Spectral Methods for Uncertainty Quantification

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PhD course on UQ - DTU

Objectives of the lecture

- Basic principle of stochastic Galerkin projection
- Discuss derivation and elementary building blocks of the Galerkin projection
- Galerkin linear models and evaluation of non-linearities.
- Show examples

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We consider a given mathematical model $\mathcal{M}$ of a physical system.

- We call data the information that prescribes the physical system among the whole class spanned by $\mathcal{M}$.
- The data can be physical and modeling constants, IC, BC, forcing terms and any other relevant characteristics.

Denoting u the solution and d the data, one has to solve

$$\mathcal{M}(u; d) = 0.$$

This notation is formal and encompasses

- various types of models: systems of ODE, PDE, integral and algebraic equations, or more generally mixed type models,
- all equations satisfied by u, including governing equations, BC, IC, constitutive laws, constraints, ...
- all unknowns (scalars, vectors, fields) involved in the model formulation.

It is further assumed that the problem has a unique solution.

We denote $\mathcal{V}$ a suitable Hilbert space for the deterministic solution u. It will be assumed that $\mathcal{V}$ is independent of the data and we call

$\mathcal{V}$ the deterministic space.

Eventually, the solution needs be discretized.
Let $\mathcal{V}^h \subset \mathcal{V}$ be the discrete deterministic approximation space,

$$\mathcal{V}^h = span\left\{\phi_1, \dots, \phi_m\right\}.$$

The corresponding discrete deterministic solution u_h is

$$u_h = \sum_{i=1}^{m} u_i \phi_i = \Phi \cdot \boldsymbol{U}^T,$$

where $\boldsymbol{U} = (u_1 \dots u_m) \in \mathbb{R}^m$. The discrete version of the problem is

$$\mathcal{M}_h(\boldsymbol{U}; d) = 0.$$

We now consider the situation where some of the **data are uncertain** and considered as random on a probability space (Θ, Σ, dP).

$$d \rightarrow D(\theta)$$

- The solution u is now also random: $u \rightarrow U(\theta)$
- U is solution of

$$\mathcal{M}(U(\theta); D(\theta)) = 0 \quad \text{a.s.}$$

We assume that

1. the problem has a unique solution a.s.
2. the solution U is a second order random quantity.

In the discrete case, we have

$$\mathcal{M}_h(\boldsymbol{U}(\theta); D(\theta)) = 0 \quad \text{a.s.}$$

Turning to the stochastic discretization, we introduce $\boldsymbol{\xi}$ a set of N random variables with probability density function p_ξ and range Ξ.

We denote $L^2(\Xi, p_\xi)$ the space of second order functionals in $\boldsymbol{\xi}$ equipped with the inner product $\langle \cdot, \cdot \rangle$ and associated norm $\| \cdot \|_{L^2(\Xi, p_\xi)}$.

The availability of a uncertainty model for the data is assumed,

$$D(\theta) = D(\boldsymbol{\xi}(\theta))$$

For the stochastic solution in $\mathcal{V} \otimes \mathrm{L}^2(\Xi, p_\xi)$, the **weak formulation of the stochastic problem** is

$$\langle \mathcal{M}(U(\boldsymbol{\xi}); D(\boldsymbol{\xi})), \beta(\boldsymbol{\xi}) \rangle = 0 \quad \forall \beta \in L^2(\Xi, p_\xi).$$

Stochastic discretization

Let $\mathcal{S}^{\mathrm{P}} \subset L^2(\Xi, p_\xi)$ defined as

$$\mathcal{S}^{\mathrm{P}} = \mathrm{span}\{\Psi_0, \dots, \Psi_{\mathrm{P}}\},$$

where the $\{\Psi_k\}$ are orthogonal functionals in ξ, *e.g.* a PC basis truncated to an order No.

$\mathcal{S}^{\mathrm{P}}$ is called the stochastic approximation space

We seek for the approximate stochastic model solution in $\mathcal{V} \otimes \mathcal{S}^{\mathrm{P}}$.

$$U(\xi) \approx U^{\mathrm{P}}(\xi) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi).$$

A procedure is need for the computation of the stochastic modes u_k

Galerkin projection

- **Weak solution of the stochastic problem** $\mathcal{M}(U(\xi); D(\xi)) = 0$
- Needs **adaptation of deterministic codes**
- Potentially more efficient than NI techniques.
- Better suited to improvement (error estimate, optimal and basis reduction, ...), thanks to functional analysis.

