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The Karhunen-Loéve Expansion

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The Karhunen-Loéve Expansion

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Abstract

We're trying to understand the math behind the Karhunen-Loéve expansion, and these are the notes we're taking along the way.

Contents

List of Figures

1. Statement of the Karhunen-Loéve expansion

Let $\{X(t)\}_{t\in[t_0,\ t_f]}$, be a real-valued stochastic process. That is, for each $\tau \in [t_0,\ t_f]$, $X(\tau)$ is a real-valued random variable.

Also, let us denote the expected value of $X(\tau)$, $\mathbb{E}[X(\tau)]$, by $\mu_X(\tau)$, for each $\tau \in [t_0,\ t_f]$.

Then, the Karhunen-Loéve theorem [1–5] states that $X(t)$ can be written as:

$$X(t) = \mu_X(t) + \sum_{k=1}^{\infty} Z_k e_k(t),\ \forall\, t \in [t_0,\ t_f]. \tag{1.1}$$

The $\{Z_k\}$s above are "zero mean, pairwise uncorrelated" real-valued random variables. That is, we have:

$$\mathbb{E}[Z_k] = 0,\ \forall\, k \in \mathbb{Z}_+,\ \text{and} \tag{1.2}$$

$$\mathbb{E}[Z_{k_1} Z_{k_2}] = 0 \text{ whenever } k_1 \neq k_2,\ \forall\, k_1, k_2 \in \mathbb{Z}_+, \tag{1.3}$$

where $\mathbb{Z}_+$ denotes the set of positive integers.

Also, the $\{e_k\}$s in Eq. (1.1) are "orthonormal". That is,

$$\int_{\tau=t_0}^{t_f} e_{k_1}(\tau)\, e_{k_2}(\tau)\, d\tau = \delta_{k_1 k_2},\ \forall\, k_1, k_2 \in \mathbb{Z}_+, \tag{1.4}$$

where $\delta_{k_1 k_2}$ denotes the Kronecker delta:

$$\delta_{k_1 k_2} \triangleq \begin{cases} 1, \text{ if } k_1 = k_2, \text{ and} \\ 0, \text{ otherwise,} \end{cases},\ \forall\, k_1, k_2 \in \mathbb{Z}_+. \tag{1.5}$$

2. Proof of the Karhunen-Loéve expansion

2.1 Proof strategy

Proving the Karhunen-Loéve expansion requires several pre-requisites. These include, (1) an understanding of the fundamentals of continuous stochastic processes, including the autocorrelation function and its properties such as symmetry and positive-semidefiniteness, the Hilbert-Schmidt integral operator and its properties such as linearity and self-adjointness, eigen-analysis of the Hilbert-Schmidt integral operator and some properties of the associated eigenvalues and eigenvectors, *etc.*, (2) the spectral theorem and various observations that can be made by applying it to the Hilbert-Schmidt integral operator, and (3) Mercer's theorem.

We haven't understood all these pre-requisites yet. For example, while we have learned about continuous stochastic processes and their properties, we still don't know how to prove the spectral theorem or Mercer's theorem. These are topics that require advanced courses in real analysis and abstract algebra.

So, while we have a good grasp of some pre-requisites, we're forced to take others on faith. So, in subsequent sections, we're going to prove some lemmas and theorems leading up to the Karhunen-Loéve expansion, but we're going to leave others without proof. Over time, as we learn more, we'll try and fill in the blanks. But until then, the proof below will necessarily be incomplete.

2.2 Some facts about continuous stochastic processes

2.2.1 The autocorrelation function R_X

We define the autocorrelation function $R_X(t_1,\ t_2)$ of the stochastic process $X(t)$ as follows:

$$\begin{aligned}
R_X(t_1,\ t_2) &\triangleq \mathbb{E}[(X(t_1) - \mu_X(t_1))(X(t_2) - \mu_X(t_2))] \\
&= \mathbb{E}[X(t_1)X(t_2) - X(t_1)\mu_X(t_2) - \mu_X(t_1)X(t_2) + \mu_X(t_1)\mu_X(t_2)] \\
&= \mathbb{E}[X(t_1)X(t_2)] - \mathbb{E}[X(t_1)\mu_X(t_2)] - \mathbb{E}[\mu_X(t_1)X(t_2)] + \mathbb{E}[\mu_X(t_1)\mu_X(t_2)] \\
&= \mathbb{E}[X(t_1)X(t_2)] - \mu_X(t_2)\mathbb{E}[X(t_1)] - \mu_X(t_1)\mathbb{E}[X(t_2)] + \mu_X(t_1)\mu_X(t_2)
\end{aligned}$$

$$
\begin{aligned}
&= \mathbb{E}[X(t_1)X(t_2)] - \mu_X(t_2)\mu_X(t_1) - \mu_X(t_1)\mu_X(t_2) + \mu_X(t_1)\mu_X(t_2) \\
&= \mathbb{E}[X(t_1)X(t_2)] - \mu_X(t_1)\mu_X(t_2),\ \forall\, t_1,\ t_2 \in [t_0,\ t_f].
\end{aligned} \tag{2.1}
$$

