On the Karhunen-Loève basis for continuous mechanical systems

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Outline: Naive look/More detailed look

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Some history

Beginning: works in Statistics and Probability and Spectral Theory in Hilbert Spaces. Some contributions:

• Kosambi (1943)
• Loève (1945)
• Karhunen (1946)
• Pougachev (1953)
• Obukhov (1954)

Applications:

• Lumley (1967): method applied to Turbulence
• Sirovich (1987): snapshot method

An important book appeared in 1996: Holmes, Lumley, Berkooz. In Solid Mechanics the applications started around 1993. In finite dimension it appears under different guises:

• Principal Component Analysis (PCA): Statistics and image processing
• Empirical orthogonal functions: Oceanography and Metereology
• Factor analysis: Psychology and Economics
Main Applications

• Data analysis: Principal Component Analysis (PCA)
• Reduced models, through Galerkin approximations
• Dynamical Systems: to understand the dynamics
• Image processing
• Signal Analysis

Two main purposes:
• order reduction by projecting high-dimensional data in lower-dimensional space
• feature extraction by revealing relevant but unexpected structure hidden in the data
Main idea of KL decomposition

In plain words  Key idea of KL is to reduce a large number of interdependent variables to a much smaller number of uncorrelated variables while retaining as much as possible of the variation in the original data.

more precisely  Suppose we have an ensemble \( \{u_k\} \) of scalar fields, each being a function defined in \( (a, b) \subset \mathbb{R} \). We work in a Hilbert space \( L^2((a, b)) \).

We want to find a (orthonormal) basis \( \{\psi_n\}_{n=1}^\infty \) of \( L^2 \) that is optimal for the given data set in the sense that the finite dimensional representation of the form

\[
\hat{u}(x) = \sum_{k=1}^{\infty} a_k \psi_k(x)
\]

describes a typical member of the ensemble better than representations of the same dimension in any other basis.

The notion of typical implies the use of an average over the ensemble \( \{u_k\} \) and optimality means maximizing the average normalized projection of \( u \) onto \( \{\psi_n\}_{n=1}^\infty \).
The mathematical problem

Suppose, for simplicity, we have just one function $\psi$

$$\max_{\psi \in L^2} \frac{E(| < u, \psi > |^2)}{\|\psi\|^2}$$

This implies

$$J(\psi) = E(| < u, \psi > |^2) - \lambda(\|\psi\|^2 - 1)$$

$$\frac{d}{ds} J(\psi + \varepsilon \phi)|_{\varepsilon=0} = 0$$

$$\int_a^b R(x, y) \psi(y) dy = \lambda \psi(x)$$

with $R(x, y) = E(u(x)u(y))$
Construction of the KL basis

• Construct $R(x, y)$ from the data
• Solve the eigenvalue problem:

$$\int_D R(x, y) \psi(y) dy = \lambda \psi(x)$$

... to get the pair $(\lambda_i, \psi_i)$
• If $u$ is the field then the N-order approximation of it is

$$\hat{u}_N(t, x) = E(u(t, x)) + \sum_{i=1}^{N} a_i(t) \psi(x)$$

• To make predictions use the Galerkin method taking the $\psi$'s as trial functions
Galerkin projections

Suppose we have a dynamical system governed by

\[
\frac{\partial v}{\partial t} = A(v) \quad v \in (a, b) \times D \to \mathbb{R}^n
\]

\[
v(0, x) = v_0(x) \quad \text{initial condition}
\]

\[
B(v) = 0 \quad \text{boundary condition}
\]

The Galerkin method is a discretization scheme for PDE based on separation of variables.
One searches solutions in the form:

\[
\hat{v}(x) = \sum_{k=1}^{\infty} a_k \psi_k(x)
\]
Reduced equations

The reduced equation is obtained making the error of the approximation orthogonal to the first N KL elements of the basis.

