Representation of Random Inputs: Chapter 5

Example 1: Consider the Helmholtz energy

$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$

with frequency-dependent random parameters,

$$\psi(P,\omega,f) = \alpha_1(f,\omega)P^2 + \alpha_{11}(f,\omega)P^4 + \alpha_{111}(f,\omega)P^6$$

frequency   random event

Challenge 1: Difficult to work with probabilities associated with random events $\omega \in \Omega$.

- Solution: Every realization $\omega \in \Omega$ yields a value q of Q in Γ. Thus work in image of probability space
$$(\Gamma, \mathcal{B}(\Gamma), \rho_Q(q))$$
instead of $(\Omega, \mathcal{F}, P)$.

Challenge 2: How do we represent random fields; e.g., $\alpha_1(f,\omega)$ - that are infinite-dimensional?

Soln: Develop a representation and approximation framework.

Example 2: Heat equation

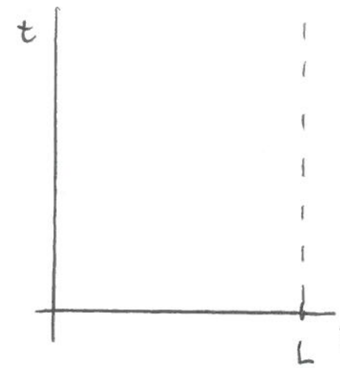
$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\alpha(x,\omega)\frac{\partial T}{\partial x}\right] + f(t,x) \qquad -1<x<1, \quad t>0$$

$$T(t,-1,\omega) = T_\ell(\omega)$$
$$T(t,1,\omega) = T_R(\omega) \quad , \ t>0$$
$$T(0,x,\omega) = T_0(\omega) \quad , \ -1<x<1$$

Motivation: Consider

$$\frac{\partial p}{\partial t} = \alpha \frac{\partial^2 p}{\partial x^2}$$

$$p(t,0) = p(t,L) = 0$$
$$p(0,x) = p_0(x)$$



Separation of Variables: Take

$$p(t,x) = T(t)X(x)$$

$$\Rightarrow X(x)\dot{T}(t) = \alpha X''(x)T(t)$$

$$\Rightarrow \frac{X''(x)}{X(x)} = \frac{\dot{T}(t)}{\alpha T(t)} = c$$

Then

$$X''(x) - cX(x) = 0 \qquad \dot{T}(t) = c\alpha T(t)$$
$$X(0) = X(L) = 0 \qquad T(t) = \beta e^{c\alpha t}$$

<u>Note</u>: Heat decays so $\alpha > 0$ and $c < 0$ so take $c = -\lambda^2$.

<u>BVP</u>: $X''(x) + \lambda^2 X(x) = 0$

$$X(0) = X(L) = 0$$

so

$$X(x) = A\cos(\lambda x) + B\sin(\lambda x)$$
$$= B\sin(\lambda_n x), \quad \lambda_n = \frac{n\pi}{L}$$

<u>General Solution</u>:

$$p(t,x) = \sum_{n=1}^{\infty} \beta_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x)$$

Determined by I.C.

Eigenfunctions (modes) - Basis functions !!

<u>Note</u>: $p_0(x) = p(0,x) = \sum_{n=1}^{\infty} \beta_n \sin(\lambda_n x)$

$$\Rightarrow \int_0^L p_0(x)\sin(\lambda_m x)\,dx = \int_0^L \sum_{n=1}^{\infty} \beta_n \sin(\lambda_n x) \cdot \sin(\lambda_m x)\,dx$$

$$\Rightarrow \beta_n = \frac{2}{L}\int_0^L p_0(x)\sin(\lambda_n x)\,dx$$

<u>Note</u>: Analogous strategy for random fields

<u>Random Fields</u>: Strategy - Represent random field $\alpha(x,\omega)$ in terms of mean function $\bar{\alpha}(x)$ and covariance function $C(x,y)$.