Stochastic discretization

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$$U(\boldsymbol{\xi}) \approx U^{\mathrm{P}}(\boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\boldsymbol{\xi}).$$

Inserting U^{P} in the weak formulation yields the stochastic residual

$$\left\langle \mathcal{M}(U^{\mathrm{P}}(\boldsymbol{\xi}); D(\boldsymbol{\xi})), \beta(\boldsymbol{\xi}) \right\rangle = \left\langle R(U^{\mathrm{P}}), \beta \right\rangle .$$

Galerkin projection

[Ghanem & Spanos, 1991]

$$\left\langle \mathcal{M}(U^{\mathrm{P}}(\xi); D(\xi)), \beta(\xi) \right\rangle = \left\langle R(U^{\mathrm{P}}), \beta \right\rangle .$$

In general, one cannot find $U^{\mathrm{P}} \in \mathcal{V} \otimes \mathcal{S}^{\mathrm{P}}$ such that

$$\left\langle R(U^{\mathrm{P}}), \beta \right\rangle = 0 \quad \forall \beta \in L^2(\Xi, p_{\xi}).$$

It is then required that $R(U^{\mathrm{P}})$ is orthogonal to the stochastic approximation space:

$$\left\langle \mathcal{M}(U^{\mathrm{P}}(\xi); D(\xi)), \beta(\xi) \right\rangle = 0 \quad \forall \beta \in \mathcal{S}^{\mathrm{P}}.$$

- This weak formulation corresponds to the stochastic Galerkin formulation.
- The actual formulation is obtained in practice by projecting all model equations on $\mathcal{S}^{\mathrm{P}}$ (see examples later).

The Galerkin projection results in a set of $\mathrm{P}+1$ coupled problems for the stochastic modes u_k of the solution.

Find $\{u_k, k = 0, \dots, \mathrm{P}+1\} \in \mathcal{V}^{\mathrm{P}+1}$ such that

$$\left\langle \mathcal{M}\left(\sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi); D(\xi)\right), \Psi_l(\xi) \right\rangle = 0, \quad l = 0, \dots, \mathrm{P}.$$

- The size of the Galerkin problem increases with P.
- Recall that $\mathrm{P} = 1 = (\mathrm{N}+\mathrm{No})!/\mathrm{N}!\mathrm{No}!$ for polynomial truncation at order No.
- This can be very costly for complex problems requiring large parametrization and large expansion order.
- Projections on the Ψ_l of the model equations can be problematic in presence of non-linearities.

The Galerkin projection for the elliptic problem:

Find $U(\boldsymbol{x},\xi) \in H_0^1 \otimes L^2(\Xi, P_\Xi)$ such that

$$A(U,V;D) = B(V) \quad \forall V(\boldsymbol{x},\xi) \in H_0^1 \otimes L^2(\Xi, P_\Xi),$$

where

$$A(U,V;D) = \mathbb{E}\left[\int_\Omega \nu(\boldsymbol{x},\xi)\boldsymbol{\nabla} U(\boldsymbol{x},\xi)\cdot\boldsymbol{\nabla} V(\boldsymbol{x},\xi)d\boldsymbol{x}\right], \quad B(V) = \mathbb{E}\left[\int_\Omega F(\boldsymbol{x},\xi)V(\boldsymbol{x},\xi)d\boldsymbol{x}\right].$$

Introducing the PC expansion of U, it comes the **coupled** set of deterministic problems:

Find $\{u_k\}_{k=0,\dots,\mathrm{P}} \in (H_0^1)^{\mathrm{P}+1}$ such that

$$\sum_{l=0}^{\mathrm{P}} a_{kl}(u_l,v) = b_k(v) \quad \forall v \in H_0^1, k = 0,\dots,\mathrm{P},$$

where

$$a_{kl}(u,v) = \int_\Omega \mathbb{E}\left[\nu(\boldsymbol{x},\xi)\Psi_k(\xi)\Psi_l(\xi)\right]\boldsymbol{\nabla} u\cdot\boldsymbol{\nabla} v d\boldsymbol{x}, \quad b_k(v) = \int_\Omega \mathbb{E}\left[f(\boldsymbol{x},\xi)\Psi_k(\xi)\right]v(\boldsymbol{x})d\boldsymbol{x}.$$

Galerkin projection of discrete deterministic problems

The previous development can be applied to models discretized at the deterministic level.
Seeking for for $\boldsymbol{U}(\boldsymbol{\xi}) \approx \boldsymbol{U}^{\mathrm{P}} \in \mathbb{R}^m \otimes \mathcal{S}^{\mathrm{P}}$, we obtain Find $\{\boldsymbol{u}_k, k = 0, \dots, \mathrm{P}+1\} \in (\mathbb{R}^m)^{\mathrm{P}+1}$ such that

$$\left\langle \mathcal{M}_h \left(\sum_{k=0}^{\mathrm{P}} \boldsymbol{u}_k \Psi_k(\boldsymbol{\xi}); D(\boldsymbol{\xi}) \right), \Psi_l(\boldsymbol{\xi}) \right\rangle = 0, \quad l = 0, \dots, \mathrm{P}.$$

For many models, apply the stochastic discretization before the deterministic discretization results in the same Galerkin problem as proceeding the reverse way, provided that $\mathcal{V}^h$ is independent of $\boldsymbol{\xi}$. Exceptions include, *e.g.*,

- Lagrangian formulations [OLM & OK, JCP 2009],
- treatment of geometric uncertainties.

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Linear problems are of practical importance in scientific computing, whether as stand-alone mathematical problems or as ingredients of numerical methods (*e.g.* iteration techniques for the resolution of non-linear problems).