\[
\begin{align*}
\text{errorequation}(t, x) &= \frac{\partial \hat{v}}{\partial t} - A(\hat{v}) \\
\text{errorinicond}(x) &= \hat{v}(0, x) - v_0(x) \\
< \text{errors}, \psi_i(x) > &= 0 \text{ for } i = 1, \ldots, N. \\
\frac{da_i}{dt}(t) &= \int_D A(\Sigma_{n=1}^N a_n(t)\psi_n(x))\psi_i(x)dx \text{ for } i = 1, \ldots, N \\
a_i(0) &= \int_D v_0(x)\psi_i(x)dx \text{ for } i = 1, \ldots, N
\end{align*}
\]
Computation of the KL basis: Direct method

In this method, the displacements of a dynamical system are measured or calculated at $N$ locations and labeled $u_1(t, x_1), u_2(t, x_2), \ldots, u_N(t, x_N)$. Sampling these displacements $M$ times, we can form the following $M \times N$ ensemble matrix:

$$U = \begin{bmatrix} u_1 & u_2 & \ldots & u_N \end{bmatrix} = \begin{bmatrix} u_1(t_1, x_1) & u_2(t_1, x_2) & \ldots & u_n(t_1, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(t_M, x_1) & u_2(t_M, x_2) & \ldots & u_n(t_M, x_N) \end{bmatrix}.$$  

Thus, the spatial correlation matrix of dimension $N \times N$ is formed as

$$\mathbf{R}_u = \frac{1}{M} U^T U.$$  

The PO modes are then given by the eigenvectors of $\mathbf{R}_u$. 

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Direct method

Algoritmo de implementação do método direto.
Algoritmo de implementação do método dos retratos.
Different guises of KL; basic ingredients

Sets:
- \( \mathcal{D} \subset \mathbb{R}^l \)
- \( \Omega \) space of events
- \( \mathbb{R}^n \) codomain of functions

\( L^2(\mathcal{D}, \mathbb{R}^n) \) is a Hilbert space of functions with inner product \( <, >_\mathcal{D} \) and associated norm \( \| \cdot \|_\mathcal{D} \). The elements of this space are deterministic functions.

\( (\Omega, \mathcal{F}, \mathbb{P}) \) is a probability space, \( \mathcal{F} \) is a sigma-algebra and \( \mathbb{P} \) a probability measure.

\( \omega \in \Omega \) is an event, that is a realization of a random function.

The mean value of a random variable \( X \) is \( E(|X|) = \int_\Omega X(z) d\mathbb{P}(z) \) with

\[
X : \quad \Omega \rightarrow \mathbb{R}^n \\
z \quad \mapsto \quad X(z)
\]

\( \Omega \) also has a Hilbert space structure, noted \( L^2(\Omega, \mathbb{R}^n) \), if we put the inner product \( <, >_\Omega = E(|XY|) \) and the associated norm is \( \| \cdot \|_\Omega \)
Basic ingredients of KL

In order to compute KL basis one needs two basic ingredients:

- a $L_2$ space of functions
- an averaging operator

In the literature we find mainly three main forms of KL decompositions. To understand their similarities and differences it is worth to think of the fields as defined in a cartesian product of two sets, that will provide the main ingredients we just mentioned

$$X : \mathcal{D} \times \Omega \rightarrow \mathbb{R}^n$$

$$(z, \omega) \mapsto X(z, \omega)$$

We have the following interpretation:

$X(z, .)$ is a random variable, that is, all possible realizations of a field for fixed $z \in \mathcal{D}$. We need the averaging operator to do statistics with this random variables, one for each $z \in \mathcal{D}$.

$X(., \omega)$ this is a realization of a field, hence a function of $L_2(\mathcal{D}, \mathbb{R}^n)$. Physical quantities are defined in terms of this field so we need the first structure.

$X(z, \omega)$ this is just an element of $\mathbb{R}^n$. 
Karhunen-Loève expansion: main hypothesis

Let us consider a random field \( \{X(z)\}_{z \in \mathcal{D}} \) defined on a probability space \((\Omega, \mathcal{F}, P)\)

\[
X : \mathcal{D} (\subset \mathbb{R}^l) \times \Omega \to \mathbb{R}^n
\]

\[
(z; \omega) \mapsto X(z; \omega)
\]

**Assumption I:** \( \{X(z)\}_{z \in \mathcal{D}} \) is a second-order random field i.e.

\[
E(\|X(z)\|^2) = E(<X(z), X(z)>) < \infty, \forall z \in \mathcal{D}
\]

\(E(.)\) denotes the ensemble average and \(<,>\) is the inner product in \(\mathbb{R}^n\).

