Lecture 5: Statistical Representation of Model Inputs

**Example:**

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Helmholtz energy
    \[
    \psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6
    \]

**UQ and SA Issues:**

- Is 6\textsuperscript{th} order term required to accurately characterize material behavior?
- **Note**: Determines molecular structure
Quantum-Informed Continuum Models

Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Helmholtz energy

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

UQ and SA Issues:

- Is 6th order term required to accurately characterize material behavior?

  • Note: Determines molecular structure

Broad Objective:

- Use UQ/SA to help bridge scales from quantum to system

Note:

- Linearly parameterized
Example 2: Pressurized Water Reactors (PWR)

Models:

• Involve neutron transport, thermal-hydraulics, chemistry.
• Inherently multi-scale, multi-physics.

CRUD Measurements: Consist of low resolution images at limited number of locations.
Pressurized Water Reactors (PWR)

Thermo-Hydraulic Equations: Mass, momentum and energy balance for fluid

\[
\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f \mathbf{v}_f) = -\Gamma
\]

\[
\alpha_f \rho_f \frac{\partial \mathbf{v}_f}{\partial t} + \alpha_f \rho_f \mathbf{v}_f \cdot \nabla \mathbf{v}_f + \nabla \cdot \sigma^R_f + \alpha_f \nabla \cdot \sigma + \alpha_f \nabla \rho_f
\]

\[
= -F^R - F + \Gamma (\mathbf{v}_f - \mathbf{v}_g)/2 + \alpha_f \rho_f g
\]

\[
\frac{\partial}{\partial t}(\alpha_f \rho_f \mathbf{e}_f) + \nabla \cdot (\alpha_f \rho_f \mathbf{e}_f \mathbf{v}_f + Th) = (T_g - T_f) H + T_f \Delta_f
\]

\[
- T_g (H - \alpha_g \nabla \cdot h) + h \cdot \nabla T - \Gamma [\mathbf{e}_f + T_f (s^* - s_f)]
\]

\[
- \rho_f \left( \frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \mathbf{v}_f) + \frac{\Gamma}{\rho_f} \right)
\]

Notes:
- Similar relations for gas and bubbly phases
- Surrogate models must conserve mass, energy, and momentum
- Many parameters are spatially varying and represented by random fields

Challenges:
- Codes can have 15-30 closure relations and up to 75 parameters.
- Codes and closure relations often "borrowed" from other physical phenomena; e.g., single phase fluids, airflow over a car (CFD code STAR-CCM+)
- Calibration necessary and closure relations can conflict.
- Inference of random fields requires high- (infinite-) dimensional theory.
Representation of Random Inputs

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

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

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

Solution: Every realization \( \omega \in \Omega \) yields a value \( q \in Q \subset \Gamma \). Work in image of probability space \( (\Gamma, \mathcal{B}(\Gamma), \rho(q)) \) instead of \( (\Omega, \mathcal{F}, P) \).

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

Solution: Develop a representation and approximation framework
Example and Motivation

Example 2: Heat equation

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

\[T(t, -1, \omega) = T_\ell(\omega) \, , \, T(t, 1, \omega) = T_r(\omega) \quad t > 0 \]

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

Motivation: Consider

\[
\frac{\partial \rho}{\partial t} = \alpha \frac{\partial^2 \rho}{\partial x^2} \quad , \quad 0 < x < L , \quad t > 0
\]

\[\rho(t, 0) = \rho(t, L) = 0 \quad t > 0 \]

\[T(0, x) = \rho_0(x) \quad 0 < x < L \]
Example and Motivation

**Motivation:** Consider

\[
\frac{\partial \rho}{\partial t} = \alpha \frac{\partial^2 \rho}{\partial x^2}, \quad 0 < x < L, \quad t > 0
\]

\[
\rho(t, 0) = \rho(t, L) = 0 \quad t > 0
\]

\[
T(0, x) = \rho_0(x) \quad 0 < x < L
\]

