

Stochastic Processes: Lecture 3

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Hilbert space

A Hilbert space H is an inner product space that is also a complete metric space w.r.t. the distance function

$$d(x, y) = \|x - y\| = \sqrt{\langle x - y, x - y \rangle}$$

induced by the inner product $\langle \cdot, \cdot \rangle$. For $x, y \in H$, this inner product satisfies

1. symmetry, i.e., $\langle x, y \rangle = \langle y, x \rangle$,
2. linearity, i.e., $\langle ax_1 + bx_2, y \rangle = a\langle x_1, y \rangle + b\langle x_2, y \rangle$,
3. positive definiteness, i.e.,

$$\langle x, x \rangle > 0, \quad x \neq 0$$

$$\langle x, x \rangle = 0, \quad x = 0.$$

L^2 -space

For a measure space X , a function $f : X \rightarrow \mathbb{R}$ is square integrable if

$$\int_X f(x)^2 dx < \infty.$$

The set of square integrable functions on X equipped with the inner product

$$\langle f_1, f_2 \rangle = \int_X f_1(x)f_2(x)dx$$

is a Hilbert space.

RKHS

A Hilbert space is a reproducing kernel Hilbert space H , if for every function $f \in H$ defined on X , there exists a function $K : X \times X \rightarrow \mathbb{R}$, such that

1. For all y , as a function of x , $K(x, y) \in H$
2. Reproducing property: for all $x \in X$,

$$f(x) = \langle K(\cdot, x), f(\cdot) \rangle.$$

Function $K(x, y)$ is the reproducing kernel of the space H .

Symmetry

Proposition 1

A reproducing kernel $K(\cdot, \cdot)$ is symmetric.

Proof.

$$K(x, y) = \langle K(\cdot, x), K(\cdot, y) \rangle = \langle K(\cdot, y), K(\cdot, x) \rangle = K(y, x).$$



Uniqueness of K

Proposition 2

If a reproducing kernel K exists, it is unique.

Proof.

Assume there exists another reproducing kernel K' . Then

$$\begin{aligned} 0 &\leq \|K(\cdot, x) - K'(\cdot, x)\|^2 \\ &= \langle K(\cdot, x) - K'(\cdot, x), K(\cdot, x) - K'(\cdot, x) \rangle \\ &= \langle K(\cdot, x) - K'(\cdot, x), K(\cdot, x) \rangle - \langle K(\cdot, x) - K'(\cdot, x), K'(\cdot, x) \rangle \\ &= \langle K(x, x) - K(x, x) \rangle - \langle K'(x, x) - K'(x, x) \rangle = 0. \end{aligned}$$

□

Positive definiteness

Proposition 3

A reproducing kernel K is positive definite.

Proof.

For any $y_1, \dots, y_n \in X$ and a_1, \dots, a_n ,

$$\begin{aligned}\sum_i \sum_j K(y_i, y_j) a_i a_j &= \sum_i \sum_j \langle K(\cdot, y_i), K(\cdot, y_j) \rangle a_i a_j \\ &= \left\langle \sum_i a_i K(\cdot, y_i), \sum_j a_j K(\cdot, y_j) \right\rangle \\ &= \left\| \sum_i a_i K(\cdot, y_i) \right\|^2 \geq 0.\end{aligned}$$

□

One-to-one relationship

Theorem 1 (Moore-Aronszajn theorem)

To every RKHS H there exists a unique symmetric, positive definite function $K(\cdot, \cdot)$. For every symmetric, positive definite function $K(\cdot, \cdot)$ there exists a unique RKHS H .

For an RKHS H , we have shown uniqueness, symmetry and positive definiteness of $K(\cdot, \cdot)$. For a symmetric, positive definite $K(\cdot, \cdot)$, let $H_0 = \text{span}\{K_x := K(x, \cdot), x \in X\}$. Define the inner product on H_0

$$\left\langle \sum_{i=1}^n a_i K_{x_i}, \sum_{j=1}^m b_j K_{x_j} \right\rangle_{H_0} = \sum_{i=1}^n \sum_{j=1}^m a_i b_j K(x_i, x_j)$$

and note it is symmetric, non-degenerate and satisfies $\langle K_x, K_y \rangle_{H_0} = K(x, y)$. Let H be the completion of H_0 , having functions

$$f(x) = \sum_{i=1}^{\infty} a_i K_{x_i}(x) \quad \text{for which} \quad \lim_{n \rightarrow \infty} \sup_{p \geq 0} \left\| \sum_{i=n}^{n+p} a_i K_{x_i} \right\|_{H_0}^2 = 0.$$