In this section, we analyze the

> structure of the Galerkin problem arising from the projection of linear models,

and examine implications regarding suitable solution strategies.

Consider a linear problem discretized at the deterministic level and recast in the matrix form

$$[A](\xi)\boldsymbol{U}(\xi) = \boldsymbol{B}(\xi).$$

Seeking the solution $\boldsymbol{U}(\xi)$ in a subspace $\mathbb{R}^m \otimes \mathcal{S}^{\mathrm{P}}$ of $\mathbb{R}^m \otimes L^2(\Xi, P_\Xi)$, the Galerkin projection gives:

$$\sum_{i=0}^{\mathrm{P}} \langle \Psi_k, [A]\Psi_i \rangle \, \boldsymbol{u}_i = \langle \Psi_k, \boldsymbol{B} \rangle, \quad k \in \{0, \dots, \mathrm{P}\}.$$

equivalent to the larger (block) system of linear equations

$$\begin{bmatrix} [A]_{00} & \cdots & [A]_{0\mathrm{P}} \\ \vdots & \ddots & \vdots \\ [A]_{\mathrm{P}0} & \cdots & [A]_{\mathrm{PP}} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \vdots \\ \boldsymbol{u}_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_0 \\ \vdots \\ \boldsymbol{b}_{\mathrm{P}} \end{pmatrix}.$$

$[A]_{ij}$ the $(m \times m)$ matrix given by $[A]_{ij} := \left\langle \Psi_i, [A]\Psi_j \right\rangle$, and $\boldsymbol{b}_i := \langle \Psi_i, \boldsymbol{B} \rangle$.

- The linear Galerkin problem couples all the stochastic modes $\boldsymbol{u}_i \in \mathbb{R}^m$ of the stochastic solution.
- It is not possible in general to compute independently the components $\boldsymbol{u}_i$.
- The size of the spectral problem is large: $m \times \dim \mathcal{S}^{\mathrm{P}} = m \times (\mathrm{P}+1)$.
- Resolution of the linear Galerkin system can be demanding.
- An understanding of the block structured system is instructive to design and apply well-suited numerical methods.

A first particular case occurs when the random data have no impact on the linear operator $[A]$ but only **on the right-hand-side $\boldsymbol{B}$**. Then

$$\langle \Psi_i, [A]\Psi_j \rangle = [A] \langle \Psi_i, \Psi_j \rangle = [A]\delta_{ij} \left\langle \Psi_i^2 \right\rangle$$

and

$$\begin{bmatrix} [A] & [0] & & \dots & [0] \\ [0] & [A] & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & [A] & [0] \\ [0] & \dots & \dots & [0] & [A] \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_{\mathrm{P}-1} \\ \boldsymbol{u}_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_0 \\ \boldsymbol{b}_1 \\ \vdots \\ \boldsymbol{b}_{\mathrm{P}-1} \\ \boldsymbol{b}_{\mathrm{P}} \end{pmatrix}$$

The stochastic modes are then $\boldsymbol{u}_i = [A]^{-1} \langle B, \Psi_i \rangle / \langle \Psi_i^2 \rangle$.
It amounts to solve the same linear system $[A]$ for $(\mathrm{P}+1)$ different right-hand sides $\Rightarrow$ single factorization.

In general, the matrix $[A]$ has a PC expansion

$$[A](\xi) = \sum_{i=0}^{\mathrm{P}} [A]_i \Psi_i(\xi) \Rightarrow [A]_{ij} = \left\langle \Psi_i, [A]\Psi_j \right\rangle = \sum_{k=0}^{\mathrm{P}} [A]_k \left\langle \Psi_i, \Psi_j \Psi_k \right\rangle,$$

and the Galerkin system can be conveniently recast as

$$\begin{bmatrix} [\overline{A}]_{00} & \cdots & [\overline{A}]_{0\mathrm{P}} \\ \vdots & \ddots & \vdots \\ [\overline{A}]_{\mathrm{P}0} & \cdots & [\overline{A}]_{\mathrm{PP}} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \vdots \\ \boldsymbol{u}_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} \overline{\boldsymbol{b}}_0 \\ \vdots \\ \overline{\boldsymbol{b}}_{\mathrm{P}} \end{pmatrix},$$

where $\overline{\boldsymbol{b}}_i := \langle B, \Psi_i \rangle / \langle \Psi_i^2 \rangle$ and

$$[\overline{A}]_{ij} := \sum_{k=0}^{\mathrm{P}} [A]_k C_{kji}, \quad C_{ijk} := \frac{\left\langle \Psi_i \Psi_j \Psi_k \right\rangle}{\left\langle \Psi_k \Psi_k \right\rangle}.$$

The third-order tensor C_{ijk} plays a fundamental role in stochastic Galerkin methods, especially in non-linear problems.

