Numerical methods for uncertainty quantification

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We often consider problems such as the elliptic PDE

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x})\nabla u(\boldsymbol{x})) = f(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in D, \\ u(\boldsymbol{x}) = g(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in \partial D. \end{cases}$$

We may be interested in a variety of things: the (forward) solution u, a quantity of interest $G(u)$, finding an optimal control f to calibrate the state u, or recovering a from available measurement data.

In practice, many of the associated quantities (diffusion coefficient a, the source term f, the boundary data g, or even the domain D) may not be perfectly known.

This has led to the study of problems where we model these uncertainties using random variables $\rightarrow$ uncertainty quantification for PDEs.

Let (Ω, Γ, P) be a probability space. A useful model problem to consider is

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x}, \omega) \nabla u(\boldsymbol{x}, \omega)) = f(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in D, \ \text{(a.e.) } \omega \in \Omega, \\ u(\boldsymbol{x}, \omega) = 0 & \text{for } \boldsymbol{x} \in \partial D, \ \text{(a.e.) } \omega \in \Omega, \end{cases}$$

where the diffusion coefficient $a(\cdot, \omega)$ is *random*. In consequence, the solution $u(\cdot, \omega)$ is a random function/field.

In order to analyze $u(\cdot, \omega)$, some approaches might be:

- Monte Carlo $\rightarrow$ slow convergence rate.
- Approximations based on lower order moments $\rightarrow$ poor accuracy.

In certain problems (such as the PDE above) the dependence of u on a is smooth. Spectral methods such as the stochastic Galerkin method and stochastic collocation, not to mention quasi-Monte Carlo methods, take advantage of this fact and can be used to obtain higher-order convergence.

Notations and preliminaries

Generalized Polynomial Chaos (gPC) expansion

[Xiu and Karniadakis (2002)] A consequence of the **generalized Cameron–Martin theorem** is that:

> *Any random process with finite variance can be expanded using orthogonal polynomials.*

A general second-order random process $X(\omega)$ can be represented as

$$X(\omega) = c_0 I_0 + \sum_{i_1=1}^{\infty} c_{i_1} I_1(\xi_{i_1}(\omega)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} c_{i_1,i_2} I_2(\xi_{i_1}(\omega), \xi_{i_2}(\omega)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} c_{i_1,i_2,i_3} I_3(\xi_{i_1}(\omega), \xi_{i_2}(\omega), \xi_{i_3}(\omega)) \cdots,$$

where $I_n(\xi_{i_1}, \ldots, \xi_{i_n})$ denotes the Wiener–Askey polynomial chaos of order n in terms of the random vector $\boldsymbol{\xi} = (\xi_{i_1}, \ldots, \xi_{i_n})$.

In particular, for $u \in L^2_P(\Omega)$,

$$u(\omega) = \sum_{j=0}^{\infty} \tilde{c}_j \Psi_j(\boldsymbol{\xi}). \tag{1}$$

Here, there is a one-to-one correspondence between the functions $I_n(\xi_{i_1}, \ldots, \xi_{i_n})$ and $\Psi_j(\boldsymbol{\xi})$.

It will be convenient to identify the random field with

$$u \equiv u(\xi_1, \xi_2, \ldots),$$

i.e., we treat it as a function of the random variables ξ_1, ξ_2, ...

Warning. The random variables ξ_j are uncorrelated, but in the non-Gaussian case not necessarily independent. Since spectral methods generally rely on ξ_j being mutually independent, a customary approach is to **assume** that the representation (1) is valid with satisfactory accuracy using mutually independent random variables (we will be implicitly guilty of this when passing onto the analysis of the parametric PDE problem). This kind of transformation can be achieved using, e.g., the Rosenblatt transformation or introducing suitable auxiliary probability density functions [Babuška et al. (2007)].