Theorem 2.2.1. *The autocorrelation function R_X is symmetric. That is, for any $t_1,\ t_2 \in [t_0,\ t_f]$, we have:*

$$
R_X(t_1,\ t_2) = R_X(t_2,\ t_1). \tag{2.2}
$$

Proof. Follows from the definition above. □

Theorem 2.2.2. *The autocorrelation function R_X is positive-semidefinite [6, 7]. That is, for any real-valued function $f:\ [t_0,\ t_f] \to \mathbb{R}$, we have:*

$$
\int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} f(\tau_1)\ R_X(\tau_1,\ \tau_2)\ f(\tau_2)\ d\tau_1\ d\tau_2\ \geq\ 0. \tag{2.3}
$$

Proof. We have:

$$
\begin{aligned}
0 &\leq \mathbb{E}\left[\left(\int_{\tau=t_0}^{t_f} f(\tau)\ (X(\tau) - \mu_X(\tau))\ d\tau \right)^2 \right] \\
&= \mathbb{E}\left[\left(\int_{\tau=t_0}^{t_f} f(\tau)\ (X(\tau) - \mu_X(\tau))\ d\tau \right) \left(\int_{\tau=t_0}^{t_f} f(\tau)\ (X(\tau) - \mu_X(\tau))\ d\tau \right) \right] \\
&= \mathbb{E}\left[\left(\int_{\tau_1=t_0}^{t_f} f(\tau_1)\ (X(\tau_1) - \mu_X(\tau_1))\ d\tau_1 \right) \left(\int_{\tau_2=t_0}^{t_f} f(\tau_2)\ (X(\tau_2) - \mu_X(\tau_2))\ d\tau_2 \right) \right] \\
&= \mathbb{E}\left[\int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} f(\tau_1)\ f(\tau_2)\ (X(\tau_1) - \mu_X(\tau_1))\ (X(\tau_2) - \mu_X(\tau_2))\ d\tau_1\ d\tau_2 \right] \\
&= \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} \mathbb{E}\left[\ f(\tau_1)\ f(\tau_2)\ (X(\tau_1) - \mu_X(\tau_1))\ (X(\tau_2) - \mu_X(\tau_2))\ \right]\ d\tau_1\ d\tau_2 \\
&= \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} f(\tau_1)\ f(\tau_2)\ \mathbb{E}\left[\ (X(\tau_1) - \mu_X(\tau_1))\ (X(\tau_2) - \mu_X(\tau_2))\ \right]\ d\tau_1\ d\tau_2 \\
&= \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} f(\tau_1)\ f(\tau_2)\ R_X(\tau_1,\ \tau_2)\ d\tau_1\ d\tau_2 \\
&= \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} f(\tau_1)\ R_X(\tau_1,\ \tau_2)\ f(\tau_2)\ d\tau_1\ d\tau_2.
\end{aligned}
$$

□

2.2.2 The Hilbert-Schmidt integral operator $\mathcal{H}_X$

Based on the autocorrelation function R_X, we define an operator $\mathcal{H}_X$, called the Hilbert-Schmidt integral operator [8].

This operator acts on a real-valued function $f:\ [t_0,\ t_f] \to \mathbb{R}$, and as a result produces another real-valued function $g:\ [t_0,\ t_f] \to \mathbb{R}$.

The relationship between the functions f and g is given by:

$$g(t) = \mathcal{H}_X(f)|_t \triangleq \int_{\tau=t_0}^{t_f} R_X(t,\tau)\ f(\tau)\ d\tau \tag{2.4}$$

Theorem 2.2.3. *$\mathcal{H}_X$ is additive. That is, for any two functions f_1 and f_2 where $f_1,\ f_2:\ [t_0,\ t_f] \to \mathbb{R}$, we have:*

$$\mathcal{H}_X(f_1 + f_2) = \mathcal{H}_X(f_1) + \mathcal{H}_X(f_2). \tag{2.5}$$

Proof. Follows from the definition in Eq. (2.4). □

Theorem 2.2.4. *$\mathcal{H}_X$ is homogeneous. That is, for every function $f:\ [t_0,\ t_f] \to \mathbb{R}$, and for every scalar $\alpha \in \mathbb{R}$, we have:*

$$\mathcal{H}_X(\alpha f) = \alpha \mathcal{H}_X(f). \tag{2.6}$$

Proof. Follows from the definition in Eq. (2.4). □

Remark 2.2.1. *Because $\mathcal{H}_X$ is both additive and homogeneous, it is said to be “linear”.*