**Separation of Variables:** Take

\[
\rho(t, x) = T(t)X(x)
\]

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

\[
\Rightarrow \frac{X''(x)}{X(x)} = \frac{\dot{T}(t)}{\alpha T(t)} = C
\]

Then

\[
X''(x) - cX(x) = 0
\]

\[
X(0) = X(L) = 0
\]

and

\[
\dot{T}(t) = c\alpha T(t)
\]

\[
\Rightarrow T(t) = \beta e^{c\alpha t}
\]

**Note:** Heat decays – Mathematical argument

\[
\int_0^L [XX'' - cX^2]dx = -\int_0^L [(X')^2 + cX^2] \, dx = 0
\]

If \(c \geq 0\), this implies that \(X(x) = k = 0\).

Thus \(c < 0\) so we take \(c = -\lambda^2\) where \(\lambda > 0\).
Motivation

Boundary Value Problem:
\[ X''(x) - cX(x) = 0 \]
\[ X(0) = X(L) = 0 \]

Solution: \( X(x) = A \cos(\lambda x) + B \sin(\lambda x) \)
\[ X(0) = 0 \Rightarrow A = 0 \]
\[ X(L) = 0 \Rightarrow \lambda L = n\pi \]

Thus
\[ X_n(x) = B_n \sin(\lambda_n x) , \lambda_n = \frac{n\pi}{L} , B_n \neq 0 \]

General Solution:
\[ \rho(t, x) = \sum_{n=1}^{\infty} B_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x) \]

Initial Condition: \( \rho_0(x) = \rho(0, x) = \sum_{n=1}^{\infty} B_n \sin(\lambda_n x) \)
\[ \Rightarrow \int_0^L \rho_0(x) \sin(\lambda_m x) dx = \int_0^L \sum_{n=1}^{\infty} B_n \sin(\lambda_n x) \sin(\lambda_m x) dx \]
\[ \Rightarrow B_n = \frac{2}{L} \int_0^L \rho_0(x) \sin(\lambda_n x) dx \]
Motivation

Boundary Value Problem:
\[ X''(x) - cX(x) = 0 \]
\[ X(0) = X(L) = 0 \]

General Solution:
\[ \rho(t, x) = \sum_{n=1}^{\infty} B_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x) \]

Initial Condition:
\[ B_n = \frac{2}{L} \int_0^L \rho_0(x) \sin(\lambda_n x) \, dx \]

Example: \( \rho_0(x) = \sin \left( \frac{\pi x}{L} \right) \)
\[ B_n = \frac{2}{L} \int_0^L \sin \left( \frac{\pi x}{L} \right) \sin \left( \frac{n\pi x}{L} \right) \, dx \]
\[ = \begin{cases} \frac{2}{L} \cdot \frac{L}{2}, & n = 1 \\ 0, & n \neq 1 \end{cases} \]

General Solution:
\[ \rho(t, x) = e^{-\alpha (\pi/L)^2 t} \sin(\pi x/L) \]

Note Decay!
Random Field Representation

**Random Fields: Strategy** – Represent random field $\alpha(x, \omega)$ in terms of mean function $\bar{\alpha}(x)$ and covariance function $c(x, y)$

**Finite-Dimensional:** $X \sim MVN(\mu, V), \ X = [X_1, \ldots, X_p]$

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

**Note:** Infinite-dimensional for functions

**Examples:** Short versus long-range interactions

1. $c(x, y) = \sigma^2 e^{-|x-y|/L}$  \hspace{1cm} **Note:** $\sigma$ normalizes
   $$\mathcal{D} = [-1, 1]$$

Limiting Behavior:

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

$(ii) \ L \to 0 \Rightarrow c(x, y) = \delta(x - y)$ Uncorrelated so easy to truncate
Random Field Representation

Examples:

2. \( c(x, y) = \min(x, y) \)  
   1-D Wiener Process
   • Used to model Brownian motion
   • Can solve eigenvalue problem explicitly