- C_{ijk} is symmetric w.r.t. the two first indices, $C_{ijk} = C_{jik}$.
- It induces block-symmetry in the spectral problem, $[\overline{A}]_{ij} = [\overline{A}]_{ji}$
- Many of the $(\mathrm{P}+1)^3$ entries are zero with many simplifications.
- For instance the first block of the Galerkin system reduces to

$$[\overline{A}]_{00} = \sum_{k=0}^{\mathrm{P}} [A]_k C_{k00} = [A]_0$$

  and the sum for the upper-right block (and lower-left block) actually reduces to $[\overline{A}]_{0\mathrm{P}} = [A]_{\mathrm{P}} / \left\langle \Psi_{\mathrm{P}}^2 \right\rangle$.
- Many other simplifications occur.
- Computational strategy for computation and storage of C_{ijk} will be discussed later (OK).

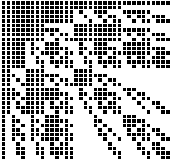
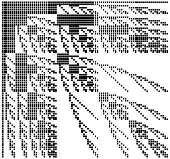
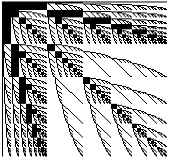
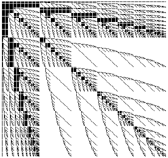
$\mathrm{N} = 4$-dim $\mathcal{S}^{\mathrm{P}} = 35$-$S = 0.58$	$\mathrm{N} = 6$-dim $\mathcal{S}^{\mathrm{P}} = 84$-$S = 0.41$
	
$\mathrm{N} = 8$-dim $\mathcal{S}^{\mathrm{P}} = 165$-$S = 0.31$	$\mathrm{N} = 10$-dim $\mathcal{S}^{\mathrm{P}} = 286$-$S = 0.23$
	

Illustration of the sparse structure of the matrices of the linear spectral problem for different dimensions, N, with $\mathrm{No} = 3$. Matrix blocks $[\bar{A}]_{ij}$ that are generally non-zero appear as black squares.

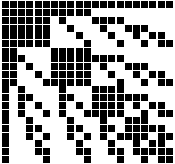
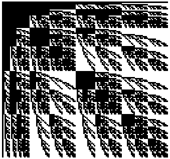
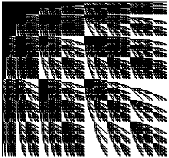
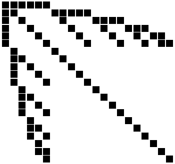
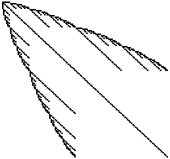
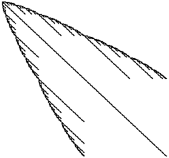
$\mathrm{No} = 2$-dim $\mathcal{S}^{\mathrm{P}} = 21$-$S = 0.52$	$\mathrm{No} = 3$-dim $\mathcal{S}^{\mathrm{P}} = 56$-$S = 0.49$
	
$\mathrm{No} = 4$-dim $\mathcal{S}^{\mathrm{P}} = 126$-$S = 0.54$	$\mathrm{No} = 5$-dim $\mathcal{S}^{\mathrm{P}} = 252$-$S = 0.55$
	

Illustration of the sparse structure of the matrices of the linear spectral problem for different expansion orders No, with $\mathrm{N} = 5$. Matrix blocks $[\bar{A}]_{ij}$ that are generally non-zero appear as black squares.

- Examples above assumes that $[A](\xi)$ has a full spectrum in $\mathcal{S}^{\mathrm{P}}$.
- When $[A](\xi)$ has a first-order expansion, the block structure of the linear spectral problem becomes even sparser.
- This behavior motivates the selection, whenever possible, of an approximation based on a first order operator.

$\mathrm{No} = 2$-dim $\mathcal{S}^{\mathrm{P}} = 21$-$S = 0.184$	$\mathrm{No} = 3$-dim $\mathcal{S}^{\mathrm{P}} = 56$-$S = 0.084$
	
$\mathrm{No} = 4$-dim $\mathcal{S}^{\mathrm{P}} = 126$-$S = 0.043$	$\mathrm{No} = 5$-dim $\mathcal{S}^{\mathrm{P}} = 252$-$S = 0.024$
	

Case of a inear stochastic operator $[A](\boldsymbol{\xi})$ having a first-order expansion.

- The main difficulty in solving discrete linear spectral problems is the size of the system.
- The structure and sparsity of the linear Galerkin problem suggests iterative solution strategies.
- Iterative solvers (*e.g.* conjugate gradient techniques for symmetric systems, and Krylov subspace methods) can be used.
- The efficiency of iterative solvers depends on the availability of appropriate preconditioners which need be adapted to the Galerkin problem.
- Construction of the preconditioners can exploit the block-structure of the linear Galerkin problem.