2.2.3 Eigenvalues and eigenfunctions of $\mathcal{H}_X$

We define λ to be an “eigenvalue” of $\mathcal{H}_X$ if there exists a function $e_\lambda:\ [t_0,\ t_f] \to \mathbb{R}$ (called the “eigenfunction” associated with λ), such that:

$$\mathcal{H}_X(e_\lambda) = \lambda\ e_\lambda. \tag{2.7}$$

That is, we have:

$$\int_{\tau=t_0}^{t_f} R_X(t,\tau)\ e_\lambda(\tau)\ d\tau = \lambda\ e_\lambda(t),\ \forall\ t \in [t_0,\ t_f]. \tag{2.8}$$

The pair (λ, e_λ) above is called an “eigenpair” of $\mathcal{H}_X$.

Theorem 2.2.5. *All eigenvalues of $\mathcal{H}_X$ are non-negative.*

Proof. Let (λ, e_λ) be an eigenpair of $\mathcal{H}_X$. Then, we have:

$$
\begin{aligned}
& \int_{\tau=t_0}^{t_f} R_X(t,\tau)\, e_\lambda(\tau)\, d\tau = \lambda\, e_\lambda(t),\ \forall\, t \in [t_0,\ t_f], \text{ by Eq. (2.8)}, \\
\Longrightarrow & \int_{\tau_2=t_0}^{t_f} R_X(t,\tau_2)\, e_\lambda(\tau_2)\, d\tau_2 = \lambda\, e_\lambda(t),\ \forall\, t \in [t_0,\ t_f], \\
\Longrightarrow & \int_{\tau_2=t_0}^{t_f} R_X(\tau_1,\tau_2)\, e_\lambda(\tau_2)\, d\tau_2 = \lambda\, e_\lambda(\tau_1),\ \forall\, \tau_1 \in [t_0,\ t_f], \\
\Longrightarrow & \int_{\tau_1=t_0}^{t_f} e_\lambda(\tau_1) \int_{\tau_2=t_0}^{t_f} R_X(\tau_1,\tau_2)\, e_\lambda(\tau_2)\, d\tau_2\, d\tau_1 = \int_{\tau_1=t_0}^{t_f} e_\lambda(\tau_1)\, \lambda\, e_\lambda(\tau_1)\, d\tau_1, \\
\Longrightarrow & \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} e_\lambda(\tau_1)\, R_X(\tau_1,\tau_2)\, e_\lambda(\tau_2)\, d\tau_1\, d\tau_2 = \lambda \int_{\tau_1=t_0}^{t_f} e_\lambda(\tau_1)^2\, d\tau_1, \\
\Longrightarrow & \lambda \underbrace{\int_{\tau_1=t_0}^{t_f} e_\lambda(\tau_1)^2\, d\tau_1}_{\geq 0} \geq 0, \text{ by the positive-semidefiniteness of } R_X \text{ (Theorem 2.2.2)} \\
\Longrightarrow & \lambda \geq 0.
\end{aligned}
$$

□

Theorem 2.2.6. *Eigenfunctions of $\mathcal{H}_X$ that correspond to distinct eigenvalues are orthogonal. That is, if $(\lambda_1, e_{\lambda_1})$ and $(\lambda_2, e_{\lambda_2})$ are eigenpairs of $\mathcal{H}_X$, and $\lambda_1 \neq \lambda_2$, then we have:*

$$
\int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau = 0. \tag{2.9}
$$

Proof. We have:

$$
\begin{aligned}
& (\lambda_1 - \lambda_2) \left[\int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau \right] \\
= & \left[\lambda_1 \int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau \right] - \left[\lambda_2 \int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau \right] \\
= & \left[\int_{\tau=t_0}^{t_f} \lambda_1\, e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau \right] - \left[\int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, \lambda_2\, e_{\lambda_2}(\tau)\, d\tau \right] \\
= & \left[\int_{t=t_0}^{t_f} \underbrace{\lambda_1\, e_{\lambda_1}(t)}_{\text{Apply Eq. (2.8)}}\, e_{\lambda_2}(t)\, dt \right] - \left[\int_{t=t_0}^{t_f} e_{\lambda_1}(t)\, \underbrace{\lambda_2\, e_{\lambda_2}(t)}_{\text{Apply Eq. (2.8)}}\, dt \right] \\
= & \left[\int_{t=t_0}^{t_f} \int_{\tau=t_0}^{t_f} R_X(t,\tau)\, e_{\lambda_1}(\tau)\, d\tau\, e_{\lambda_2}(t)\, dt \right] - \left[\int_{t=t_0}^{t_f} e_{\lambda_1}(t) \int_{\tau=t_0}^{t_f} R_X(t,\tau)\, e_{\lambda_2}(\tau)\, d\tau\, dt \right] \\
= & \left[\int_{t=t_0}^{t_f} \int_{\tau=t_0}^{t_f} R_X(t,\tau)\, e_{\lambda_1}(\tau)\, e_{\lambda_2}(t)\, dt\, d\tau \right] - \left[\int_{t=t_0}^{t_f} \int_{\tau=t_0}^{t_f} e_{\lambda_1}(t)\, R_X(t,\tau)\, e_{\lambda_2}(\tau)\, dt\, d\tau \right] \\
= & \left[\int_{\tau_1=t_0}^{t_f} \int_{\tau=t_0}^{t_f} R_X(\tau_1,\tau)\, e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau_1)\, d\tau_1\, d\tau \right] - \left[\int_{\tau_2=t_0}^{t_f} \int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau_2)\, R_X(\tau_2,\tau)\, e_{\lambda_2}(\tau)\, d\tau_2\, d\tau \right] \\
= & \left[\int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} R_X(\tau_1,\tau_2)\, e_{\lambda_1}(\tau_2)\, e_{\lambda_2}(\tau_1)\, d\tau_1\, d\tau_2 \right] - \left[\int_{\tau_2=t_0}^{t_f} \int_{\tau_1=t_0}^{t_f} e_{\lambda_1}(\tau_2)\, R_X(\tau_2,\tau_1)\, e_{\lambda_2}(\tau_1)\, d\tau_2\, d\tau_1 \right]
\end{aligned}
$$

$$= \left[\int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} e_{\lambda_2}(\tau_1)\, R_X(\tau_1,\tau_2)\, e_{\lambda_1}(\tau_2)\, d\tau_1\, d\tau_2 \right] - \left[\int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} e_{\lambda_2}(\tau_1)\, R_X(\tau_2,\tau_1)\, e_{\lambda_1}(\tau_2)\, d\tau_1\, d\tau_2 \right]$$

$$= \int_{\tau_1=t_0}^{t_f} \int_{\tau_2=t_0}^{t_f} e_{\lambda_2}(\tau_1) \underbrace{[R_X(\tau_1,\tau_2) - R_X(\tau_2,\tau_1)]}_{=\,0,\text{ by the symmetry of } R_X \text{ (Theorem 2.2.1)}} e_{\lambda_1}(\tau_2)\, d\tau_1\, d\tau_2$$

$$= 0.$$

$$\implies \text{Either } \underbrace{(\lambda_1 - \lambda_2) = 0}_{\text{Not possible because } \lambda_1 \neq \lambda_2}, \text{ or } \underbrace{\left[\int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau \right] = 0}_{\text{Only possibility}}.$$

$$\implies \int_{\tau=t_0}^{t_f} e_{\lambda_1}(\tau)\, e_{\lambda_2}(\tau)\, d\tau = 0.$$

□

2.2.4 Self-adjointness of $\mathcal{H}_X$

For any two functions f and g, where $f,\ g:\ [t_0,\ t_f] \to \mathbb{R}$, we define the "inner product" of f and g, denoted by $\langle f,\ g\rangle$, to be:

$$\langle f,\ g\rangle \triangleq \int_{\tau=t_0}^{t_f} f(\tau)\, g(\tau)\, d\tau. \tag{2.10}$$

Theorem 2.2.7. *$\mathcal{H}_X$ is a self-adjoint operator. That is, for any two functions f and g where $f,\ g:$ $[t_0,\ t_f] \to \mathbb{R}$, we have:*

$$\langle f,\ \mathcal{H}_X(g)\rangle = \langle \mathcal{H}_X(f),\ g\rangle \tag{2.11}$$

Proof. We have:

$$\begin{aligned}
\langle f,\ \mathcal{H}_X(g)\rangle &= \int_{\tau=t_0}^{t_f} f(\tau)\, \mathcal{H}_X(g)(\tau)\, d\tau, \text{ from Eq. (2.10)} \\
&= \int_{\tau=t_0}^{t_f} f(\tau) \int_{t=t_0}^{t_f} R_X(\tau,\ t)\, g(t)\, dt\, d\tau, \text{ from Eq. (2.4)} \\
&= \int_{\tau=t_0}^{t_f} \int_{t=t_0}^{t_f} f(\tau)\, R_X(\tau,\ t)\, g(t)\, dt\, d\tau, \\
&= \int_{t=t_0}^{t_f} g(t) \int_{\tau=t_0}^{t_f} \underbrace{R_X(\tau,\ t)}_{=\,R_X(t,\ \tau),\text{ by symmetry of } R_X \text{ (Theorem 2.2.1)}} f(\tau)\, d\tau\, dt, \\
&= \int_{t=t_0}^{t_f} g(t) \underbrace{\int_{\tau=t_0}^{t_f} R_X(t,\ \tau)\, f(\tau)\, d\tau}_{=\,\mathcal{H}_X(f)(t),\text{ by Eq. (2.4)}} dt, \\
&= \int_{t=t_0}^{t_f} \mathcal{H}_X(f)(t)\, g(t)\, dt,
\end{aligned}$$

$= \langle \mathcal{H}_X(f),\ g\rangle$, by Eq. (2.10).