In practice, we use a truncated gPC expansion (both in dimension and the number of terms). Furthermore, note that $\mathbb{E}[u] = \tilde{c}_0$ and $\mathrm{Var}[u] = \sum_{k \geq 1} \tilde{c}_k^2 \mathbb{E}[\Psi_k^2]$.

If the random variables ξ_j are independent, we can represent the polynomial chaos using tensorized orthogonal polynomials. Let $\mathscr{F} := \{\boldsymbol{\nu} \in \mathbb{N}_0^\infty;\ |\mathrm{supp}(\boldsymbol{\nu})| < \infty\}$ denote the set of all finitely supported multi-indices, with support $\mathrm{supp}(\boldsymbol{\nu}) := \{i \in \mathbb{N};\ \nu_i \neq 0\}$. Then

$$X(\omega) = \sum_{\boldsymbol{\nu} \in \mathscr{F}} c_{\boldsymbol{\nu}} \Psi_{\boldsymbol{\nu}}(\boldsymbol{\xi}), \tag{2}$$

where

$$\Psi_{\boldsymbol{\nu}}(\boldsymbol{\xi}) = \prod_{j \in \mathrm{supp}(\boldsymbol{\nu})} \Psi_j(\xi_j). \tag{3}$$

The polynomials Ψ_j can be chosen according to the distribution of the random variables ξ_j; see the Askey scheme on the next page.

Table: The Askey scheme for certain continuous random variables. If the random variables $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$ in (2) are i.i.d., then the factors $\Psi_j(\xi_j)$ in (3) should be chosen according to this table.

Random variables ξ_j	Polynomial basis $\{\Psi_j(\xi_j)\}_{j\geq 0}$	Support
Gaussian	Hermite polynomials	$(-\infty, \infty)$
gamma	Laguerre polynomials	$[0, \infty)$
beta	Jacobi polynomials	$[a, b]$
uniform	Legendre polynomials	$[a, b]$
arcsine	Chebyshev polynomials (1^{st} kind)	$[a, b]$

Each polynomial in the Askey scheme forms a complete basis in the Hilbert space determined by its corresponding support.

Example (Legendre polynomials supported on $[-1/2, 1/2]$[†])

By carrying out the Gram–Schmidt procedure on the monomial basis $(1, x, x^2, \ldots, x^n)$ with respect to $\langle p, q \rangle = \int_{-1/2}^{1/2} p(x)q(x)\,\mathrm{d}x$, we obtain

$$L_0(x) = 1,$$

$$L_1(x) = x - \frac{\langle L_0, x\rangle}{\langle L_0, L_0\rangle} L_0 = x - \frac{\int_{-1/2}^{1/2} x\,\mathrm{d}x}{\int_{-1/2}^{1/2} \mathrm{d}x} \cdot 1 = x,$$

$$L_2(x) = x^2 - \frac{\langle L_0, x^2\rangle}{\langle L_0, L_0\rangle} L_0 - \frac{\langle L_1, x^2\rangle}{\langle L_1, L_1\rangle} L_1 = x^2 - \frac{\int_{-1/2}^{1/2} x^2\,\mathrm{d}x}{\int_{-1/2}^{1/2} \mathrm{d}x} - \frac{\int_{-1/2}^{1/2} x^3\,\mathrm{d}x}{\int_{-1/2}^{1/2} x^2\,\mathrm{d}x} x$$

$$= x^2 - \tfrac{1}{12},$$

$$L_3(x) = x^3 - \tfrac{3}{20}x, \quad L_4(x) = x^4 - \tfrac{3}{14}x^2 + \tfrac{3}{560}, \ldots$$

These are the (monic) Legendre polynomials supported on $[-1/2, 1/2]$.

[†] The "standard" Legendre polynomials are defined on $[-1, 1]$ and usually denoted P_n.