One-to-one relationship

The reproducing property holds on this completion:

$$\langle f, K_x \rangle_H = \sum_{i=1}^{\infty} a_i \langle K_{x_i}, K_x \rangle_{H_0} = \sum_{i=1}^{\infty} K(x_i, x) = f(x).$$

To prove uniqueness, let G be another Hilbert space on which K is the reproducing kernel. Then

$$\langle K_x, K_y \rangle_G = K(x, y) = \langle K_x, K_y \rangle_H.$$

By linearity, $\langle \cdot, \cdot \rangle_G = \langle \cdot, \cdot \rangle_H$ on H_0 , so $H_0 \subset G$. But G is complete, so it contains H , the completion of H_0 . Finally, we need to show $G \subset H$. Let $f \in G$. Because $H \subset G$ and closed, $f = f_H + f_{H^\perp}$. Then

$$f(x) = \langle K_x, f \rangle_G = \langle K_x, f_{H^\perp} \rangle_G + \langle K_x, f_H \rangle_G = \langle K_x, f_H \rangle_G = \langle K_x, f_H \rangle_H = f_H(x),$$

where we use the fact that $K_x \in H$.

Roughness of RKHS

Proposition 4

Norm convergence implies pointwise convergence in an RKHS H .

Proof.

For any sequence $f_n \in H$,

$$|f_n(x) - f(x)| = |\langle K(\cdot, x), f_n(\cdot) - f(\cdot) \rangle| \leq \|K(\cdot, x)\| \|f_n(\cdot) - f(\cdot)\|$$

□

Roughness of RKHS

L^2 is rougher than an RKHS: norm convergence does not imply pointwise convergence. Consider $L^2([0, 1])$ and the function

$$g_n(x) = x^n$$

g_n converges to $g(x) = 0$ in norm:

$$\|g_n\|^2 = \int_0^1 x^{2n} dx = \frac{1}{2n+1} \rightarrow 0.$$

But $g_n(1) = 1 \neq 0$.

Mercer's theorem

Let $K(\cdot, \cdot) : X \times X \rightarrow \mathbb{R}$ be a symmetric function and define the integral operator $T_K : L^2(X) \rightarrow L^2(X)$

$$T_K f(\cdot) = \int K(\cdot, x) f(x) dx.$$

T_K is positive definite if for all $f \in L^2$, $\langle f, T_K f \rangle > 0$.

Theorem 2

If K is continuous and T_K is positive definite, then T_K has eigenfunctions $\phi_i \in L^2$ ($\|\phi_i\| = 1$) with eigenvalues $\lambda_i > 0$ and for all $x, y \in X$,

$$K(x, y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \phi_i(y)$$

Fourier decompositions and RKHS

Theorem 3

Let $K(\cdot, \cdot)$ be an L^2 kernel. For all $f \in L^2$, define the Fourier coefficients as

$$f_i = \int f(x)\phi_i(x)dx.$$

For all $f, g \in L^2$ the inner product on the RKHS of K is

$$\langle f, g \rangle = \sum_i \frac{f_i g_i}{\lambda_i},$$

and $f \in \text{RKHS}$ if

$$\|f\|^2 = \sum_i \frac{f_i^2}{\lambda_i} < \infty.$$

Fourier decompositions and RKHS

Proof.

The Fourier expansions for $f(\cdot)$ and $K(x, \cdot)$ are

$$f(\cdot) = \sum_i f_i \phi_i(\cdot) \quad \text{and} \quad K(x, \cdot) = \sum_i \lambda_i \phi_i(x) \phi_i(\cdot).$$

Then the above inner product satisfies

$$\langle K(\cdot, x), f(\cdot) \rangle = \sum_i \frac{f_i \lambda_i \phi_i(x)}{\lambda_i} = \sum_i f_i \phi_i(x) = f(x)$$

so $K(\cdot, x)$ is a reproducing kernel and has corresponding norm

$$\|f\|^2 = \sum_i f_i^2 / \lambda_i.$$

□

Karhunen-Loeve

Let $\{X(t), t \in \mathcal{T}\}$ be a zero mean, second order ($E(X_t^2) < \infty$) stochastic process. Its covariance function $E(X(s)X(t)) = K(s, t)$ is continuous.