3. \( c(x, y) = \sigma^2 e^{-(x-y)^2/2L^2} \)  
   Gaussian

\[
C = \Phi \Lambda \Phi^{-1} = \Phi \Lambda \Phi^T
\]

\[
= \begin{bmatrix}
\phi^1 & \cdots & \phi^p
\end{bmatrix}
\begin{bmatrix}
\lambda_1 \\
& \ddots \\
& & \lambda_p
\end{bmatrix}
\begin{bmatrix}
\phi^1 \\
\vdots \\
\phi^p
\end{bmatrix}
\]

\[
= [\lambda_1 \phi^1, \ldots, \lambda_p \phi^p] = \sum_{p=1}^{p} \lambda_n \phi^n (\phi^n)^T
\]

MATLAB: covariance_exp.m, covariance_min.m, covariance_Gaussian.m

Properties of \( c(x,y) \):

1. Finite-dimensional: e.g., \( C = V \) symmetric and positive definite

\[
C = \Phi \Lambda \Phi^{-1} = \Phi \Lambda \Phi^T
\]
Random Field Representation

**Mercer’s Theorem:** (Infinite Dimensional) – 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

\[
\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}
\]

and

\[
\int_{\mathcal{D}} \phi_n(x) \phi_m(x) dx = \delta_{mn} \quad \text{Note: Eigenfunctions are orthonormal}
\]

**Karhunen-Loeve Expansion:**

\[
\alpha(x, \omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)
\]
Random Field Representation

Karhunen-Loève Expansion:

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

Statistical Properties: Take

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

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

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

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

Recall: For random variables \( X, Y \)

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

Notation: \( \mathbb{E}[Y] = \langle Y \rangle = \int y \rho(y) dy \)
Random Field Representation

**Statistical Properties:** Because $\beta(x, \omega)$ has zero mean,

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

Since eigenfunctions are orthogonal,

\[
\lambda_k \phi_k(x) = \int_{\mathbb{D}} c(x, y)\phi_k(y)dy = \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega) \rangle \sqrt{\lambda_n\lambda_k}\phi_n(x)
\]

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

\[
\lambda_k \int_{\mathbb{D}} \phi_k(x)\phi_{\ell}(x)dx = \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_\ell(\omega) \rangle \sqrt{\lambda_n\lambda_k}\delta_{n\ell}
\]

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

**Note:**

\[
k = \ell \quad \Rightarrow \quad \langle Q_k(\omega)Q_\ell(\omega) \rangle = 1
\]

\[
k \neq \ell \quad \Rightarrow \quad \langle Q_k(\omega)Q_\ell(\omega) \rangle = 0
\]

\[
\Rightarrow \langle Q_k(\omega)Q_\ell(\omega) \rangle = \delta_{k\ell}
\]
Random Field Representation

**Karhunen-Loeve Expansion:**

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

where

\[
\int_{\mathcal{D}} c(x, y) \phi_n(y) \, dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}
\]

**Result:** The random variables satisfy

(i) \( \mathbb{E}[Q_n] = 0 \) \quad Zero mean

(ii) \( \mathbb{E}[Q_n Q_m] = \delta_{mn} \) \quad Mutually orthogonal and uncorrelated

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

\[
\int_{\mathcal{D}} c(x, y) \phi_n(y) \, dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}
\]
Common Choices for $c(x,y)$

1. Radial Basis Function:

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

so

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

Analytic Solution:

$$\lambda_n = \begin{cases} \frac{2L}{1 + L^2 w_n^2} , & \text{if } n \text{ is even}, \\ \frac{2L}{1 + L^2 v_n^2} , & \text{if } n \text{ is odd} \end{cases}$$

$$\phi_n(x) = \begin{cases} \frac{\sin(w_n x)}{\sqrt{1 - \frac{\sin(2w_n)}{2w_n}}} , & \text{if } n \text{ is even}, \\ \frac{\cos(v_n x)}{\sqrt{1 + \frac{\sin(2v_n)}{2v_n}}} , & \text{if } n \text{ is odd} \end{cases}$$