Let $\langle p, q\rangle = \int p(x)q(x)\,\mathrm{d}\mu(x)$, where μ is a positive measure with finite moments (e.g., $\mathrm{d}\mu(x) = \rho(x)\,\mathrm{d}x$ where ρ is the density associated with one of the polynomials in the Askey scheme). All (monic) orthogonal polynomials associated with $\mathrm{d}\mu$ admit to a *three-term recurrence relation*

$$p_0(x) = 1, \quad p_1(x) = (x - \alpha_1)p_0(x),$$
$$p_{k+1}(x) = (x - \alpha_{k+1})p_k(x) - \beta_{k+1}p_{k-1}(x),$$

where

$$\alpha_{k+1} = \frac{\langle xp_k, p_k\rangle}{\langle p_k, p_k\rangle} \quad \text{and} \quad \beta_{k+1} = \frac{\langle p_k, p_k\rangle}{\langle p_{k-1}, p_{k-1}\rangle}.$$

Example (Legendre polynomials supported on $[-1/2, 1/2]$)

$$\alpha_k = 0 \ \forall k \quad \text{and} \quad \beta_k = \frac{(k-1)^2}{16k^2 - 32k + 12}, \quad k \geq 2.$$

Example (Hermite polynomials)

$$\alpha_k = 0 \ \forall k \quad \text{and} \quad \beta_k = \frac{k-1}{2}, \quad k \geq 2.$$

Note that the three-term recurrence given on the previous page does not automatically give orthonormal polynomials. For example, the orthonormal Legendre polynomials on $[-1/2, 1/2]$ can be obtained by

$$\hat{L}_0(x) = \frac{L_0(x)}{\sqrt{\langle L_0, L_0 \rangle}} = 1,$$

$$\hat{L}_1(x) = \frac{L_1(x)}{\sqrt{\langle L_1, L_1 \rangle}} = 2\sqrt{3}x,$$

$$\hat{L}_2(x) = \frac{L_2(x)}{\sqrt{\langle L_2, L_2 \rangle}} = 6\sqrt{5}x^2 - \frac{\sqrt{5}}{2},$$

$$\hat{L}_3(x) = \frac{L_3(x)}{\sqrt{\langle L_3, L_3 \rangle}} = 20\sqrt{7}x^3 - 3\sqrt{7}x,$$

$$\hat{L}_4(x) = \frac{L_4(x)}{\sqrt{\langle L_4, L_4 \rangle}} = 210x^4 - 45x^2 + \frac{9}{8},$$

and so on.

Karhunen–Loève expansion

Let $a(\boldsymbol{x}, \omega)$ be a random field with mean

$$\overline{a}(\boldsymbol{x}) = \int_\Omega a(\boldsymbol{x}, \omega)\,\mathrm{d}P(\omega), \quad \boldsymbol{x} \in D,$$

and a (continuous) symmetric, positive definite covariance

$$K(\boldsymbol{x}, \boldsymbol{x}') = \int_\Omega (a(\boldsymbol{x}, \omega) - \overline{a}(\boldsymbol{x}))(a(\boldsymbol{x}', \omega) - \overline{a}(\boldsymbol{x}'))\,\mathrm{d}P(\omega).$$

Mercer's theorem: the covariance operator $\mathcal{C}\colon L^2(D) \to L^2(D)$

$$(\mathcal{C}u)(\boldsymbol{x}) = \int_D K(\boldsymbol{x}, \boldsymbol{x}')u(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}', \quad \boldsymbol{x} \in D,$$

is compact. Hence, there exists a countable sequence of eigenvalues $\{\lambda_k\}_{k\geq 1}$ and corresponding eigenfunctions $\{\psi_k\}_{k\geq 1}$ satisfying $\mathcal{C}\psi_k = \lambda_k\psi_k$ such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$ for $k \geq 1$ and $\lambda_k \to 0$ and the eigenfunctions form an orthonormal basis for $L^2(D)$.

