Lecture for 11/4/21

— KL expansion (sketch)
  HW 2 (released tomorrow)

— Polynomial chaos in higher dimensions (multiple sources of uncertainty)

Next week

- stochastic reachability (TJ Sullivan)
- ZDR guest speaker rescheduled
  — adjust draft deadline

Def. (eigenfunction/eigenvalue). Let L be a linear operator on some function space. Then we say a nonzero f in that func. space is an eigenfunction of L w/ eigenvalue λ (a scalar) if

$$L(f) = \lambda f.$$

Ex. function space $= C^\infty(\mathbb{R})$

$\quad\quad\quad\quad\quad\quad\quad\quad \|$ continuous, infinitely differentiable functions with all continuous higher order derivatives

$L = \frac{d}{dt}$

- f is an eigenfunc. of L w/ eigenvalue λ if

$$\frac{d}{dt} f = \lambda f$$

ex. $f(x) = e^x$

$\underline{f(t) = f_0 e^{\lambda t}}$ = eigenfunc. w/ eigenval. λ

$\{u(\vec{x};\xi)\}_{\vec{x}\in D}$ $\xi = RV$

$K: D \times D \longrightarrow \mathbb{R}$

$K(\vec{x},\vec{y}) = \operatorname{cov}(u(\vec{x};\xi), u(\vec{y};\xi))$ (covariance function)

Def. The covariance operator L on function space $\mathcal{L}^2(\mathbb{R})$ is

$$L(f)(\vec{y}) = \int_D K(\vec{x},\vec{y})\, f(\vec{x})\, d\vec{x}$$

Ex. An eigenfunction ϕ_K of the cov. operator w/ eigenvalue λ_K satisfies

$$L(\phi_K) = \lambda_K \phi_K$$

$$\int_D K(\vec{x},\vec{y})\, \phi_K(\vec{x})\, d\vec{x} = \lambda_K\, \phi_K(\vec{y}).$$

- (1) Cov. kernels have infinitely many eigenfunc. ϕ_K w/ eigenvalues λ_K

- (2) Cov. kernels have their $\lambda_K \longrightarrow 0$ as $K \to \infty$ (*) HW

Def. Given a stochastic process $\alpha(\vec{x};\xi)$,
you can write this as

e.g., for PDE, would be. $u(x,t;\xi)$

$$\boxed{\alpha(\vec{x};\xi) = \bar{\alpha}(\vec{x}) + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\, \alpha_k(\xi)\, \phi_k(\vec{x})}$$

This is the Karhunen-Loeve Expansion.

mean func. $\bar{\alpha}(\underline{\vec{x}}) = \mathbb{E}[\alpha(\underline{\vec{x}};\xi)]$

- assumes you know (or have selected) the mean $\bar{\alpha}(x)$ and the cov. function $K(\vec{x},\vec{y})$ for the stochastic process $\alpha(\vec{x};\xi)$

- convergence "is only always good" when $\underline{\xi}$ is Gaussian
  - (ϕ_k, λ_k) are eigenfunc./value pairs for the covariance operator **and** ϕ_k are orthonormal

$$\int_{\mathcal{D}} K(\vec{x},\vec{y})\, \phi_k(\vec{x})\, d\vec{x} = \lambda_k\, \phi_k(\vec{y})$$

Ralph Smith text (pg. 110)

$\mathcal{D}$: domain for $\vec{x}$

- HW 2 (soil permeability): retrieving λ_k and ϕ_k from data given $\bar{\alpha}$, $K(\vec{x},\vec{y})$

The $\alpha_K(\xi)$ coeff. functions of ξ :

HW
$K(x,y) = e^{-|x+y|}$
ϕ_K (closed form soon.)

$$\alpha(\vec{x};\xi) - \bar{\alpha}(\vec{x}) = \sum_{i=1}^{\infty} \sqrt{\lambda_i}\, \alpha_i(\xi)\, \phi_i(\vec{x})$$

Mult. through by some $\phi_K(\xi)$ and integrating (but now w.r.t. $\vec{x}$),

any kind of "mult. through and integrate and.... it's nice b/c of orthogonality" called Galerkin projection

RHS
$$= \sum_{i=1}^{\infty} \sqrt{\lambda_i}\, \alpha_i(\xi) \overbrace{\int_{\mathcal{D}} \phi_i(\vec{x})\, \phi_K(\vec{x})\, d\vec{x}}^{\text{orthonormality}}$$
$$= \sqrt{\lambda_K}\, \alpha_K(\xi)\, (1)$$

$$\text{LHS} = \int_{\mathcal{D}} \left(\alpha(\vec{x};\xi) - \alpha(\vec{x})\right) \phi_K(\vec{x})\, dx$$

$$\boxed{\alpha_K(\xi) = \frac{1}{\sqrt{\lambda_K}} \int_{\mathcal{D}} \left(\alpha(\vec{x};\xi) - \bar{\alpha}(\vec{x})\right) \phi_K(\vec{x})\, d\vec{x}}$$

- HW 2 (est. $\alpha_K(\xi)$ as well)

$$\mathbb{E}(\alpha_K(\xi)) = \frac{1}{\sqrt{\lambda_K}} \int_{\mathcal{D}} \left(\cancel{\mathbb{E}(\alpha(\vec{x};\xi)) - \underbrace{\bar{\alpha}(\vec{x})}_{=\mathbb{E}(\alpha(\vec{x};\xi))}}^{0}\right) \phi_K(\vec{x})\, d\vec{x}$$
$= 0$

$\text{cov}(\alpha_k(\xi), \alpha_j(\xi)) \underset{\uparrow \text{HW2}}{=} \delta_{kj}$

[use: def. of ϕ_k as a eigenfunc. of $K(\vec{x}, \vec{y})$]

Ex. 1D Heat Eq.