**Assumption II:** \( \{X(z)\}_{z \in \mathcal{D}} \) is continuous in quadratic mean i.e.

\[
\|X(z + h) - X(z)\|_{L^2(\Omega, \mathbb{R}^n)}^2 \to 0 \text{ as } h \to 0.
\]
Under Assumption I and II

- \( \forall z \in \mathcal{D}, X(z) \in L^2(\Omega, \mathbb{R}^n) \) (with \( \langle Y_1, Y_2 \rangle_\Omega = E(\langle Y_1, Y_2 \rangle) \)).

- Second order moment characteristics:
  \[
  m_X(z) = E(X(z)) \\
  R_X(z_1, z_2) = E(X(z_1) \otimes X(z_2)) \\
  C_X(z_1, z_2) = E((X(z_1) - E(X(1))) \otimes (X(z_2) - E(X(z_2))))
  \]

- When the random field is mean zero valued, then \( C_X = R_X \). We will assume in the sequel that \( \{X(z)\}_{z \in \mathcal{D}} \) is a mean zero valued field.

- The correlation function \( C_X \) is continuous on \( \mathcal{D} \times \mathcal{D} \).
The self-adjoint operator

According to our assumptions, the integral operator,

\[ Q : \ L^2(D, \mathbb{R}^n) \rightarrow L^2(D, \mathbb{R}^n) \]

\[ \psi \mapsto (Q\psi)(z) = \int_D C_X(z, z')\psi(z')dz' , \]

with kernel \( C_X(z, z') \), defines a continuous self-adjoint Hilbert-Schmidt operator on the Hilbert space \( L^2(D, \mathbb{R}^n) \).
**Eigenvalues property:**

The operator $Q$ has a countable number of eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n \geq \cdots$, i.e.

$$(Q\psi_n)(z) = \lambda_n \psi_n(z)$$

where

$$\psi_1, \cdots, \psi_n, \cdots,$$

denote the associated eigenfunctions.

The set of eigenfunctions constitutes a orthonormal basis of $L^2(D, \mathbb{R}^n)$

$$<\psi_n, \psi_m>_D = \int_D <\psi_n(z), \psi_m(z)> dz = \delta_{nm}$$

where $<,>_D$ denotes the inner product in $L^2(D, \mathbb{R}^n)$ with the associated norm $\|\cdot\|_D$. 
**Karhunen-Loève Theorem**

The Karhunen-Loève theorem states that a continuous second-order random field can be expanded in a series of the eigenfunctions, \( \psi_n \), as

\[
X(z) = \sum_{n=1}^{\infty} \xi_n \psi_n(z) \quad \text{(in } L^2(\Omega, \mathbb{R}^n)) \]

where \( \xi_1, \xi_2, \ldots, \xi_n, \ldots \) are scalar uncorrelated random variables defined by

\[
\xi_n = \int_D < X(z), \psi_m(z) > \, dz
\]

with

\[
E(\xi_n \xi_m) = \lambda_n \delta_{nm} = \begin{cases} 
\lambda_n & \text{if } n = m \\
0 & \text{if } n \neq m 
\end{cases}
\]

The \( \{\psi_k\} \) are named the KL modes (also, Principal Orthogonal modes, POM).
Energy property

The eigenvalues, $\lambda_n$, of $Q$ are related to the mean “energy” of the random field according to the following relation

$$E(\|X\|^2_{\langle,\rangle_D}) = \sum_{n=1}^{\infty} \lambda_n.$$
Optimality property

The Karhunen-Loève expansion satisfies the following optimality property:

\[
E\left(\|X - \sum_{k=1}^{q} \xi_k \psi_k(z)\|^2_D\right) \leq E\left(\|X - \sum_{k=1}^{q} \tilde{\xi}_k \tilde{\psi}_k(z)\|^2_D\right)
\]

for any integer \(q\) and any arbitrary orthogonal basis \((\tilde{\psi}_k)_{k \geq 1}\) of \(L^2(D, \mathbb{R}^n)\) where \(\tilde{\xi}_1, \tilde{\xi}_2, \cdots, \tilde{\xi}_k, \cdots\) are scalar random variables given by

\[
\tilde{\xi}_k = \int_D <X(z), \psi_k(z)> \, dz
\]