**Note:** $L$ is correlation length, which quantifies smoothness or relation between values of $x$ and $y$.

**Note:** $w_n$ and $v_n$ are the solutions of the transcendental equations

$$Lw + \tan(w) = 0 \quad \text{for even } n,$$

$$1 - Lv \tan(v) = 0 \quad \text{for odd } n.$$
Common Choices for $c(x,y)$

1. Radial Basis Function:

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

Note: $L$ is correlation length

so

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

Limiting Cases:

(i) $c(x, y) = 1$ Fully correlated ($L \to \infty$)

$$\int_{\mathcal{D}} \phi_n(y) dy = \lambda_n \phi_n(x) = k_n$$

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

Take

$$\phi_1(x) = \phi_1(y) = \frac{\sqrt{2}}{2}$$

$$\lambda_1 = 2$$

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

(ii) $c(x, y) = \delta(x - y)$ Uncorrelated ($L \to 0$)

Then

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

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

Note: Because uncorrelated, we cannot truncate series!
Construction of $c(x,y)$

**Question:** If we know underlying distribution $\omega \in \Omega$, can we approximate the covariance function $c(x,y)$? Yes … via sampling!

**Example:** Consider the Helmholtz energy

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

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

**Note:** Assume we can evaluate $\alpha(x_j, \omega^k)$ for various polarizations $x_j = P_j$ and values $\omega^k$ from the underlying distribution.

**Required Steps:**

- Approximation of the covariance function $c(x,y)$
- Approximation of the eigenvalue problem

$$\int_\mathcal{D} c(x,y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D} \quad \text{with} \quad \int_\mathcal{D} \phi_n(x) \phi_m(x) dx = \delta_{mn}$$
Construction of $c(x,y)$

**Step 1:** Approximation of covariance function $c(x,y)$

For $N_{MC}$ Monte Carlo samples $\omega^k$, covariance function approximated by

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

where the centered field is

$$\alpha_c(x, \omega^k) = \alpha(x, \omega^k) - \bar{\alpha}(x)$$

and the mean is

$$\bar{\alpha}(x) \approx \frac{1}{N_{MC}} \sum_{j=1}^{N_{MC}} \alpha(x, \omega^j)$$
Construction of $c(x,y)$

**Step 2 (Nystrom’s Method):** Approximate eigenvalue problem

\[
\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \quad \text{for } x \in \mathcal{D} \quad \text{with} \quad \int_{\mathcal{D}} \phi_n(x) \phi_m(x) dx = \delta_{mn}
\]

Consider composite quadrature rule with $N_{quad}$ points and weights $\{(x_j, w_j)\}$.

**Discretized Eigenvalue Problem:**

\[
\sum_{j=1}^{N_{quad}} c(x_i, x_j) \phi_n(x_j) w_j = \lambda_n \phi_n(x_i) , \quad i = 1, \ldots, N_{quad}
\]

**Matrix Eigenvalue Problem:**

\[CW\phi_n = \lambda_n \phi_n\]

where

\[\phi_n^i = \phi_n(x_i)\]

\[C_{ij} = c(x_i, x_j)\]

\[W = \text{diag}(w_1, \ldots, w_{N_{quad}})\]

**Symmetric Matrix Eigenvalue Problem:**

\[W^{1/2} CW^{1/2} \tilde{\phi}_n = \lambda_n \tilde{\phi}_n\]

where

\[\tilde{\phi}_n = W^{1/2} \phi_n \Rightarrow \phi_n = W^{-1/2} \tilde{\phi}_n\]

\[\tilde{\phi}_n^T \tilde{\phi}_n = 1 \Rightarrow \phi_n^T W \phi_1 = 1\]

\[W^{1/2} = \text{diag}(\sqrt{w_1}, \ldots, \sqrt{w_{N_{quad}}})\]
Algorithm to Approximate $c(x,y)$