□

2.3 The spectral theorem

From Theorem 2.2.7, we know that $\mathcal{H}_X$ is a self-adjoint operator. More specifically, $\mathcal{H}_X$ is a *compact* self-adjoint operator *on a Hilbert space* [9, 10]. We don't know exactly what the word "compact" means, and we also don't know what a Hilbert space is. Understanding the proper meanings of these terms requires taking graduate-level courses in real analysis and abstract algebra, which we don't have time for at the moment. So, we're just taking these facts on faith for the time-being.

Theorem 2.3.1 (Spectral theorem)**.** *Given a compact self-adjoint operator $\mathcal{H}_X$ on a Hilbert space, there exists an orthonormal basis of eigenvectors of $\mathcal{H}_X$ that span the space.*

Proof. We think the proof is well beyond our scope at this time. To learn the proof, some useful resources to consult include [11–16]. □

The spectral theorem tells us the following:

Observation 2.3.1. *We can find a countable set of eigenpairs $\{(\lambda_k, e_{\lambda_k})\}_{k\in\mathbb{Z}_+}$ of $\mathcal{H}_X$.*

Observation 2.3.2. *By Theorem 2.2.5, all the λ_ks above will be non-negative.*

Observation 2.3.3. *Without loss of generality, we can assume that the λ_ks above are in descending order.*

Observation 2.3.4. *We have:*

$$\lim_{k\to\infty} \lambda_k = 0. \tag{2.12}$$

Observation 2.3.5. *By the orthonormality of the e_{λ_k}s, we have:*

$$\langle e_{\lambda_{k_1}},\ e_{\lambda_{k_2}}\rangle = \int_{t=t_0}^{t_f} e_{\lambda_{k_1}}(t)\, e_{\lambda_{k_2}}(t)\, dt = \delta_{k_1 k_2},\ \forall\, k_1,\ k_2 \in \mathbb{Z}_+. \tag{2.13}$$

Observation 2.3.6. *Because each e_{λ_k} above is an eigenvector of $\mathcal{H}_X$, with eigenvalue λ_k, we have the following from Eqs. 2.7 and 2.8:*

$$\mathcal{H}_X\left(e_{\lambda_k}\right) = \lambda_k\, e_{\lambda_k},\ \forall\, k \in \mathbb{Z}_+,\ \text{and} \tag{2.14}$$

$$\begin{aligned}\mathcal{H}_X\left(e_{\lambda_k}\right)(t) &= \int_{\tau=t_0}^{t_f} R_X(t,\tau)\, e_{\lambda_k}(\tau)\, d\tau \\ &= \lambda_k\, e_{\lambda_k}(t),\ \forall\, t \in [t_0,\ t_f],\ \forall\, k \in \mathbb{Z}_+.\end{aligned} \tag{2.15}$$

Observation 2.3.7. *Because the e_{λ_k}s span the space of functions, we can write any function $f:\ [t_0,\ t_f] \to \mathbb{R}$ as a linear combination of the e_{λ_k}s. That is, given any such function f, we can find coefficients $\{c_k\}_{k\in\mathbb{Z}_+}$ such that:*

$$f = \sum_{k=1}^{\infty} c_k e_{\lambda_k}, \text{ or} \tag{2.16}$$

$$f(t) = \sum_{k=1}^{\infty} c_k e_{\lambda_k}(t),\ \forall\, t \in [t_0,\ t_f]. \tag{2.17}$$

Observation 2.3.8. *Based on the linear combination above, the result of applying the $\mathcal{H}_X$ operation on any function $f:\ [t_0,\ t_f] \to \mathbb{R}$ can be written as:*

$$\begin{aligned}
\mathcal{H}_X(f) &= \mathcal{H}_X\left(\sum_{k=1}^{\infty} c_k\, e_{\lambda_k}\right), \text{ from Eq. (2.16)} \\
&= \sum_{k=1}^{\infty} c_k\, \mathcal{H}_X\left(e_{\lambda_k}\right), \text{ from the linearity of } \mathcal{H}_X \text{ (Theorems 2.2.3, 2.2.4)} \\
&= \sum_{k=1}^{\infty} c_k\, \lambda_k\, e_{\lambda_k}, \text{ from Eq. (2.14), or} && (2.18) \\
\mathcal{H}_X(f)(t) &= \sum_{k=1}^{\infty} c_k\, \lambda_k\, e_{\lambda_k}(t),\ \forall\, t \in [t_0,\ t_f]. && (2.19)
\end{aligned}$$

