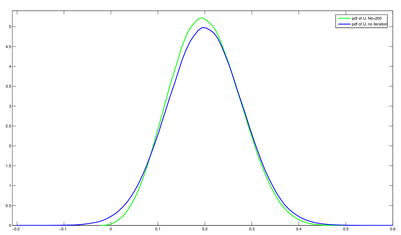
Constrained Representations: Numerical example

Benchmark SODE (Reagan et.al 2004) $\frac{du}{dt} = -u(u+10)(u-1)\,, \quad u(t=0) = U_0 + U_1\xi$
Attractors $u = -10,\ u = 1$ and saddle point $u = 0$.

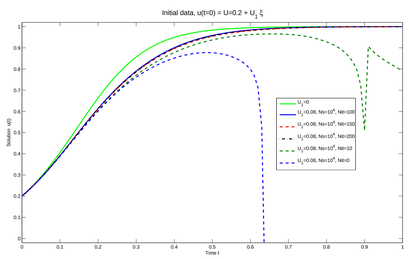
<u>Numerical method:</u> Spectral stochastic Galerkin. $u(t) \sim u_n(t) = \sum_{i=0}^{n} u_i(t)\Psi_i$.

For $i = 1, \ldots, n$: $\quad \frac{du_i}{dt} = \mathbb{E}_\xi[-u_n(u_n+10)(u_n-1)\Psi_i]\,, \quad u_i(t=0) = U_i$

Modified problem: $\quad \frac{du_i}{dt} = \mathbb{E}_\xi[-\tilde{u}_n(\tilde{u}_n+10)(\tilde{u}_n-1)\Psi_i]\,, \quad u_i(t=0) = \tilde{U}_i \quad \tilde{u}_n(t) = \sum_{i=0}^{n} \tilde{u}_i(t)\Psi_i$



Pdf's of $U, \tilde{U}$.



Time evolution of $\mathbb{E}[u(t)]$ and $\mathbb{E}[\tilde{u}(t)]$.

Adapted Representations: Objectives

- Obtain a distributionally equivalent representation of functions through low-dimensional L^2 projections.
- Instead of expanding $u(\boldsymbol{\xi})$ along polynomials in $\boldsymbol{\xi}$, we expand it on polynomials in $\boldsymbol{\eta} = \boldsymbol{A}\boldsymbol{\xi}$ where $\boldsymbol{A}$ is an isometry.
- with proper choice of $\boldsymbol{A}$, the measure of the solution is concentrated along the dominant η_1 dimension.

Adapted Representations: Formulation

Consider the solution, $u(\boldsymbol{\xi})$, of some ODE, PDE, ADE, or AE. $\quad \boldsymbol{\xi} : (L^2(\Omega, \Sigma, P) \mapsto \mathbb{R}^d$ is a d-dimensional Gaussian random variable.

Then also: $u : (L^2(\Omega, \Sigma(\boldsymbol{\xi}), P) \mapsto H$ for some function space H.

Consider a functional $h : H \mapsto \mathbb{R}$. $\quad$ Then we have:

$$h(\boldsymbol{\xi}) = h_0 + \sum_{|\boldsymbol{\alpha}|=1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Let : $\eta_1 = \sum_{|\boldsymbol{\alpha}|=1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$,

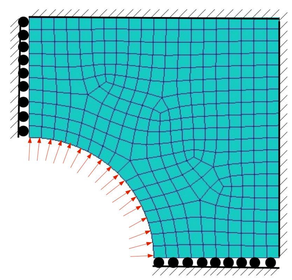
Complete the isometry $\boldsymbol{A}$ through any orthogonalization process resulting in : $\boldsymbol{\eta} = \boldsymbol{A}\boldsymbol{\xi}$.
Then in L^2:

$$\begin{aligned} h(\boldsymbol{\xi}) &= h_0 + \hat{h}_1\eta_1 + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}) \\ &= h_0 + \hat{h}_1\eta_1 + \sum_{\substack{|\boldsymbol{\alpha}|>1 \\ \boldsymbol{\alpha}=(|\boldsymbol{\alpha}|,0,\cdots,0)}} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\eta_1) + \sum_{\substack{|\boldsymbol{\alpha}|>1 \\ \boldsymbol{\alpha}\neq(|\boldsymbol{\alpha}|,0,\cdots,0)}} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}) \end{aligned}$$

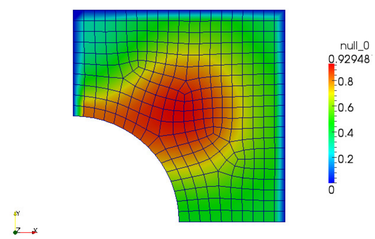
The 1D Approximation is obtained as the projection of the solution on $L^2(\Omega, \Sigma(\eta_1), P)$:

$$h(\boldsymbol{\xi}) \stackrel{d}{=} h_0 + \hat{h}_1\eta_1 + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\eta_1)$$

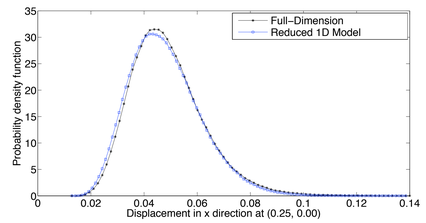
Adapted Representations: Numerical Example from Elasticity



Plane-Stress with Internal Pressure.



Spatial Variation of one coordinate of the Optimal 1D.



PDF at QOI with 10 parametric dimensions and 1-adapted dimension.

References

1. Reagan, H. N. Najm, B. J. Debusschere, O. P. Le Maitre, M. Knio, and R. G. Ghanem. Spectral stochastic uncertainty quantification in chemical systems. 8(3):607–632, 2004.

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