It is optimal in the sense that given a fixed number \(q\) of modes, no other linear decomposition can contain as much energy as the KL expansion.
Summary: Karhunen-Loève Theorem

\( \{X(z)\}_{z \in \mathcal{D}} \) defined on a probability space \((\Omega, \mathcal{F}, P)\)

Covariance matrix function \( C_X(z_1, z_2) \)

\[
X(z; \omega) = \sum_{n=1}^{\infty} \xi_n(\omega) \psi_n(z) \text{ in } L^2(\Omega, \mathbb{R}^n)
\]

with

\[
\psi_n : \text{ eigenfunctions (} Q \psi)(z) = \int_{\mathcal{D}} C_X(z, z') \psi(z') dz'
\]

\[
\int_{\mathcal{D}} \langle \psi_n(z) \psi_m(z) \rangle dz = \begin{cases} 
1 & \text{if } n = m \\
0 & \text{if } n \neq m 
\end{cases} \text{ in } L^2(\mathcal{D}, \mathbb{R}^n)
\]

\[
\xi_n : \text{ scalar random variables } \xi_n(\omega) = \int_{\mathcal{D}} \langle X(z, \omega), \psi_m(z) \rangle dz
\]

\[
E(\xi_n \xi_m) = \begin{cases} 
\lambda_n & \text{if } n = m \\
0 & \text{if } n \neq m
\end{cases}
\]
Applications to Random Mechanics

In random mechanics, the random characteristics have often modeled using random fields \( \{u(z)\}_{z \in \mathcal{D}} \) where the domain \( \mathcal{D} \) is

- either \( \mathcal{D} = \mathcal{D}_x \subset \mathbb{R}^p \) (with \( p = 1, 2, \) or \( 3 \)) static problems
- or \( \mathcal{D} = \mathcal{D}_t \times \mathcal{D}_x \subset \mathbb{R} \times \mathbb{R}^p \) dynamics problems

Without loss of generality, we assume \( \mathcal{D}_t = [0, T] \) where \( T \in \mathbb{R}^+ \).

In order to find a flow model that still reveals the main features contained in the dynamics, one often searches for an expansion in the variables separated form

\[
  u(t, x) = \sum_{k=1}^{\infty} a_k(t) \phi_k(x)
\]

where \( \phi_k \) are deterministic \( \mathbb{R}^n \)-valued functions, and \( \{a_k(t)\}_{t \in \mathcal{D}_t} \) are scalar time random processes.

Let us see how to adapt the KL theory to these cases.


**Approach 1**

Apply the KL theorem to random field \{u(t, x)\}_{(t, x) \in \mathcal{D}} with covariance matrix function \(C_u(t_1, x_1, t_2, x_2)\)

\[
u(t, x; \omega) = \sum_{n=1}^{\infty} \xi_n(\omega)\psi_n(t, x) \text{ in } L^2(\Omega, \mathbb{R}^n)
\]

with

\[
\psi_n: \text{ eigenfunctions } (Q\psi)(t, x) = \int_{\mathcal{D}} C_X(t, x, t', x')\psi(t', x')dt' dx' \\
\int_{\mathcal{D}} \langle \psi_n(t, x)\psi_m(t, x) \rangle dt dx = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases} \text{ in } L^2(\mathcal{D}, \mathbb{R}^n)
\]

\[
\xi_n: \text{ scalar random variables } \xi_n(\omega) = \int_{\mathcal{D}} \langle X(t, x, \omega), \psi_m(t, x) \rangle dt dx \\
E(\xi_n\xi_m) = \begin{cases} \lambda_n & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}
\]
**Approach 2**