2.4 Mercer's theorem

Theorem 2.4.1 (Mercer's theorem)**.** *The autocorrelation function R_X can be written as:*

$$R_X(t_1, t_2) = \sum_{k=1}^{\infty} \lambda_k\, e_{\lambda_k}(t_1)\, e_{\lambda_k}(t_2),\ \forall\, t_1,\ t_2 \in [t_0,\ t_f]. \tag{2.20}$$

Proof. We don't know the proof of this theorem yet, because it involves learning about various convergence criteria such as absolute convergence, uniform convergence, *etc*. But we're working on it. Once we understand the proof, we'll put it in here. Some useful resources to consult include [10, 17, 18]. □

2.5 Finally, the Karhunen-Loéve expansion

From the stochastic process $\{X(t)\}_{t\in[t_0,\ t_f]}$, we define the random variables $\{Z_k\}_{k\in\mathbb{Z}_+}$ as follows:

$$Z_k \triangleq \int_{t=t_0}^{t_f} \left(X(t) - \mu_X(t)\right) e_{\lambda_k}(t)\, dt,\ \forall\, k \in \mathbb{Z}_+. \tag{2.21}$$

The e_{λ_k}s above are, of course, the eigenvectors of $\mathcal{H}_X$ discussed in §2.3.

Theorem 2.5.1. *The Z_ks above are all zero-mean random variables.*

Proof. We have:

$$\begin{aligned}
\mathbb{E}\left[Z_k\right] &= \mathbb{E}\left[\int_{t=t_0}^{t_f} \left(X(t) - \mu_X(t)\right) e_{\lambda_k}(t)\, dt\right], \text{ from Eq. (2.21)} \\
&= \int_{t=t_0}^{t_f} \mathbb{E}\left[X(t) - \mu_X(t)\right]\, e_{\lambda_k}(t)\, dt, \\
&= \int_{t=t_0}^{t_f} \left(\mathbb{E}\left[X(t)\right] - \mu_X(t)\right)\, e_{\lambda_k}(t)\, dt, \\
&= \int_{t=t_0}^{t_f} \left(\mu_X(t) - \mu_X(t)\right)\, e_{\lambda_k}(t)\, dt, \\
&= 0, \ \forall\, k \in \mathbb{Z}_+.
\end{aligned} \tag{2.22}$$

□

Theorem 2.5.2. *The Z_ks above are all pairwise-uncorrelated.*

Proof. We have:

$$\begin{aligned}
\mathbb{E}\left[Z_{k_1} Z_{k_2}\right] &= \mathbb{E}\left[\left(\int_{t=t_0}^{t_f} \left(X(t) - \mu_X(t)\right) e_{\lambda_{k_1}}(t)\, dt\right)\left(\int_{t=t_0}^{t_f} \left(X(t) - \mu_X(t)\right) e_{\lambda_{k_2}}(t)\, dt\right)\right], \text{ from Eq. (2.21)} \\
&= \mathbb{E}\left[\left(\int_{t_1=t_0}^{t_f} \left(X(t_1) - \mu_X(t_1)\right) e_{\lambda_{k_1}}(t_1)\, dt_1\right)\left(\int_{t_2=t_0}^{t_f} \left(X(t_2) - \mu_X(t_2)\right) e_{\lambda_{k_2}}(t_2)\, dt_2\right)\right] \\
&= \mathbb{E}\left[\int_{t_1=t_0}^{t_f}\int_{t_2=t_0}^{t_f} \left(X(t_1) - \mu_X(t_1)\right) e_{\lambda_{k_1}}(t_1) \left(X(t_2) - \mu_X(t_2)\right) e_{\lambda_{k_2}}(t_2)\, dt_1\, dt_2\right] \\
&= \int_{t_1=t_0}^{t_f}\int_{t_2=t_0}^{t_f} \mathbb{E}\left[\left(X(t_1) - \mu_X(t_1)\right)\left(X(t_2) - \mu_X(t_2)\right)\right] e_{\lambda_{k_1}}(t_1)\, e_{\lambda_{k_2}}(t_2)\, dt_1\, dt_2 \\
&= \int_{t_1=t_0}^{t_f}\int_{t_2=t_0}^{t_f} R_X(t_1, t_2)\, e_{\lambda_{k_1}}(t_1)\, e_{\lambda_{k_2}}(t_2)\, dt_1\, dt_2, \text{ from Eq. (2.1)} \\
&= \int_{t_1=t_0}^{t_f} e_{\lambda_{k_1}}(t_1) \left[\int_{t_2=t_0}^{t_f} R_X(t_1, t_2)\, e_{\lambda_{k_2}}(t_2)\, dt_2\right] dt_1 \\
&= \int_{t_1=t_0}^{t_f} e_{\lambda_{k_1}}(t_1)\ \left[\mathcal{H}_X(e_{\lambda_{k_2}})(t_1)\right] dt_1, \text{ from Eq. (2.4)} \\
&= \int_{t_1=t_0}^{t_f} e_{\lambda_{k_1}}(t_1)\ \left[\lambda_{k_2}\, e_{\lambda_{k_2}}(t_1)\right] dt_1, \text{ from Eq. (2.14)} \\
&= \lambda_{k_2} \int_{t_1=t_0}^{t_f} e_{\lambda_{k_1}}(t_1)\, e_{\lambda_{k_2}}(t_1)\, dt_1 \\
&= \lambda_{k_2}\, \delta_{k_1 k_2} \text{ (from Observation 2.3.5)}, \ \forall\, k_1,\ k_2 \in \mathbb{Z}_+.
\end{aligned} \tag{2.23}$$