<u>Gaussian Process</u>: Probability distribution for functions

<u>Finite Dimensional</u>: $X \sim BVN(\mu, V)$, $X = [X_1, \dots, X_p]$

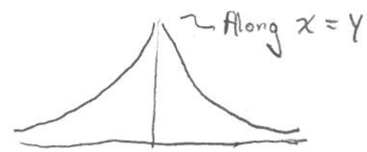
$$V = \begin{bmatrix} var(X_1) & cov(X_1,X_2) & \cdots & \\ cov(X_2,X_1) & var(X_2) & & \\ \vdots & & \ddots & \\ & & & var(X_p) \end{bmatrix}$$

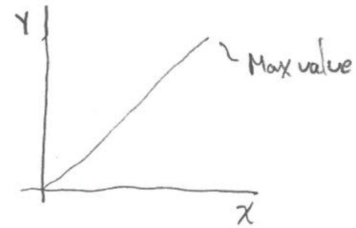
<u>Note</u>: V is symmetric and positive def.

<u>Note</u>: Infinite-dimensional for functions

<u>Examples</u>: Short versus long-range interactions

i.) $C(x,y) = \sigma^2 e^{-|x-y|/L}$





- Exponential isotropic
- $D = [-1, 1]$

MATLAB: covariance_exp.m

<u>Note</u>: $\sigma^2 = \frac{1}{2L}$ normalizes
- See additional notes on (iv, v)

<u>Limiting Behavior</u>:

i) $L \to \infty \Rightarrow C(x,y) = 1$ Fully correlated so cannot truncate

ii) $L \to 0 \Rightarrow C(x,y) = \delta(x-y)$ Uncorrelated and easy to truncate

2.) $C(x,y) = \min(x,y)$ 1-D Wiener Process: Used to model Brownian motion

Notes: a) Can solve eigenvalue problem explicitly
b) >> covariance_min

3.) $C(x,y) = \sigma^2 e^{-(x-y)^2/2L^2}$ Gaussian
$\uparrow$ Signal variance

<u>Karhunen-Loeve Expansion:</u>

$$\alpha(x,\omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n}\, \phi_n(x) Q_n(\omega)$$

Note: λ_n and $\phi_n(x)$ are eigenvalues and eigenfunctions of the covariance function $C(x,y)$; that is

$$\int_D C(x,y)\phi_n(y)dy = \lambda_n \phi_n(x) \quad \text{for } x \in D. \quad (+)$$

<u>Motivation for (+):</u>

1.) Finite-dimensional; e.g., $C = V$ symmetric + positive definite

$$C = \Phi \Lambda \Phi^{-1} = \Phi \Lambda \Phi^T = \begin{bmatrix} \phi^1 \cdots \phi^P \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_P \end{bmatrix} \begin{bmatrix} \phi^1 \\ \vdots \\ \phi^P \end{bmatrix}$$

$$= \begin{bmatrix} \lambda_1 \phi^1 \cdots \lambda_P \phi^P \end{bmatrix} \begin{bmatrix} \phi^1 \\ \vdots \\ \phi^P \end{bmatrix} = \sum_{n=1}^{P} \lambda_n \underset{p\times 1}{\phi^n} \underset{1\times p}{(\phi^n)^T}$$

2.) Infinite-dimensional: Mercer's theorem – If $C(x,y)$ is symmetric and positive definite, it can be expressed as

$$C(x,y) = \sum_{n=1}^{\infty} \lambda_n \phi_n(x) \phi_n(y)$$

where

$$\int_D C(x,y)\phi_n(y)dy = \lambda_n \phi_n(x)$$

and

$$\int_D \phi_n(x)\phi_m(x)dx = \delta_{mn} = \begin{cases} 1, & m=n \\ 0, & m \neq n \end{cases}$$

<u>Statistical Properties of $\alpha(x,\omega)$:</u> Take

$$\alpha(x,\omega) = \bar{\alpha}(x) + \beta(x,\omega)$$

where $\beta(x,\omega)$ has zero mean and covariance function $C(x,y)$. Take

$$\beta(x,\omega) = \sum_{n=1}^{\infty} \sqrt{\lambda_n}\, \phi_n(x) Q_n(\omega)$$

$$\Rightarrow \beta(x,\omega)\beta(y,\omega) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} Q_n(\omega) Q_m(\omega) \sqrt{\lambda_n \lambda_m}\, \phi_n(x)\phi_m(y)$$