Preconditioning with the mean operator

- One can expect the diagonal blocks $[\bar{A}]_{ii}$ of the Galerkin system to be dominant.

$$[\bar{A}]_{ii} = \sum_{k=0}^{P} [A]_k \frac{\langle \Psi_k \Psi_i \Psi_i \rangle}{\langle \Psi_i \Psi_i \rangle}$$

- The mean operator $[A]_0$ is always present in this summation.
- It is expected to be dominant for reasonable variability in $[A](\xi)$.
- It suggests the preconditioner

$$[P] = \begin{bmatrix} [A]_0 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & [A]_0 \end{bmatrix}.$$

Owing to the diagonal block structure of $[P]$, only the inversion of $[A]_0$ is required:

$$[P]^{-1} = \begin{bmatrix} ([A]_0)^{-1} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & ([A]_0)^{-1} \end{bmatrix}.$$

The preconditioned Galerkin problem can now be expressed as:

$$[P]^{-1} \begin{bmatrix} [\overline{A}]_{00} & \dots & [\overline{A}]_{0\mathrm{P}} \\ \vdots & \ddots & \vdots \\ [\overline{A}]_{\mathrm{P}0} & \dots & [\overline{A}]_{\mathrm{PP}} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \vdots \\ \vdots \\ \boldsymbol{u}_\mathrm{P} \end{pmatrix} = [P]^{-1} \begin{pmatrix} \boldsymbol{b}_0 \\ \vdots \\ \vdots \\ \boldsymbol{b}_\mathrm{P} \end{pmatrix}.$$

Resolution of the preconditioned problem also factorizes in a series of $\mathrm{P}+1$ problems each with dimension m.

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Many models involve non-linearities of various types and their treatment is critical in stochastic Galerkin methods

Let $\{\Psi_k(\xi)\}_{k=0}^{\mathrm{P}}$ be an orthogonal basis of $\mathcal{S}^{\mathrm{P}} \subset L_2(\Xi, P_\Xi)$, and f a non-linear functional $u, v, \ldots$:

$$u, v, \cdots \in \mathbb{R} \mapsto f(u, v, \ldots) \in \mathbb{R}.$$

For random arguments, $U(\xi), V(\xi), \cdots \in \mathbb{R} \otimes \mathcal{S}^{\mathrm{P}}$, we generally have $f(U, V, \ldots) =: G(\xi) \notin \mathbb{R} \otimes \mathcal{S}^{\mathrm{P}}$, but if $G(\xi) \in \mathbb{R} \otimes L_2(\Xi, P_\Xi)$ it has an orthogonal projection on $\mathcal{S}^{\mathrm{P}}$,

$$G(\xi) \approx \widehat{G} = \sum_{k=0}^{\mathrm{P}} g_k \Psi_k, \quad g_k = \frac{\langle f(U, V, \ldots), \Psi_k \rangle}{\langle \Psi_k^2 \rangle}.$$

The problem is therefore to derive efficient strategies to compute the expansion coefficients g_k of $\hat{G}(\xi)$ from the expansion coefficients of its arguments $U(\xi), V(\xi), \ldots$.

Polynomial non-linearities

The product of two quantities appears in many models.

It corresponds to the case $G(\xi) = W(\xi) = U(\xi)V(\xi)$ for $U, V \in \mathcal{S}^{\mathrm{P}}$ having known expansions. Clearly,

$$W(\xi) = \sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} u_i v_j \Psi_i(\xi) \Psi_j(\xi).$$

and in general $W(\xi) \notin \mathcal{S}^{\mathrm{P}}$ though it is in $L_2(\Xi, P_\Xi)$. Therefore, $\widehat{W}$, the orthogonal projection of W on $\mathcal{S}^{\mathrm{P}}$, has expansion coefficients

$$w_k = \frac{\langle W, \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} u_i v_j C_{ijk}.$$

The result of the orthogonal projection of UV is called the Galerkin product of U and V and is denoted $U * V$.
The Galerkin product introduces **truncation errors** by disregarding the components of UV orthogonal to $\mathcal{S}^{\mathrm{P}}$.

Polynomial non-linearities

Higher order polynomial non-linearities are also frequent.

Consider first the triple product $G(\xi) = U(\xi)V(\xi)W(\xi)$ One can again perform an exact Galerkin projection of the triple product:

$$\widehat{UVW} := \sum_{m=0}^{\mathrm{P}} \widehat{uvw}_m \Psi_m = \sum_{m=0}^{\mathrm{P}} \Psi_m \left(\sum_{j,k,l=0}^{\mathrm{P}} T_{jklm} u_j v_k w_l \right),$$

$$T_{jklm} \equiv \frac{\langle \Psi_j \Psi_k \Psi_l \Psi_m \rangle}{\langle \Psi_m \Psi_m \rangle}.$$

- This exact Galerkin projection of the triple product involves the **fourth order tensor T_{jklm}**.
- T_{jklm} is sparse with many symmetries .
- However, computation and storage of T_{jklm} becomes quickly prohibitive when P increases.
- The exact Galerkin projection can hardly be extended further to higher order polynomial non-linearities.

Polynomial non-linearities

It is often preferred to rely on approximations for polynomial non-linearities of order larger than 2. For the triple product, an immediate approximation is

$$\widehat{UVW} \approx U * (V * W) = \widehat{U\widehat{VW}}.$$

This strategy can be extended to higher degree polynomial non-linearities by using successive Galerkin products. For instance,

$$\widehat{ABC \dots D} \approx A * (B * (C * (\dots * D))).$$

This procedure does not provide the exact Galerkin projection, since every intermediate product disregards the part orthogonal to $\mathcal{S}^{\mathrm{P}}$. Even for the triple product it is remarked that, in general

$$U * (V * W) \neq (U * V) * W \neq (U * W) * V.$$

The order in which the successive Galerkin products are applied affects the result.