**Inputs:**

(i) Quadrature formula with nodes and weights $\{(x_j, w_j)\}$

(ii) Functions evaluations $\{\alpha(x_j, \omega^k)\}, j = 1, \ldots, N_{\text{quad}}, \quad k = 1, \ldots, N_{\text{Mc}}$

**Output:** Eigenvalues, eigenvectors and KL modes

1) Center the process

$$\alpha_c(x_i, \omega^k) = \alpha(x_i, \omega^k) - \frac{1}{N_{\text{MC}}} \sum_{j=1}^{N_{\text{MC}}} \alpha(x_i, \omega^j)$$

for $i = 1, \ldots, N_{\text{quad}}$ and $k = 1, \ldots, N_{\text{MC}}$.

2) Form covariance matrix $C = [C_{ij}]$ that discretizes covariance function $c(x, y)$

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

for $i, j = 1, \ldots, N_{\text{quad}}$. 
Algorithm to Approximate $c(x,y)$

**Output:** Eigenvalues, eigenvectors and KL modes

(3) Let $W = \text{diag}(w_1, \ldots, w_{N_{\text{quad}}})$ and solve

\[ W^{1/2} C w^{1/2} \tilde{\phi}_n = \lambda_n \tilde{\phi}_n \]

for $n = 1, \ldots, N_{\text{quad}}$.

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

(5) Exploit the decay in the eigenvalues $\lambda_n$ to choose a KL truncation level $N_{KL}$ and compute discretized KL modes $Q_n(\omega)$. Consider

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

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

\[ \Rightarrow Q_n(\omega) = \frac{1}{\sqrt{\lambda_n}} \int_{\mathcal{D}} \alpha_c(x, \omega) \phi_n(x) dx \]

\[ \approx \frac{1}{\sqrt{\lambda_n}} \sum_{j=1}^{N_{\text{quad}}} w_j \alpha_c(x_j, \omega) \phi_n^j. \]
Algorithm to Approximate $c(x,y)$

**Output:** Eigenvalues, eigenvectors and KL modes

(6) Sample $\omega^k$ and construct surrogate $\tilde{Q}_n(\omega^k)$; e.g., polynomial, spectral polynomial, Gaussian process.

**Example:** Consider the Helmholtz energy

$$\alpha(x, \omega) = \alpha_1(\omega)x^2 + \alpha_{11}x^4 + \alpha_{111}x^6$$

for $x \in [0, 1]$

Mean Values: Based on DFT

$$\bar{\alpha}_1 = -389.4 , \bar{\alpha}_{11} = 761.3 , \bar{\alpha}_{111} = 61.5.$$

Distribution:

$$\alpha = [\alpha_1, \alpha_{11}, \alpha_{111}] \sim \mathcal{U}([\alpha_{1\ell}, \alpha_{1r}] \times [\alpha_{2\ell}, \alpha_{2r}] \times [\alpha_{3\ell}, \alpha_{3r}])$$

where $\alpha_{1\ell} = \bar{\alpha}_1 - 0.2\bar{\alpha}_1, \alpha_{1r} = \bar{\alpha} + 0.2\bar{\alpha}_1$ with similar intervals for $\alpha_{11}$ and $\alpha_{111}$

Eigenvalues: $\lambda_1 = 417.88, \lambda_2 = 1.2$ and $\lambda_3 = 0.009$ so truncate series at $N_{KL} = 3$

MATLAB: covariance_construct.m
Example and Motivation

Example 2: Heat equation

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

\[
T(t, -1, \omega) = T_\ell(\omega), \quad T(t, 1, \omega) = T_r(\omega), \quad t > 0
\]

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

Note: Well-posedness requires

\[
0 < \alpha_{\min} \leq \alpha(x, \omega) \leq \alpha_{\max}
\]

Take

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

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