□

Theorem 2.5.3 (The Karhunen-Loéve theorem)**.** *The stochastic process* $\{X(t)\}_{t\in[t_0,\ t_f]}$ *can be written in terms of the random variables* $\{Z_k\}_{k\in\mathbb{Z}_+}$*, as follows:*

$$X(t) = \mu_X(t) + \sum_{k=1}^{\infty} Z_k e_{\lambda_k}(t),\ \forall\, t \in [t_0,\ t_f]. \tag{2.24}$$

This is true in the following sense:

$$\lim_{N\to\infty} \mathbb{E}\left[\left(X(t) - \left(\mu_X(t) + \sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)\right)^2\right] = 0,\ \forall\, t \in [t_0,\ t_f]. \tag{2.25}$$

Proof. We have:

$$\begin{aligned}
&\lim_{N\to\infty} \mathbb{E}\left[\left(X(t) - \left(\mu_X(t) + \sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)\right)^2\right] \\
&= \lim_{N\to\infty} \mathbb{E}\left[\left([X(t) - \mu_X(t)] - \sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)^2\right] \\
&= \lim_{N\to\infty} \mathbb{E}\left[(X(t) - \mu_X(t))^2 + \left(\sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)^2 - 2\ (X(t) - \mu_X(t)) \left(\sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)\right] \\
&= \lim_{N\to\infty} \left(\mathbb{E}\left[(X(t) - \mu_X(t))^2 \right] + \mathbb{E}\left[\left(\sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)^2\right] - \mathbb{E}\left[2\ (X(t) - \mu_X(t)) \left(\sum_{k=1}^{N} Z_k e_{\lambda_k}(t)\right)\right]\right) \\
&= \lim_{N\to\infty} \left(R_X(t,\ t) + \mathbb{E}\left[\left(\sum_{k_1=1}^{N} Z_{k_1} e_{\lambda_{k_1}}(t)\right)\left(\sum_{k_2=1}^{N} Z_{k_2} e_{\lambda_{k_2}}(t)\right)\right] - 2\,\mathbb{E}\left[\sum_{k=1}^{N} (X(t) - \mu_X(t))\, Z_k e_{\lambda_k}(t)\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\mathbb{E}\left[\sum_{k_1=1}^{N}\sum_{k_2=1}^{N} Z_{k_1} Z_{k_2} e_{\lambda_{k_1}}(t) e_{\lambda_{k_2}}(t)\right] - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[(X(t) - \mu_X(t))\, Z_k\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\sum_{k_1=1}^{N}\sum_{k_2=1}^{N} e_{\lambda_{k_1}}(t) e_{\lambda_{k_2}}(t) \mathbb{E}\left[Z_{k_1} Z_{k_2}\right] - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[(X(t) - \mu_X(t))\, Z_k\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\sum_{k_1=1}^{N}\sum_{k_2=1}^{N} e_{\lambda_{k_1}}(t) e_{\lambda_{k_2}}(t) \lambda_{k_2} \delta_{k_1 k_2} - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[(X(t) - \mu_X(t))\, Z_k\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\sum_{k=1}^{N} \lambda_k e^2_{\lambda_k}(t) - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[(X(t) - \mu_X(t))\, Z_k\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\sum_{k=1}^{N} \lambda_k e^2_{\lambda_k}(t) - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[(X(t) - \mu_X(t)) \int_{\tau=t_0}^{t_f} (X(\tau) - \mu_X(\tau))\, e_{\lambda_k}(\tau)\, d\tau\right]\right) \\
&= R_X(t,\ t) + \lim_{N\to\infty} \left(\sum_{k=1}^{N} \lambda_k e^2_{\lambda_k}(t) - 2 \sum_{k=1}^{N} e_{\lambda_k}(t)\, \mathbb{E}\left[\int_{\tau=t_0}^{t_f} (X(t) - \mu_X(t))\, (X(\tau) - \mu_X(\tau))\, e_{\lambda_k}(\tau) d\tau\right]\right)
\end{aligned}$$