- transient heat conduction problem
- spatially varying random conductivity parameter

$$u_t(x,t) = \frac{d}{dx}\left[\alpha(x;\xi)\, u_x(x,t)\right] + 1 \quad (*)$$

$x \in [-1,1]$

$t \in [0,T]$

ξ = real RV

1. Represent $\alpha(x,\xi)$ by the KL expansion
2. Plug into $(*)$
3. Integrate and use orthogonality ....
4. ... get deterministic set of PDEs

"Paul Constantine Primer"

High dim. polynomial chaos

- $\vec{\xi}$ = random vector ($\xi_1, \ldots, \xi_n$ are RVs)
  ξ_i are identically distributed

Burgers' eqn: $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$ $\quad u: \mathbb{R}_x \times \mathbb{R}_{t\geq 0} \to \mathbb{R}$

$$u(x, t=0; \vec{\xi}) = \underline{\xi_1} \sin(x) + \underline{\xi_2}$$

- assume $\vec{\xi} \sim N(0, I_{2\times 2})$

ξ_i are uncorrelated (needed for "classic" PC)

Not Gauss? Generalized polynomial chaos ... fine, but be careful w/ convergence

Ernst et al. (2011–2015)

?

Def. The (truncated) high-dim. PCE is

$$u(x,t;\vec{\xi}) = \sum_{0 \leq |\vec{K}| \leq M} \underline{u_{\vec{K}}(x,t)}\, \underline{\Psi_{\vec{K}}(\vec{\xi})}$$

multi-index $\vec{K} \in \mathbb{N}_0^2$ (size of vec. = # of components of $\vec{\xi}$)

$\vec{K} = (K_1, K_2)$ $\quad K_1, K_2 = 0, 1, 2, \ldots$

- <u>size</u> of multi-index $|\vec{K}| = K_1 + K_2 = \|\vec{K}\|_1$

$M = 3$

$\vec{K}$ is 2×1

sum over : $0 \leq |\vec{K}| \leq M$

$\{(K_1, K_2) \in \mathbb{N}_0^2 \mid K_1 + K_2 \leq 3\}$

$(0,0)$	$\lvert K \rvert = 0$
$(1,0)$, $(0,1)$	$\lvert K \rvert = 1$
$(2,0)$, $(0,2)$, $(1,1)$	$\lvert K \rvert = 2$
$(1,2)$, $(2,1)$, $(3,0)$, $(0,3)$	$\lvert K \rvert = 3$

$K_1 + K_2 \leq |M|$

- factorially many terms in the <u>sum</u>
- caution! might be slower than MC
- heuristically (biased experience), low M are still giving o.k. approximations

Now, $\{\Psi_{\vec{K}}\}$ are supposed to be orthog. w.r.t. PDF of $\vec{\xi}$

Define $\underline{\Psi_{\vec{K}}(\vec{\xi})} = \underline{\Psi_{K_1}(\xi_1)}\,\underline{\Psi_{K_2}(\xi_2)}$.

$$\int_{\mathcal{D}} \Psi_{\vec{K}}(\vec{\xi})\,\Psi_{\vec{J}}(\vec{\xi})\,d\vec{\xi}$$

$\vec{\xi} \sim N(0, I_{2\times 2})$

$$\|$$

split the density into product. of marginals

$$\int_{\mathcal{D}} \Psi_{K_1}(\xi_1)\Psi_{K_2}(\xi_2)\Psi_{j_1}(\xi_1)\Psi_{j_2}(\xi_2)\,\underline{d\xi_1\,d\xi_2}$$

$\|$ Fubini's thm.

* independence of the ξ_i

$$\left(\int_{\mathcal{D}_1} \underbrace{\Psi_{K_1}(\xi_1)\Psi_{j_1}(\xi_1)}_{\text{orthog.}}\,d\xi_1\right)\left(\int_{\mathcal{D}_2} \underbrace{\Psi_{K_2}(\xi_2)\Psi_{j_2}(\xi_2)}_{\text{orthog.}}\,d\xi_2\right)$$

$\mathcal{D} = \mathcal{D}_1 \times \mathcal{D}_2$

$$\left(h_{K_1}\,\delta_{K_1,j_1}\right)\left(h_{K_2}\,\delta_{K_2,j_2}\right) = \begin{cases} h_{K_1}h_{K_2} & \text{if } K_1 = j_1 \text{ and } K_2 = j_2 \\ 0 & \text{else} \end{cases}$$

$= h_{K_1}h_{K_2}\,\delta_{\vec{K}=\vec{J}}$ so orthogonal.

$\vec{K} = \vec{J}$ if and only if

$(K_1, K_2) = (j_1, j_2) \iff K_1 = j_1$ and $K_2 = j_2$