<u>Recall:</u> For R.V X, Y

$$\text{cov}(X,Y) = \mathbb{E}[XY] - \mathbb{E}(X)\mathbb{E}(Y)$$

<u>Notation:</u> $\mathbb{E}(Y) = \langle Y \rangle = \int y\, p(y)\, dy$

Because $\beta(x,\omega)$ has zero mean,

$$
\begin{aligned}
c(x,y) &= \mathbb{E}[\beta(x,\omega)\beta(y,\omega)] \\
&= \langle \beta(x,\omega)\beta(y,\omega)\rangle \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \langle Q_n(\omega)Q_m(\omega)\rangle \sqrt{\lambda_n\lambda_m}\,\phi_n(x)\phi_m(y)
\end{aligned}
$$

Since eigenfunctions are orthogonal,

$$
\begin{aligned}
\lambda_k \phi_k(x) &= \int_D C(x,y)\phi_k(y)\,dy \\
&= \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega)\rangle \sqrt{\lambda_n\lambda_k}\,\phi_n(x).
\end{aligned}
$$

Multiplication by $\phi_\ell(x)$ and integration yields

$$
\lambda_k \int_D \phi_k(x)\phi_\ell(x)\,dx = \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega)\rangle \sqrt{\lambda_n\lambda_k}\,\delta_{n\ell}
$$

$$
\Rightarrow \lambda_k \delta_{k\ell} = \sqrt{\lambda_k\lambda_\ell}\,\langle Q_k(\omega)Q_\ell(\omega)\rangle
$$

Note: $k=\ell \Rightarrow \langle Q_k(\omega)Q_\ell(\omega)\rangle = 1$

$k \neq \ell \Rightarrow \langle Q_k(\omega)Q_\ell(\omega)\rangle = 0$

$\Rightarrow \langle Q_k(\omega)Q_\ell(\omega)\rangle = \delta_{k\ell}$

RESULT: The random variables satisfy

i) $\mathbb{E}(Q_n) = 0$ — Zero mean

ii) $\mathbb{E}(Q_n Q_m) = \delta_{mn}$ — Mutually orthogonal & uncorrelated

(+)

Question: How do we choose $c(x,y)$ and compute solutions to

$$
\int_D C(x,y)\phi_n(y)\,dy = \lambda_n \phi_n(x)?
$$

Common Choices for $c(x,y)$:

1.) $C(x,y) = e^{-|x-y|/2L}$, $D = [-1,1]$, L is correlation length

Radial basis functions

So

$$
\int_{-1}^{1} e^{-|x-y|/L}\phi_n(y)\,dy = 2L\,\phi_n(x)
$$

Analytic Solution:

$$
\lambda_n = \begin{cases} \dfrac{2L}{1+L^2\omega_n^2}, & n \text{ even} \\[2ex] \dfrac{2L}{1+L^2 v_n^2}, & n \text{ even} \end{cases}
$$

$$
\phi_n(x) = \begin{cases} \dfrac{\sin(\omega_n x)}{\sqrt{1-\frac{\sin(2\omega_n)}{2\omega_n}}}, & n \text{ even} \\[3ex] \dfrac{\cos(v_n x)}{\sqrt{1+\frac{\sin(2v_n x)}{2v_n}}}, & n \text{ odd} \end{cases}
$$

Note: ω_n, v_n are solutions to

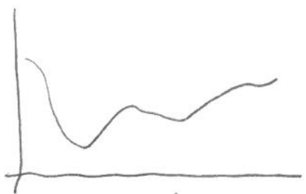
$L\omega + \tan(\omega) = 0$, even n

$1 - Lv\tan(v) = 0$, odd n

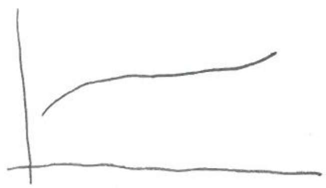
Note: Function or Kernel often represented by

$$C(x,y) = \sigma^2 e^{-|x-y|/2L}$$

- Here correlation length L describes smoothness or relation between values of x and y.

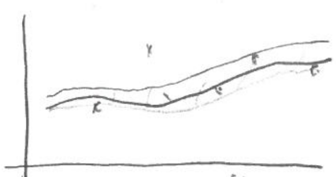


L small

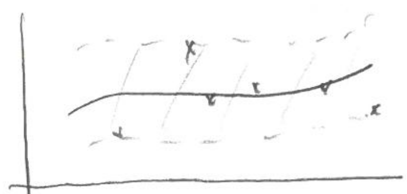


L large

- σ^2 quantifies how function varies from its mean (signal variance)



σ^2 small



σ^2 large

Note: $C(x,y)$ often called covariance function, autocorrelation function, or autocovariance function.