For fixed $t \in D_t$,

Apply the KL theorem to random field $\{u(t, x)\}_{x \in D_x}$

with the covariance matrix function $C_u(t, x_1, t, x_2)$

$$u(t, x; \omega) = \sum_{n=1}^{\infty} \xi_n(t, \omega) \psi_n(t, x) \text{ in } L^2(\Omega, \mathbb{R}^n)$$

with

$$\begin{cases} 
\psi_n(t, .) : \text{ eigenfunctions } (Q \psi)(x) = \int_{D_x} C_X(t, x, t, x') \psi(x') dx' \\
\int_{D_x} \langle \psi_n(t, x) \psi_m(t, x) \rangle dt dx = \begin{cases} 
1 & \text{ if } n = m \\
0 & \text{ if } n \neq m \end{cases} \text{ in } L^2(D, \mathbb{R}^n) \\
\xi_n(t, .) : \text{ scalar random variables } \xi_n(t, \omega) = \int_{D_x} \langle X(t, x, \omega), \psi_m(t, x) \rangle dx \\
E(\xi_n(t, .) \xi_m(t, .)) = \begin{cases} 
\lambda_n & \text{ if } n = m \\
0 & \text{ if } n \neq m \end{cases}
\end{cases}$$
Approach 3

$L^2([0, T] \times \Omega, \mathbb{R}^n)$ with $< Y, Z >_{[0, T] \times \Omega} = \mathcal{E}(< Y, Z >)$ with $\mathcal{E}(.) = \frac{1}{T} \int_0^T E(.) dt$.

Apply KL theorem the random field $\{u(., x)\}_{x \in \mathcal{D}_x}$ with the covariance matrix function $C_u(x, x') = \mathcal{E}(u(., x) \otimes u(., x'))$

$$u(x; t, \omega) = \sum_{n=1}^{\infty} \xi_n(t, \omega)\psi_n(x)$$

with

$$\begin{cases} 
\psi_n(.) : & \text{eigenfunctions } (Q\psi)(x) = \int_{\mathcal{D}_x} C_u(x, x')\psi(x')dx' \\
\int_{\mathcal{D}_x} <\psi_n(x)\psi_m(x)> dx = \begin{cases} 1 & \text{if } n = m \\
0 & \text{if } n \neq m \end{cases} \text{ in } L^2(\mathcal{D}_x, \mathbb{R}^n) \\
\xi_n : & \text{scalar random processes } \xi_n(t, \omega) = \int_{\mathcal{D}_x} <u(t, x, \omega)\psi_m(x)> dx \\
\mathcal{E}(\xi_n\xi_m) = \begin{cases} \lambda_n & \text{if } n = m \\
0 & \text{if } n \neq m \end{cases} \text{ in } L^2([0, T] \times \Omega, \mathbb{R})
\end{cases}$$
Approach 3: discrete case, random process: \( \{u(t)\}_{[0,T]} \)

\[
\begin{align*}
  u &: [0,T] \times \Omega \to \mathbb{R}^n \\
  (t,\omega) &\mapsto u(t;\omega)
\end{align*}
\]

\( L^2([0,T] \times \Omega, \mathbb{R}^n) \) with \( <Y,Z>_{[0,T] \times \Omega} = \mathcal{E}(<Y,Z>) \) with \( \mathcal{E}(\cdot) = \frac{1}{T} \int_0^T E(\cdot) dt \).

Covariance matrix \( \mathcal{C}_u = \mathcal{E}(u(\cdot)u(\cdot)^T) \)

\[ u(t,\omega) = \sum_{n=1}^{\infty} \xi_n(t,\omega)\psi_n \]

\[
\begin{align*}
  \psi_n &\text{: eigenvectors } \mathcal{C}_u \psi_n = \lambda_n \psi_n \\
  \psi_n\psi_m^T = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases} \text{ in } \mathbb{R}^n
\end{align*}
\]

\[
\begin{align*}
  \xi_n &\text{: scalar random processes } \xi_n(t,\omega) = <u(t,\omega)\psi_m> \\
  \mathcal{E}(\xi_n\xi_m) = \begin{cases} \lambda_n & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases} \text{ in } L^2([0,T] \times \Omega, \mathbb{R})
\end{align*}
\]
Some remarks

1. The existence of the Karhunen-Loève expansion as described in approach 3 does not require any assumption on stationarity and ergodicity properties.