Theorem 4

Assume that λ_i and ϕ_i satisfy the following equation:

$$\int_{\mathcal{T}} K(s, t)\phi_i(t)dt = \lambda_i\phi_i(s),$$

where $\{\phi_i, i \in \mathbb{N}\}$ are orthogonal eigenfunctions in L^2 and $\{\lambda_i, i \in \mathbb{N}\}$ are eigenvalues. Furthermore, specify

$$\xi_i = \frac{1}{\sqrt{\lambda_i}} \int_{\mathcal{T}} X(t)\phi_i(t)dt.$$

Then,

$$X(t) = \sum_{i=1}^{\infty} \sqrt{\lambda_i}\xi_i\phi_i(t)$$

as the following holds uniformly:

$$\lim_{p \rightarrow \infty} E \left(X(t) - \sum_{i=1}^p \sqrt{\lambda_i}\xi_i\phi_i(t) \right)^2 = 0$$

Karhunen-Loeve

Theorem 4 (cont.)

Conversely, if $X(t) = \sum_{i=1}^{\infty} \sqrt{\lambda_i} \xi_i \phi_i(t)$ for $\{\xi_i\} \stackrel{iid}{\sim} (0, 1)$, then

$$\int_{\mathcal{T}} K(s, t) \phi_i(t) dt = \lambda_i \phi_i(s).$$

Proof.

We'll use the whiteboard for this one. □

KL and RKHS

Let $\{X(t), t \in \mathcal{T}\}$ be a zero mean, second order ($E(X_t^2) < \infty$) Gaussian process with covariance function $E(X(s)X(t)) = K(s, t)$. When equipped with the covariance as inner product, the space

$$H_X = \text{span}\{X(t), t \in \mathcal{T}\}$$

is isometrically isomorphic to the RKHS of K . If $X_m, X_n \in H_X$, i.e.,

$$X_m = \sum_i a_i X(t_i), \quad X_n = \sum_i b_i X(t_i),$$

then $\langle X_m, X_n \rangle = E(X_m X_n)$ is a valid inner product. The spaces are isometrically isomorphic because

$$\langle X(s), X(t) \rangle = E(X(s)X(t)) = K(t, s) = \langle K(t, \cdot), K(s, \cdot) \rangle.$$

KL and RKHS

Theorem 5

If $\{X(t), t \in \mathcal{T}\}$ is a zero mean, second order Gaussian process with covariance function $E(X(s)X(t)) = K(s, t)$, then the sample path $X(\cdot)$ a.s. does not belong to the RKHS of K .

Heuristic proof: recall that (for $f, g \in L^2$) the inner product on the RKHS of K is

$$\langle f, g \rangle = \sum_i \frac{f_i g_i}{\lambda_i},$$

where λ_i are the eigenvalues of K . Define the truncated KL expansion

$$X_p(t) = \sum_{i=1}^p \sqrt{\lambda_i} \xi_i \phi_i(t),$$

and note that

$$E\left(\|X_p\|^2\right) = E\left(\sum_{i=1}^p \frac{\sqrt{\lambda_i} \xi_i \sqrt{\lambda_i} \xi_i}{\lambda_i}\right) = \sum_{i=1}^p E(\xi_i^2) = p \rightarrow \infty.$$

Truncated KL expansion

Again, the KL expansion uses coefficients λ_i and functions ϕ_i that satisfy the integral equation

$$\int_{\mathcal{T}} K(s, t)\phi_i(t)dt = \lambda_i\phi_i(s).$$

Theorem 6

Among all truncated expansions that take the form

$$X_p(t) = \sum_{i=1}^p \sqrt{l_i} x_i \psi_i(t), \quad \text{for} \quad \int \psi_i(t)\psi_j(t)dt = \delta_{ij},$$

the truncated KL expansion minimizes the integrated mean squared error

$$\int E(e_p^2(t))dt, \quad \text{where} \quad e_p(t) = \sum_{i>p} \sqrt{l_i} x_i \psi_i(t).$$

Truncated KL expansion

Proof. The expected squared error is

$$\begin{aligned} E(e_p^2(t)) &= E\left(\sum_{i>p} \sum_{j>p} \sqrt{l_i l_j} x_i x_j \psi_i(t) \psi_j(t)\right) \\ &= E\left(\sum_{i>p} \sum_{j>p} \psi_i(t) \psi_j(t) \int \int X(t_1) X(s_1) \psi_i(t_1) \psi_j(s_1) ds_1 dt_1\right) \\ &= \sum_{i>p} \sum_{j>p} \psi_i(t) \psi_j(t) \int \int K(t_1, s_1) \psi_i(t_1) \psi_j(s_1) ds_1 dt_1. \end{aligned}$$