Choice 2: $C(x,y) = \min(x,y)$, $D = [0,1]$

Analytic Solution: From

$$\int_0^1 \min(x,y)\,\phi_n(y)\,dy = \lambda_n \phi_n(x)$$

we obtain $\phi_n(0) = 0$. For fixed x,

$$\int_0^x y\,\phi_n(y)\,dy + x\int_x^1 \phi_n(y)\,dy = \lambda_n \phi_n(x)$$

$$\Rightarrow \int_x^1 \phi_n(y)\,dy = \lambda_n \phi_n'(x)$$

and $\phi_n'(1) = 0$. Differentiate to obtain Sturm-Liouville BVP

$$\lambda_n \phi_n''(x) + \phi_n(x) = 0$$

$$\phi_n(0) = \phi_n'(1) = 0$$

Eigenvalues and eigenfunctions:

$$\lambda_n = \frac{1}{(n+\frac{1}{2})^2\pi^2}$$

$$\phi_n(x) = \sqrt{2}\,\sin(x/\sqrt{\lambda_n})$$

3.) Limiting Cases of 1)

$$c(x,y) = e^{-|x-y|/2L} \quad , \quad D = [0,1]$$

a) $C(x,y) = 1$ Fully correlated $(L \to \infty)$

$$\int_D \phi_n(y)\,dy = \lambda_n \phi_n(x) = k \text{ ~ Constant}$$

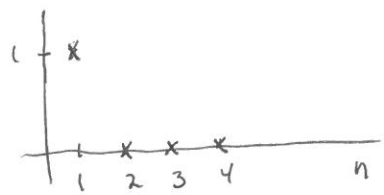
Recall: $C(x,y) = 1 = \sum_{n=1}^{\infty} \lambda_n \phi_n(x) \phi_n(y)$

Here

$$\phi_1(x) = \phi_1(y) = 1$$

$$\lambda_1 = 1$$

$$\lambda_n = 0 \text{ for } n = 2,3,\ldots$$



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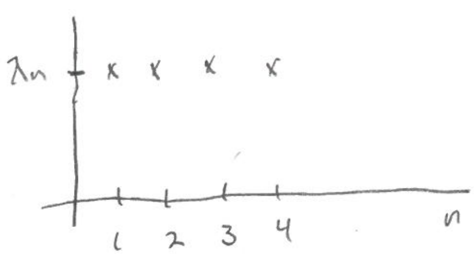
b) $C(x,y) = \delta(x-y)$ Uncorrelated $(L \to 0)$

Not positive definite

Then

$$\phi_n(x) = \lambda_n \phi_n(x)$$

$$\Rightarrow \lambda_n = 1 \text{ for all } n$$



Conclusion: Uncorrelated so cannot truncate series

Summary Thus Far... We have random process or field $\alpha(x,\omega)$ that we represent as

$$\alpha(x,\omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \underbrace{\sqrt{\lambda_n}\,\phi_n(x)}_{\text{Deterministic}} \underbrace{Q_n(\omega)}_{\text{Random}}$$

where

$$\int_D C(x,y)\phi_n(y)\,dy = \lambda_n \phi_n(x) \quad , \quad x \in D$$

and

$$\int_D \phi_n(x)\phi_m(x)\,dx = \delta_{mn}.$$

One choice for covariance function:

$$C(x,y) = e^{-|x-y|/2L}$$

Notes: i) We can use eigenvalue decay to truncate sum; i.e.,

$$\alpha(x,\omega) \simeq \alpha^N(x,\omega) = \bar{\alpha}(x) + \sum_{n=1}^{N_{KL}} \sqrt{\lambda_n}\,\phi_n(x) Q_n(\omega)$$

ii) The random variables satisfy

$$\mathbb{E}[Q_n] = 0$$

$$\mathbb{E}[Q_n Q_m] = \delta_{mn}$$

iii) If a Gaussian process, uncorrelated implies independent and

$$Q = [Q_1, \cdots, Q_P] \sim N(0, I_P)$$

with

$$\rho_Q(q) = \prod_{i=1}^{P} \frac{1}{\sqrt{2\pi}} e^{-q_i^2/2}$$

Question: If we know the underlying distribution $\omega \in \Omega$, can we approximate the covariance function $C(x,y)$? Yes, do it through sampling.

e.g.) Consider

$$\alpha(P,\omega) = \alpha_{I}(\omega)P^{2} + \alpha_{II}(\omega)P^{4} + \alpha_{III}P^{6}$$

and take $x = P$, for $x = P \in [0,1]$.