Inverse and square root

Inverse and division are also common non-linearities.

For the inversion, one has to determine the expansion coefficients of the inverse U^{-1} of $U(\xi)$,

$$U^{-1}(\xi) = \frac{1}{U(\xi)} = \left(\sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi) \right)^{-1},$$

such that

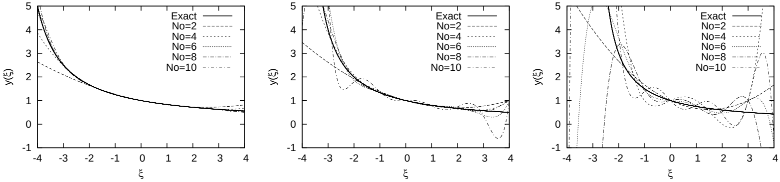
$$U^{-1}(\xi) U(\xi) = 1 \quad \text{a.s.}$$

U^{-1} is sought in $\mathcal{S}^{\mathrm{P}}$ and the previous equation needs to be interpreted in a weak sense. Using the Galerkin multiplication tensor, it comes

$$\begin{pmatrix} \sum_{j=0}^{\mathrm{P}} C_{j00} u_j & \cdots & \sum_{j=0}^{\mathrm{P}} C_{j\mathrm{P}0} u_j \\ \vdots & \ddots & \vdots \\ \sum_{j=0}^{\mathrm{P}} C_{j0\mathrm{P}} u_j & \cdots & \sum_{j=0}^{\mathrm{P}} C_{j\mathrm{P}\mathrm{P}} u_j \end{pmatrix} \begin{pmatrix} u_0^{-1} \\ \vdots \\ u_{\mathrm{P}}^{-1} \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ 0 \end{pmatrix}.$$

Due to truncature error, the above definition corresponds to the pseudo-spectral inverse $U^{*-1}$of U.

Inverse and square root



Pseudo-spectral approximation at different orders of the inverse $Y(\xi) = \widehat{U^{-1}}(\xi)$ of $U(\xi) = 1 + \alpha\xi$ with $\xi \sim \mathrm{N}(0, 1)$: $\alpha = 1/5$ (left), $1/4$ (center) and $1/3$ (right). Wiener-Hermite expansions are used.

Extend immediately to the evaluation of U/V

Inverse and square root

The Galerkin product can also serve to approximate square roots.

Given $U(\xi) > 0$ we have

$$U^{1/2}(\xi)U^{1/2}(\xi) = U(\xi).$$

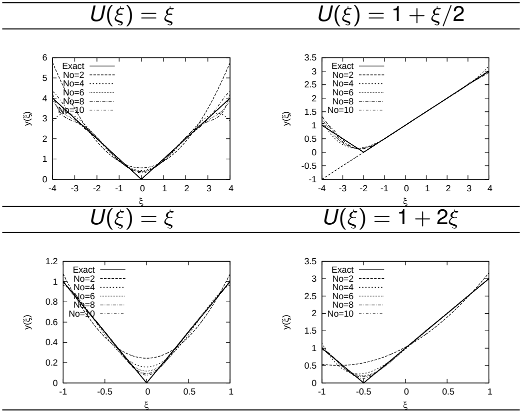
The approximate $U^{*1/2} \in \mathcal{S}^{\mathrm{P}}$ of $U^{1/2}$ solves

$$\begin{pmatrix} \sum_{j=0}^{\mathrm{P}} C_{j00} {u^{1/2}}_j & \cdots & \sum_{j=0}^{\mathrm{P}} C_{j\mathrm{P}0} {u^{1/2}}_j \\ \vdots & \ddots & \vdots \\ \sum_{j=0}^{\mathrm{P}} C_{j0\mathrm{P}} {u^{1/2}}_j & \cdots & \sum_{j=0}^{\mathrm{P}} C_{j\mathrm{PP}} {u^{1/2}}_j \end{pmatrix} \begin{pmatrix} {u^{1/2}}_0 \\ \vdots \\ {u^{1/2}}_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} u_0 \\ \vdots \\ u_{\mathrm{P}} \end{pmatrix}.$$

This non-linear system can be solved using standard techniques (Newton-Raphson iterations) Choosing for the initial guess $U^{*1/2}(\xi) = \pm\sqrt{u_0}$ allows for the selection of the positive or negative square root of $U(\xi)$.

Absolute values

Application to the approximation of absolute values



Convergence with No of the pseudo-spectral approximation on $\mathcal{S}^{\mathrm{No}}$ of $Y(\xi) = |U(\xi)|$ for different $u(\xi)$. Top plots: $\xi \sim \mathrm{N}(0,1)$ and Wiener-Hermite expansions. Bottom plots: $\xi \sim \mathcal{U}(-1,1)$ and Wiener-Legendre expansions.