The Karhunen–Loève (KL) expansion of random field $a(\boldsymbol{x}, \omega)$ can be written as

$$a(\boldsymbol{x}, \omega) = \bar{a}(\boldsymbol{x}) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} \psi_k(\boldsymbol{x}) \xi_k(\omega).$$

Remarks:

- The KL expansion minimizes the mean square truncation error:

$$\left\| a(\boldsymbol{x}, \omega) - \bar{a}(\boldsymbol{x}) - \sum_{k=1}^{N} \sqrt{\lambda_k} \psi_k(\boldsymbol{x}) \xi_k(\omega) \right\|_{L^2(\Omega; L^2(D))} = \left(\sum_{k=N+1}^{\infty} \lambda_k \right)^{1/2}.$$

- The random variables ξ_k are centered and uncorrelated, but not necessarily independent (in non-Gaussian setting). The remarks made on pg. 6 apply here as well.
- The KL expansion is a special case of gPC expansion, where the polynomial order has been truncated to be at most 1.

Stochastic Galerkin method

Let $D \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, be a bounded domain with Lipschitz boundary. We call $\boldsymbol{x} \in D$ the *spatial variable*.

For the remainder of the slides I will restrict the analysis to the "uniform setting", i.e., the input random field $a(\boldsymbol{x}, \boldsymbol{y}) \equiv a(\boldsymbol{x}, \boldsymbol{y}(\omega))$ is assumed to be given as a KL expansion

$$a(\boldsymbol{x}, \boldsymbol{y}) = \overline{a}(\boldsymbol{x}) + \sum_{j \geq 1} y_j \psi_j(\boldsymbol{x}), \quad \boldsymbol{x} \in D,$$

where $y_j \overset{\text{i.i.d.}}{\sim} \mathit{Unif}(-1/2, 1/2)$. Furthermore, we assume that it satisfies the summability conditions $\overline{a} \in L^\infty(D)$, $\psi_j \in L^\infty(D)$ for $j \geq 1$ with $(\|\psi_j\|_{L^\infty(D)})_{j \geq 1} \in \ell^p(\mathbb{N})$ for some $0 < p \leq 1$.

We may then proceed to analyze the following parametric PDE.

Let $U := [-1/2, 1/2]^{\mathbb{N}}$ and suppose that $\boldsymbol{y} := (y_1, y_2, \ldots) \in U$. Our model problem is to find the function $u\colon D \times U \to \mathbb{R}$ satisfying

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = f(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in D,\ \boldsymbol{y} \in U, \\ u(\boldsymbol{x}, \boldsymbol{y}) = 0 & \text{for } \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in U, \end{cases}$$

where we assume that $a(\boldsymbol{x}, \boldsymbol{y})$ is given by the KL expansion on the previous page satisfying the summability condition and the following ellipticity condition: there exist constants $a_{\min}, a_{\max} > 0$ such that

$$0 < a_{\min} \le a(\boldsymbol{x}, \boldsymbol{y}) \le a_{\max} < \infty \quad \text{for all } \boldsymbol{x} \in D,\ \boldsymbol{y} \in U.$$

Let $V := H_0^1(D)$ and $V' := H^{-1}(D)$. Let $f \in L^2(D)$. The variational formulation of this parametric PDE is: find $u \in L^2(U; V) := \{g\colon U \to V;\ \|g\|_{L^2(U,V)}^2 := \int_U \|g(\cdot, \boldsymbol{y})\|_V^2 \,\mathrm{d}\boldsymbol{y} < \infty\}$ such that

$$\int_U \int_D a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y} = \int_U \int_D f(\boldsymbol{x}) v(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y}$$

for all $v \in L^2(U; V)$.

Generally, we can let the physical domain $D \subset \mathbb{R}^d$ to be a bounded domain with Lipschitz boundary. However, let us assume a bit more:

- The physical domain $D \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, is a convex and bounded polyhedron with plane faces.

This assumption ensures that we have a conforming FE space. To this end, let V_h denote the FE subspace of V spanned by piecewise linear FE basis functions $(\phi_j)_{j=1}^{M_h}$. Here, h denotes the (uniform) mesh width and M_h denotes the number of degrees of freedom.