2. The Karhunen-Loève expansion as described in approach 3 usually depends on the time parameter $T$.

3. If the random field $\{u(t, x)\}_{(t, x) \in \mathcal{D}_t \times \mathcal{D}_x}$ is weakly stationary with respect to the time variable, $(C_u(t, x, t', x') = C_u(t - t', x, x'))$ then approach 2 and approach 3 give the same results. Moreover, the KL expansion does not depend on the time parameter $T$. 
**KL modes and Equivalent linear system**

Let us consider the discrete nonlinear case: \( U(t) \in \mathbb{R}^n \)

\[
M\ddot{U}(t) + C\dot{U}(t) + F(U(t)) = Bw(t)
\]

where \( \{w(t)\}_t \) is a Gaussian white noise process
\( \{U(t)\} \): stationary process

Then, the KL modes of the stationary nonlinear response coincide with the KL modes of the stationary response of the associated equivalent linear system given by the true stochastic linearization method:

\[
M\ddot{U}(t) + C\dot{U}(t) + K_{eq}U(t) = Bw(t)
\]

where \( K_{eq} \) minimizes

\[
E((F(U) - KU)^T(F(U) - KU))
\]
How to compute the PO modes?

The techniques to estimate the covariance function of a random field depends on its properties. If the random field is non-stationary, there is a general method for estimating its second-moment characteristics that assumes several realizations of the random field are available.

If the random field is weakly stationary with respect to the time variable, there is a method for estimating $C_u(x_1, x_2)$ based on a single realization of the random field. Two methods can be used to compute de PO modes:
- Direct method
- Snapshot method
Vibro-impact beam

Some results are presented here obtained from simulated data generated from a mathematical model of a linear clamped beam impacting a flexible barrier.
Simulation of the experiment

\[ EI \frac{\partial^4 w(x, t)}{\partial x^4} + \rho A \frac{\partial^2 w(x, t)}{\partial t^2} = F_f(t) \delta(x - x_f) + \sum_{i=1}^{N} F_b(w(x_{ci}, t)) \delta(x - x_{ci}) \]

- Ten mode shapes of the associated linear system

\[ \hat{w}(x, t) = \sum_{i=1}^{10} q_i(t) \phi_i(x) \]

- Galerkin method (10 DOF)

\[ \ddot{Q} + [2\omega_i \tau_i] \dot{Q} + [\omega_i^2] Q + F_{ci}(Q) = BF_f(t) \]

where modal damping were added to the discretized model.
Comparison between PO modes $\psi_i$ and linear modes $\phi_i$

The first two KLs significantly differs from the first two mode shapes reflecting the influence of the barrier upon the system.
Reduced-order model formulation:

From the PO modes \( \psi_i \), we have construct a reduced model.

\[
EI \frac{\partial^4 w(x, t)}{\partial x^4} + \rho A \frac{\partial^2 w(x, t)}{\partial t^2} = F_f(t) \delta (x - x_f) + \sum_{i=1}^{N} F_b(w(x_{ci}, t)) \delta (x - x_{ci}),
\]

- \( n \) KL modes with \((1 \leq n \leq 10)\)

\[
\hat{w}(x, t) = \sum_{i=1}^{n} a_i(t) \psi_i(x)
\]

- Galerkin method \((n \text{ DOF})\)

\[
\ddot{A} + [2\omega_i \tau_i] \dot{A} + F_{KL}(A) = B_{KL} F_f(t)
\]

where same modal damping were added to the discretized model.
This figure presents a comparison between the original and the reduced-order models constructed with 5 and 10 PO modes.

The result is clearly not as good as expected and the full reduced-order model is not yet capable of reproducing the original response. A probable explanation for this result is that the use of the modal damping ratios for the first and second KLMs is inappropriate as they are physically different.
Concluding remarks

- In order to use the KL theory to expand a random field in the variables separated (time-random variables and spatial variable), it is necessary to use the adequate spatial covariance function.
- The use of the PO modes to develop the reduced-order model in the presence of damping may not be robust.