Note: We assume that we can evaluate $\alpha(x_j, \omega^k)$ for varies frequencies $x_j = f_j$ and values ω^k from the underlying distribution.

Sampling-Based Covariance Function:

$$C(x,y) \simeq C^{N_{mc}}(x,y)$$

$$= \frac{1}{N_{mc}-1}\sum_{k=1}^{N_{mc}} \alpha_c(x,\omega^k)\,\alpha_c(y,\omega^k)$$

where

$$\alpha_c(x,\omega^k) = \alpha(x,\omega^k) - \underbrace{\frac{1}{N_{mc}}\sum_{j=1}^{N_{mc}} \alpha(x,\omega^j)}_{\bar{\alpha}(x)}$$

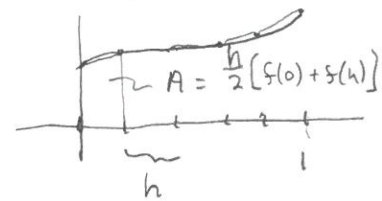
Approximation of Eigenvalue Problem: Consider approximation of

$$\int_0^1 C(x,y)\,\phi_n(y)\,dy = \lambda_n \phi_n(x)$$

$$\int_0^1 \phi_n(x)\,\phi_m(x)\,dx = \delta_{mn}$$

Consider quadrature rule with nodes and weights $\{(x_j, w_j)\}$.

Examples; i) Composite trapezoid

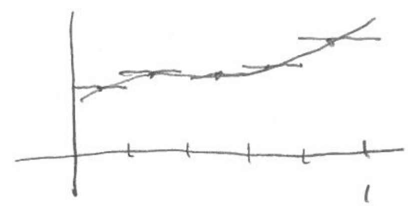


$$h = \frac{1}{N-1}$$

$$x_j = jh,\ j = 0,\dots,N$$

$$w_j = \left[\frac{h}{2}, h, \dots, h, \frac{h}{2}\right]$$

ii) Composite midpoint



iii) Gaussian

iv) Monte Carlo

Discretized Problem:

$$\sum_{j=1}^{N_{quad}} w_j\, C(x_i, x_j)\,\phi_n(x_j) = \lambda_n \phi_n(x_i),\quad i = 1,\dots,N_{quad}$$

Let $\phi_n^i = \phi_n(x_i)$ $\quad W = \mathrm{diag}(w_1, \dots, w_{N_{quad}})$

$C_{ij} = C(x_i, x_j)$

Discretized Eigenvalue Problem:

$$CW\phi_n = \lambda_n \phi_n$$

Symmetric Eigenvalue Problem:

$$W^{1/2} C W^{1/2} \tilde{\phi}_n = \lambda_n \tilde{\phi}_n$$

where

$$\tilde{\phi}_n = W^{1/2}\phi_n$$

$$\tilde{\phi}_n^T \tilde{\phi}_n = 1$$

Compute eigenvectors by $\phi_n = W^{-1/2}\tilde{\phi}_n$.

Note: Nystom's method

$$\phi_n^T W \phi_n = 1.$$

Complete Algorithm:

Input: i) Quadrature formula with nodes & weights $\{(x_j, w_j)\}$.

ii) Function evaluations $\{\alpha(x_j, \omega^k)\}$, $j=1,\dots,N_{quad}$, $k=1,\dots,N_{mc}$