Moreover, we let $\|u\|_V := \|\nabla u\|_{L^2(D)}$ for $u \in H_0^1(D)$ (the Poincaré inequality ensures that this is equivalent to the usual $H^1(D)$-norm).

Let us denote

$$B(u,v) := \int_U \int_D a(\boldsymbol{x},\boldsymbol{y}) \nabla u(\boldsymbol{x},\boldsymbol{y}) \cdot \nabla v(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y},$$

$$F(v) := \int_U \int_D f(\boldsymbol{x}) v(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}$$

so our weak formulation is: find $u \in L^2(U;V)$ such that $B(u,v) = F(v)$ for all $v \in L^2(U;V)$.

Lemma (Lax–Milgram)

Let $\mathcal{H}$ be a (real) Hilbert space. Let $b\colon \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ be a bilinear form such that

- *there exists a constant $C > 0$ such that for all $u, v \in \mathcal{H}$, $|b(u,v)| \le C\|u\|\|v\|$.*
- *there exists a constant $c > 0$ such that for all $v \in \mathcal{H}$, $|b(v,v)| \ge c\|v\|^2$.*

Then for all $F \in \mathcal{H}'$, there exists a unique $u \in \mathcal{H}$ such that for all $v \in \mathcal{H}$, $b(u,v) = F(v)$. Furthermore, we have the a priori *estimate $\|u\| \le c^{-1}\|F\|_{\mathcal{H}'}$.*

The Lax–Milgram lemma implies that our weak formulation has a unique solution $u \in L^2(U;V)$.

Recall that $\mathscr{F} := \{\boldsymbol{\nu} \in \mathbb{N}_0^\infty;\ |\mathrm{supp}(\boldsymbol{\nu})| < \infty\}$ denotes the set of all finitely supported multi-indices, with support $\mathrm{supp}(\boldsymbol{\nu}) := \{i \in \mathbb{N};\ \nu_i \neq 0\}$. Let $\varnothing \neq \Lambda \subseteq \mathscr{F}$ be a collection of multi-indices.

[Cohen et al. (2010)] propose the following discretizations:

Stochastic discretization

Let $X_\Lambda := \{v_\Lambda(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{\nu}\in\Lambda} v_{\boldsymbol{\nu}}(\boldsymbol{x})\hat{L}_{\boldsymbol{\nu}}(\boldsymbol{y});\ v_{\boldsymbol{\nu}} \in V\}$, where $\{\hat{L}_{\boldsymbol{\nu}}\}_{\boldsymbol{\nu}\in\mathscr{F}}$ is the basis of tensorized (orthonormal) Legendre polynomials $\hat{L}_{\boldsymbol{\nu}}(\boldsymbol{y}) = \prod_{i\in\mathrm{supp}(\boldsymbol{\nu})} \hat{L}_{\nu_i}(y_i)$. The Galerkin approximation $u_\Lambda = \sum_{\boldsymbol{\nu}\in\Lambda} u_{\boldsymbol{\nu}}\hat{L}_{\boldsymbol{\nu}} \in X_\Lambda$ of u is the unique solution to the problem

$$B(u_\Lambda, v_\Lambda) = F(v_\Lambda) \quad \text{for all } v_\Lambda \in X_\Lambda.$$

Stochastic and spatial discretization

Let $X_{\Lambda,h} = \{v_{\Lambda,h}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{\nu}\in\Lambda} v_{\boldsymbol{\nu}}(\boldsymbol{x})\hat{L}_{\boldsymbol{\nu}}(\boldsymbol{y});\ v_{\boldsymbol{\nu}} \in V_h\}$. The Galerkin approximation $u_{\Lambda,h} = \sum_{\boldsymbol{\nu}\in\Lambda} u_{\boldsymbol{\nu},h}\hat{L}_{\boldsymbol{\nu}} \in X_{\Lambda,h}$ of u is the unique solution to

$$B(u_{\Lambda,h}, v_{\Lambda,h}) = F(v_{\Lambda,h}) \quad \text{for all } v_{\Lambda,h} \in X_{\Lambda,h}. \tag{4}$$