Min and Max operators

Consider the Max (Min) operator

$$u, v \in \mathbb{R} \mapsto Max(u, v) = \begin{cases} u, & u \geq v \\ v, & u < v \end{cases}$$

In the deterministic case, the $Min(u, v)$ and $Max(u, v)$ are smallest and largest zeros of

$$x \in \mathbb{R} \mapsto g(x; u, v) = -(x-u)(x-v)(x-w) \in \mathbb{R}, \quad w := \frac{u+v}{2}.$$

For Newton-Raphson iterations the zeros of g are determine through the sequence $\{x^n\}$

$$x^{n+1} = h(x^n) := x^n - \frac{g(x^n; u, v)}{g'(x^n, u, v)} = x^n + \frac{(x^n-u)(x^n-v)(x^n-w)}{3(x^n)^2 - 6wx^n + uv + uw + vw}.$$

Min and Max operators

In the stochastic case the sequence becomes

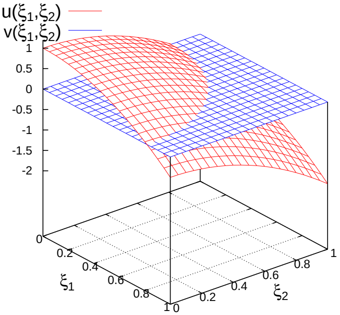
$$X^{n+1} = X^n + \frac{(X^n - U)(X^n - V)(X^n - W)}{3\,(X^n)^2 - 6WX^n + UV + UW + VW}$$
$$\approx X^n + (X^n - U) * (X^n - V) * (X^n - W) * \Big(3\,(X^n)^{*2}$$
$$-6W * X^n + U * V + U * W + V * W\Big)^{*-1}.$$

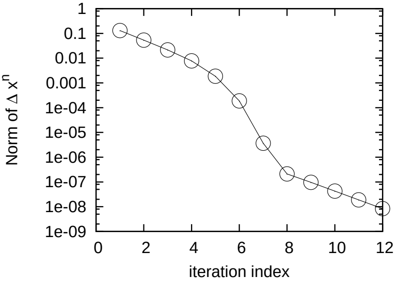
The selection of the Max (resp. Min) is made from appropriate selection of X^0, through

$$X^0 = \alpha\sqrt{\|U\|^2_{P_\Xi} + \|V\|^2_{P_\Xi}},$$

for some $\alpha > 1$ (resp. $\alpha < -1$).

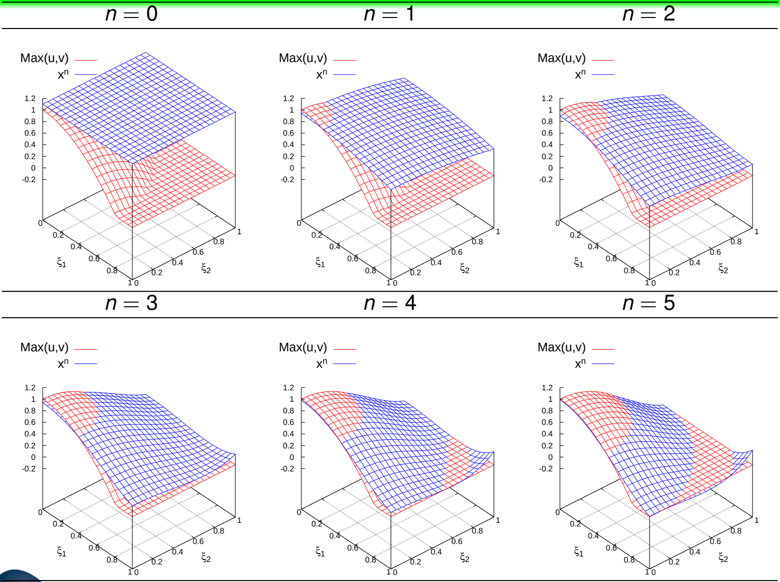
Min and Max operators





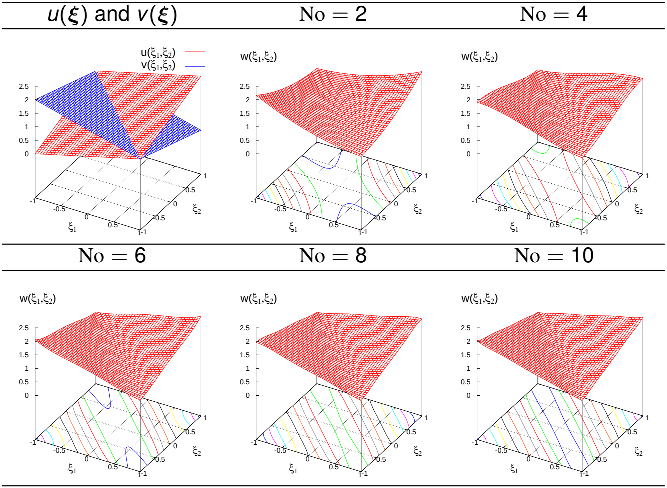
Left: $U(\xi_1, \xi_2)$ and $V(\xi_1, \xi_2)$ for which $Max(U, V)$ is sought. Only a portion of the stochastic domain Ξ is shown for clarity. Right: convergence of the sequence $\{X^n\}$ measured by the stochastic norm of $\Delta X^n = X^n - X^{n-1}$ approximating $Max(U, V)$.