Output: Eigenvalues, eigenvectors and KL modes

1.) Center process

$$\alpha_c(x_i, \omega^k) = \alpha(x_i,\omega^k) - \frac{1}{N_{mc}}\sum_{m=1}^{N_{mc}} \alpha(x_i,\omega^m)$$

for $i=1,\dots,N_{quad}$ and $k=1,\dots,N_{mc}$

2) Form covariance matrix (discretized covariance function)

$$C_{ij} = \frac{1}{N_{mc}-1}\sum_{k=1}^{N_{mc}} \alpha_c(x_i,\omega^k)\,\alpha_c(x_j,\omega^k)$$

for $i,j=1,\dots,N_{quad}$

3.) Let $W = \mathrm{diag}(w_1,\dots,w_{N_{quad}})$ and solve

$$W^{1/2} C W^{1/2}\tilde{\phi}_n = \lambda_n \tilde{\phi}_n \quad , n=1,\dots,N_{quad}$$

4.) Compute $\phi_n = W^{-1/2}\tilde{\phi}_n$

5.) Choose a KL truncation level N_{KL} and compute discretized KL modes $Q_n(\omega)$. Consider

$$\alpha(x,\omega) = \bar{\alpha}(x) + \sum_{n=1}^{N_{KL}} \sqrt{\lambda_n}\,\phi_n(x)\,Q_n(\omega)$$

$$\Rightarrow \alpha_c(x,\omega) = \sum_{n=1}^{N_{KL}} \sqrt{\lambda_n}\,\phi_n(x)\,Q_n(\omega)$$

$$\Rightarrow Q_n(\omega) = \frac{1}{\sqrt{\lambda_n}}\int_0^1 \alpha_c(x,\omega)\,\phi_n(x)\,dx$$

$$\simeq \frac{1}{\sqrt{\lambda_n}}\sum_{j=1}^{N_{quad}} w_j\,\alpha_c(x_j,\omega)\,\phi_n^j$$

6.) Sample at ω^k and build surrogate

$$\tilde{Q}_n(\omega^k);$$

e.g., Polynomial, spectral expansion

Example: Consider

$$\alpha(x,\omega) = \Psi(x,\omega)$$
$$= \alpha_I(\omega)x^2 + \alpha_{II}(\omega)x^4 + \alpha_{III}x^6$$

on $x \in [0,1]$ with

$$\mathbb{E}[\alpha_1] = -389.4$$
$$\mathbb{E}[\alpha_2] = 761.3$$
$$\mathbb{E}[\alpha_3] = 61.5$$

and assume that $\alpha = [\alpha_I, \alpha_{II}, \alpha_{III}] \sim \mathcal{U}([\alpha_{Il}, \alpha_{Ir}] \times [\alpha_{IIl}, \alpha_{IIr}] \times [\alpha_{IIIl}, \alpha_{IIIr}])$.

where $\alpha_{Il} = \bar{\alpha}_1 - 0.2\bar{\alpha}_1$, $\alpha_{Ir} = \bar{\alpha}_1 + 0.2\bar{\alpha}_1$.

Results: $\lambda_1 = 417.88$ Thus $N_{KL} = 3$

$\lambda_2 = 1.2$

$\lambda_3 = 0.009$

Note:
- $C(x,y)$ is symmetric nonnegative definite for trapezoid rule but has 0 eigenvalue.
- $\omega \in \mathbb{R}^3$ for our example

Observation: How do we do inverse problem when we cannot directly sample field? E.g.,

$$\Psi(P,\omega,f) = \alpha_I(f,\omega)P^2 + \alpha_{II}(f,\omega)P^4 + \alpha_{III}(f,\omega)P^6$$

1. Employ parametric covariance function; e.g.,
$$C(x,y) = e^{-|x-y|/2L}$$
and estimate L

2.) Employ polynomial surrogate for field; To come later.

Final Note: Heat equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\alpha(x,\omega)\frac{\partial T}{\partial x}\right] \quad , -1<x<1,\ t>0$$

$$\left.\begin{aligned} T(t,-1,\omega) &= T_\ell(\omega) \\ T(t,1,\omega) &= T_R(\omega) \end{aligned}\right\} t>0$$

$$T(0,x,\omega) = T_0(\omega) \quad , -1<x<1$$

Well-posedness requires: $0 < \alpha_{min} \le \alpha(x,\omega) < \alpha_{max}$. Take

$$\alpha(x,\omega) = \alpha_{min} + e^{\bar{\alpha}(x) + \sum_{n=1}^{\infty}\sqrt{\lambda_n}\,\phi_n(x)Q_n(\omega)}$$

Parameters: $Q = [T_\ell, T_R, T_0, Q_1, \ldots, Q_N]$