Since $X_{\Lambda,h}$ is a finite-dimensional space and $L^2(U;V) \simeq L^2(U) \otimes V$, (4) is equivalent to

$$B(u_{\Lambda,h}, \phi_i \hat{L}_{\boldsymbol{\nu}}) = F(\phi_i \hat{L}_{\boldsymbol{\nu}}) \quad \text{for all } i \in \{1, \dots, M_h\},\ \boldsymbol{\nu} \in \Lambda.$$

Meanwhile, the Galerkin approximation can be written as $u_{\Lambda,h} = \sum_{j,\boldsymbol{\eta}} c_{j,\boldsymbol{\eta}} \phi_j \hat{L}_{\boldsymbol{\eta}}$ using undetermined coefficients $(c_{j,\boldsymbol{\eta}})_{j,\boldsymbol{\eta}}$. Plugging this into the above yields

$$\sum_{j,\boldsymbol{\eta}} c_{j,\boldsymbol{\eta}} B(\phi_j \hat{L}_{\boldsymbol{\eta}}, \phi_i \hat{L}_{\boldsymbol{\nu}}) = F(\phi_i \hat{L}_{\boldsymbol{\nu}}).$$

We can recast this as a matrix equation

$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{b},$$

where $\boldsymbol{A} = (B(\phi_i \hat{L}_{\boldsymbol{\nu}}, \phi_j \hat{L}_{\boldsymbol{\eta}}))_{(i,\boldsymbol{\nu}),(j,\boldsymbol{\eta})}$ is the $(M_h|\Lambda|) \times (M_h|\Lambda|)$ stiffness matrix, $\boldsymbol{c} = (c_{i,\boldsymbol{\nu}})_{(i,\boldsymbol{\nu})}$, and $\boldsymbol{b} = (F(\phi_i \hat{L}_{\boldsymbol{\nu}}))_{(i,\boldsymbol{\nu})}$ is the load vector.

Here and in what follows, the indexing of matrix/vector elements has been done using multi-indices, with $(i, \boldsymbol{\nu}) \in \{1, \dots, m\} \times \Lambda$ and $(j, \boldsymbol{\eta}) \in \{1, \dots, m\} \times \Lambda$. The ordering of the multi-indices is assumed to be consistent with the matrix equation $\boldsymbol{A}\boldsymbol{c} = \boldsymbol{b}$ (for example, rows/columns are indexed in lexicographic ordering).

If $a(\boldsymbol{x}, \boldsymbol{y})$ has a KL-like expansion

$$a(\boldsymbol{x}, \boldsymbol{y}) = \bar{a}(\boldsymbol{x}) + \sum_{k \geq 1} y_k \psi_k(\boldsymbol{x}), \quad \boldsymbol{y} = (y_1, y_2, \ldots) \in U,$$

where $\bar{a} \in L^\infty(D)$ and $(\|\psi_k\|_{L^\infty})_{k \geq 1} \in \ell^p(\mathbb{N})$ for some $0 < p \leq 1$, then

$$B(\phi_i \hat{L}_{\boldsymbol{\nu}}, \phi_j \hat{L}_{\boldsymbol{\eta}}) = \overbrace{\int_U \hat{L}_{\boldsymbol{\nu}} \hat{L}_{\boldsymbol{\eta}} \, \mathrm{d}\boldsymbol{y}}^{= \|\hat{L}_{\boldsymbol{\nu}}\|^2 \delta_{\boldsymbol{\nu}, \boldsymbol{\eta}} = \boldsymbol{I}} \int_D \bar{a} \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\boldsymbol{x}$$
$$+ \sum_{k \geq 1} \int_U y_k \hat{L}_{\boldsymbol{\nu}} \hat{L}_{\boldsymbol{\eta}} \, \mathrm{d}\boldsymbol{y} \int_D \psi_k \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\boldsymbol{x}$$

The stochastic and deterministic parts are completely independent!