Min and Max operators



First terms of the sequence $\{X^n\}$ in the pseudo-spectral approximation of $Max(U, V)$ on a two dimensional stochastic space.
Wiener-Legendre expansions with $N = 5$

Min and Max operators



Convergence with truncation order No of $W(\xi)$ approximating $Max(U, V)(\xi)$. The random variables $U(\xi)$ and $V(\xi)$ are linear in ξ_1 and ξ_2 as depicted in the top-left plot.

Other non-linearities

For sufficiently differentiable non-linearities one can rely on Taylor series

$$f(u) = f(\hat{u}) + (u - \hat{u})f'(\hat{u}) + \frac{(u-\hat{u})^2}{2} f''(\hat{u}) + \cdots$$

In the stochastic case, it is common to expand the series about the mean u_0 of U, at which $f'(u_0)$, $f''(u_0)$, $\cdots$ can be evaluated.
Successive powers of $\delta U := U - u_0$ can be evaluated in a pseudo-spectral fashion

$$\mathcal{S} \ni F(U) \approx f(u_0) + \delta U f'(u_0) + \frac{\delta U * \delta U}{2} f''(u_0) + \frac{\delta U * \delta U * \delta U}{6} f'''(u_0) + \cdots$$

- Convergence of the approximation needs be carefully analyzed.
- Impact of the pseudo spectral error is critical.
- Radius of convergence often unknown.

Other non-linearities

Integration approach for differentiable non-linearities [Debusschere *et al*, 2004]

If $f(\cdot)$ is analytical with derivative $f'(\cdot)$, f can be defined as some integral of f' along a deterministic integration path.

Let $Y(s,\xi)$ be a stochastic processes of $L^2(\Xi, P_\Xi)$, and consider $G(s,\xi) := f(Y)$:

$$Y = Y(s,\xi) = \sum_{k=0}^{\mathrm{P}} y_k(s)\Psi_k(\xi), \quad G = G(s,\xi) = \sum_{k=0}^{\mathrm{P}} g_k(s)\Psi_k(\xi).$$

Therefore, we have

$$\begin{aligned}
\int_{s_1}^{s_2} \frac{\partial G}{\partial s} \mathrm{d}s &= \int_{s_1}^{s_2} G' \frac{\partial Y}{\partial s} \mathrm{d}s \\
\sum_{k=0}^{\mathrm{P}} \Psi_k \int_{s_1}^{s_2} \frac{\mathrm{d}g_k}{\mathrm{d}s} \mathrm{d}s &= \sum_{k=0}^{\mathrm{P}} \Psi_k \left[g_k(s_2) - g_k(s_1)\right] \\
&= \sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} \Psi_i \Psi_j \int_{s_1}^{s_2} g_i'(s) \frac{\mathrm{d}y_j}{\mathrm{d}s} \mathrm{d}s.
\end{aligned}$$

Other non-linearities

The integration path is set such that for all $k = 0, \ldots, \mathrm{P}$

$$Y(s_1, \xi) = \hat{U}, \quad Y(s_2, \xi) = U, \tag{1}$$

we obtain

$$F(U(\xi))_k = F(\hat{U})_k + \sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} C_{ijk} \int_{\hat{u}_j}^{u_j} f_i' \, \mathrm{d}y_j, \quad \forall k = 0, \ldots, \mathrm{P}.$$

Provided that

- the PC expansion of $F(\hat{U})$ is known,
- the PC expansion of $F'(\cdot)$ is easily computed along the integration path,

the computation of $F(U)$ amounts to solve a set of coupled ODEs.

Other non-linearities

Example: exponential $f(u) = \exp(u)$.

We simply set $Y(s, \xi) = sU(\xi)$, $s_1 = 0$ and $s_2 = 1$.
Since $\exp(u)' = u$, we obtain the the set of coupled ODEs:

$$\frac{\mathrm{d}g_k}{\mathrm{d}s} = \sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} C_{ijk} u_i g_k, \quad k = 0, \ldots, \mathrm{P},$$

to be integrated up to $s = 1$ from the initial condition

$$g_k(s = 0) = \langle \exp 0, \Psi_k \rangle = \delta_{k,0} \quad k = 0, \ldots, \mathrm{P}.$$

- Standard techniques for ODEs can be used.
- Integration and stochastic truncation error control is critical.

Other non-linearities

Non-intrusive projections

- For general non-linearities $F(U, V, \dots)$ it is possible to proceed by non-intrusive projection techniques:

$$f_k := \frac{\langle F(U, V, \dots), \Psi_k \rangle}{\langle \Psi_k^2 \rangle}. \tag{2}$$

- Results in hybrid Galerkin / non-intrusive approaches when used in intermediate step of a Galerkin projection method (case of complex non-linear model).

$$\nabla \cdot (\nu(U) \nabla U) = g \text{ with BCs.} \tag{3}$$

- Interest can be questionable.

Questions & Discussion