$$
\begin{aligned}
&= R_X(t,\ t) + \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) - 2\, \sum_{k=1}^{N} e_{\lambda_k}(t)\ \int_{\tau=t_0}^{t_f} e_{\lambda_k}(\tau)\ \mathbb{E}\left[\left(X(t) - \mu_X(t)\right) \left(X(\tau) - \mu_X(\tau)\right) \right] d\tau \right) \\
&= R_X(t,\ t) + \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) - 2\, \sum_{k=1}^{N} e_{\lambda_k}(t)\ \int_{\tau=t_0}^{t_f} e_{\lambda_k}(\tau)\ R_X(t,\ \tau)\ d\tau \right) \\
&= R_X(t,\ t) + \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) - 2\, \sum_{k=1}^{N} e_{\lambda_k}(t) \left(\mathcal{H}_X(e_{\lambda_k})(t)\right) \right) \\
&= R_X(t,\ t) + \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) - 2\, \sum_{k=1}^{N} e_{\lambda_k}(t) \lambda_k e_{\lambda_k}(t) \right) \\
&= R_X(t,\ t) + \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) - 2\, \sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) \right) \\
&= R_X(t,\ t) + \lim_{N\to\infty}\left(-\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) \right) \\
&= R_X(t,\ t) - \lim_{N\to\infty}\left(\sum_{k=1}^{N} \lambda_k\, e_{\lambda_k}^2(t) \right) \\
&= R_X(t,\ t) - \sum_{k=1}^{\infty} \lambda_k\, e_{\lambda_k}^2(t) \\
&= 0, \forall\, t \in [t_0,\ t_f], \text{ by Mercer's theorem (Theorem 2.4.1).}
\end{aligned}
$$

□

References

[1] https://en.wikipedia.org/wiki/Karhunen%E2%80%93Lo%C3%A8ve_theorem.

[2] J. Burkardt. Covariance, correlation, and the KL expansion, 2012. https://people.sc.fsu.edu/~jburkardt/m_src/svd_snowfall/kl_2012.pdf.

[3] P. Constantine. A primer on stochastic Galerkin methods. Technical report, 2007. https://inside.mines.edu/~pconstan/docs/constantine-primer.pdf.

[4] A. Alexanderian. A brief note on the Karhunen-Loéve expansion, 2015. http://users.ices.utexas.edu/~alen/articles/KL.pdf.

[5] O. Le Maître and O. M. Knio. *Spectral methods for uncertainty quantification, with applications to computational fluid dynamics*. Springer Science & Business Media, 2010.

[6] J. Stewart. Positive definite functions and generalizations, an historical survey. *Rocky Mountain Journal of Mathematics*, 6(3):409–434, 1976. http://projecteuclid.org/download/pdf_1/euclid.rmjm/1250130219.

[7] https://en.wikipedia.org/wiki/Positive-definite_kernel.

[8] https://en.wikipedia.org/wiki/Hilbert\OT1\textendashSchmidt_integral_operator.

[9] https://en.wikipedia.org/Compact_operator_on_Hilbert_space.

[10] https://patternsofideas.wordpress.com/2016/12/12/mercers-theorem-and-svms/.

[11] http://analysisyawp.blogspot.com/.

[12] https://en.wikipedia.org/wiki/Spectral_theorem.

[13] P. R. Halmos. What does the spectral theorem say? *The American Mathematical Monthly*, 70(3):241–247, 1963. http://www.math.wsu.edu/faculty/watkins/Math502/pdfiles/spectral.pdf.

[14] T. M. Apostol. *Mathematical analysis*. Addison-Wesley Reading, MA, 2^{nd} edition, 1974.

[15] W. Rudin. *Principles of mathematical analysis*. McGraw-Hill, New York, 3^{rd} edition, 1964.

[16] R. R. Goldberg. *Methods of real analysis*. Oxford and IBH Publishing, 1970.

[17] https://en.wikipedia.org/wiki/Mercer%27s_theorem.

[18] https://math.stackexchange.com/questions/2133637/inequality-in-mercers-theorem-proof.

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