Note the similarity of the previous expression with the matrix Kronecker product illustrated on the next slide!

Let us enumerate the rows and columns of the $nm \times nm$ Kronecker product $E \otimes F$ by the multi-indices $\boldsymbol{i}, \boldsymbol{j} \in \{1, \ldots, n\} \times \{1, \ldots, m\}$ in lexicographic order, see Table below for an illustration. Using this convention, the elements of the Kronecker product can be expressed concisely as

$$(E \otimes F)_{\boldsymbol{i},\boldsymbol{j}} = E_{i_1,j_1} F_{i_2,j_2}, \quad \boldsymbol{i}, \boldsymbol{j} \in \{1, \ldots, n\} \times \{1, \ldots, m\},$$

where $\boldsymbol{i} = (i_1, i_2)$ and $\boldsymbol{j} = (j_1, j_2)$ are ordered pairs.

Table: Enumeration of the columns and rows of the Kronecker product $E \otimes F$ by the multi-indices $\boldsymbol{i}, \boldsymbol{j} \in \{1, \ldots, n\} \times \{1, \ldots, m\}$ in lexicographic order.

column/row index	$(1,1)$	$(1,2)$	$\cdots$	$(1,m)$	$(2,1)$	$\cdots$	(n,m)
$(1,1)$	$E_{1,1}F_{1,1}$	$E_{1,1}F_{1,2}$	$\cdots$	$E_{1,1}F_{1,n}$	$E_{1,2}F_{1,1}$	$\cdots$	$E_{1,n}F_{1,m}$
$(1,2)$	$E_{1,1}F_{2,1}$	$E_{1,1}F_{2,2}$	$\cdots$	$E_{1,1}F_{2,n}$	$E_{1,2}F_{2,1}$	$\cdots$	$E_{1,n}F_{2,m}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$(1,m)$	$E_{1,1}F_{m,1}$	$E_{1,1}F_{m,2}$	$\cdots$	$E_{1,1}F_{m,m}$	$E_{1,2}F_{m,1}$	$\cdots$	$E_{1,n}F_{m,m}$
$(2,1)$	$E_{2,1}F_{1,1}$	$E_{2,1}F_{1,2}$	$\cdots$	$E_{2,1}F_{1,n}$	$E_{2,2}F_{1,1}$	$\cdots$	$E_{2,n}F_{1,m}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
(n,m)	$E_{n,1}F_{m,1}$	$E_{n,1}F_{m,2}$	$\cdots$	$E_{n,1}F_{m,m}$	$E_{n,2}F_{m,1}$	$\cdots$	$E_{n,n}F_{m,m}$

This allows us to write the stiffness matrix as

$$\boldsymbol{A} = \sum_{k \geq 0} (\boldsymbol{R}_k \otimes \boldsymbol{S}_k),$$

where we have the ordinary FE stiffness matrices

$$\boldsymbol{R}_0 = \left(\int_D \bar{a} \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\boldsymbol{x} \right)_{i,j} \quad \text{and} \quad \boldsymbol{R}_k = \left(\int_D \psi_k \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\boldsymbol{x} \right)_{i,j}$$

and their "stochastic" counterparts

$$\boldsymbol{S}_0 = \boldsymbol{I} \quad \text{and} \quad \boldsymbol{S}_k = \left(\int_U y_k \hat{L}_{\boldsymbol{\nu}} \hat{L}_{\boldsymbol{\eta}} \, \mathrm{d}\boldsymbol{y} \right)_{\boldsymbol{\nu},\boldsymbol{\eta}}.$$

All of these matrices are sparse!

Remark. If the tensorized orthogonal polynomials $\{\hat{L}_{\boldsymbol{\nu}}\}_{\boldsymbol{\nu} \in \mathscr{F}}$ are not normalized, then the formulae for the matrices $\boldsymbol{S}_k$, $k \geq 0$, are slightly different. Note also that if the orthogonal polynomial family is not chosen according to the Askey scheme, then the matrices $\boldsymbol{S}_k$ are no longer sparse in general.

Evaluation of the triple product expectations

In order to construct the matrices

$$\boldsymbol{S}_k = \left(\int_U y_k \hat{L}_{\boldsymbol{\nu}} \hat{L}_{\boldsymbol{\eta}} \, \mathrm{d}\boldsymbol{y} \right)_{\boldsymbol{\nu},\boldsymbol{\eta}}, \tag{5}$$

one needs to be able to compute the associated integrals. Since these are integrals of polynomials, a simple approach is to use Gaussian quadratures.

It is also possible to design recursive formulae for these quantities. To wit:

$$\int_{-1/2}^{1/2} y^r \hat{L}_p(y) \hat{L}_q(y) \, \mathrm{d}y = 2^{-r} c(r, |p-q|, \max\{p,q\}),$$

where $c(0,k,\ell) = \delta_{k,0}$ and $c(r,k,\ell) = \sqrt{\beta_{\ell+1-k}} c(r-1,k-1,\ell) + \sqrt{\beta_{\ell-k}} c(r-1,k+1,\ell)$, with $\beta_k := k^2/(4k^2-1)$. These formulae can be obtained trivially by integrating the three-term recurrence over the support; see, e.g., Appendix in [Hakula et al. (2015)]. Since (5) is a *product of univariate integrals* (Fubini), the recursion or Gaussian quadratures are simple to implement.

Remark. We could also consider the case where the input random field $a(\boldsymbol{x}, \boldsymbol{y})$ is given by a gPC expansion

$$a(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{\mu} \in \mathscr{F}} a_{\boldsymbol{\mu}}(\boldsymbol{x}) \hat{L}_{\boldsymbol{\mu}}(\boldsymbol{y}), \quad a_{\boldsymbol{\mu}}(\boldsymbol{x}) = \int_U a(\boldsymbol{x}, \boldsymbol{y}) \hat{L}_{\boldsymbol{\mu}}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}.$$

Then one ends up with the decomposition

$$\boldsymbol{A} = \sum_{\boldsymbol{\mu} \in \mathscr{F}} (\boldsymbol{R}'_{\boldsymbol{\mu}} \otimes \boldsymbol{S}'_{\boldsymbol{\mu}}),$$

where

$$\boldsymbol{R}'_{\boldsymbol{\mu}} = \left(\int_D a_{\boldsymbol{\mu}} \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\boldsymbol{x} \right)_{i,j} \quad \text{and} \quad \boldsymbol{S}'_{\boldsymbol{\mu}} = \left(\int_U \hat{L}_{\boldsymbol{\nu}} \hat{L}_{\boldsymbol{\eta}} \hat{L}_{\boldsymbol{\mu}} \, \mathrm{d}\boldsymbol{y} \right)_{\boldsymbol{\nu}, \boldsymbol{\eta}}.$$

Again, one can compute the elements of $\boldsymbol{S}'_{\boldsymbol{\mu}}$ using either Gaussian quadrature or recursively based on the three-term recurrence relation; cf., e.g., Appendix in [Hakula et al. (2015)].

Note that the underlying idea behind the stochastic Galerkin method is the following: the mapping $\boldsymbol{y} \mapsto u(\cdot, \boldsymbol{y})$ is smooth (in fact, it is analytic), so using orthogonal polynomials as the basis functions will produce higher-order convergence rates as we will later see.

So far, we have not addressed the issue of *how* to choose the index set Λ.

A simple approach would be to work with a dimensionally truncated problem (i.e., $\boldsymbol{y} \in [-1/2, 1/2]^s$ and $\varnothing \neq \Lambda \subseteq \mathbb{N}_0^s$) and using, e.g., a total degree index set Λ. Next lecture, we will discuss this topic as well as convergence rates for the stochastic Galerkin method.

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