The integrated expected squared error is then

$$\begin{aligned} \int E(e_p^2(t)) dt &= \sum_{i>p} \sum_{j>p} \left(\int \psi_i(t) \psi_j(t) dt\right) \int \int K(t_1, s_1) \psi_i(t_1) \psi_j(s_1) ds_1 dt_1 \\ &= \sum_{i>p} \int \int K(t_1, s_1) \psi_i(t_1) \psi_i(s_1) ds_1 dt_1. \end{aligned}$$

Truncated KL expansion

Proof continued. We are interested in the optimization problem

$$\min \int E(e_p^2(t))dt, \quad \text{a.s.} \quad \int \psi_i(t)\psi_j(t)dt = \delta_{ij}.$$

We therefore minimize the objective function

$$Q = \sum_{i>p} \int \int K(t_1, s_1)\psi_i(t_1)\psi_i(s_1)ds_1dt_1 - \lambda_i \left(\int \psi_i^2(t)dt - 1 \right)$$

by taking the following functional derivative and setting equal to 0:

$$\frac{dQ}{d\psi_i}(t) = 2 \int K(t, s)\psi_i(s)ds - 2\lambda_i\psi_i(t) = 0.$$

Thus, we obtain the Fredholm equation

$$\int_{\mathcal{T}} K(t, s)\phi_i(s)ds = \lambda_i\phi_i(t).$$

Analytic example: Brownian motion on $\mathcal{T} = [0, 1]$

Let $s \leq t$, the covariance function for Brownian motion is

$$\begin{aligned} K(s, t) &= E(B_s B_t) = E(B_s(B_t - B_s + B_s)) \\ &= E(B_s^2) = s. \end{aligned}$$

Thus, the KL expansion corresponds to the integral equation

$$\int \min(s, t) \phi(s) ds = \lambda \phi(t)$$

or

$$\int_0^t s \phi(s) ds + t \int_t^1 \phi(s) ds = \lambda \phi(t),$$

and thus $\phi(0) = 0$.

Analytic example: Brownian motion on $\mathcal{T} = [0, 1]$

Taking the first derivative of both sides of

$$\int_0^t s\phi(s)ds + t \int_t^1 \phi(s)ds = \lambda\phi(t)$$

gives

$$\int_t^1 \phi(s)ds = \lambda \frac{d}{dt} \phi(t).$$

Taking the second derivative gives the ODE

$$-\phi(t) = \lambda \frac{d^2}{dt^2} \phi(t),$$

which is solved by

$$\phi(t) = A \sin(t/\sqrt{\lambda}) + B \cos(t/\sqrt{\lambda}).$$

Analytic example: Brownian motion on $\mathcal{T} = [0, 1]$

... which is solved by

$$\phi(t) = A \sin(t/\sqrt{\lambda}) + B \cos(t/\sqrt{\lambda}).$$

But $\phi(0) = 0$, so $B = 0$ and $\phi(t) = A \sin(t/\sqrt{\lambda})$. To get eigenvalues, substitute $\phi(t)$ into the first derivative equations:

$$A \int_t^1 \sin(s/\sqrt{\lambda}) ds = A\lambda \cos(t/\sqrt{\lambda})/\sqrt{\lambda} \quad \implies$$

$$A\sqrt{\lambda} \left(\cos(t/\sqrt{\lambda}) - \cos(1/\sqrt{\lambda}) \right) = A\sqrt{\lambda} \cos(t/\sqrt{\lambda}) \quad \implies$$

$$\cos(1/\sqrt{\lambda}) = 0 \quad \implies$$

$$\lambda_i = \frac{4}{(2i-1)^2\pi^2}, \quad i \geq 1.$$

Analytic example: Brownian motion on $\mathcal{T} = [0, 1]$

Use the orthogonality of ϕ_i to get A :

$$\begin{aligned} 1 &= \int_0^1 \phi_i^2(t) dt = A^2 \int_0^1 \sin^2(t/\sqrt{\lambda}) dt \\ &= A^2 \int_0^1 \sin^2\left(\left(i - \frac{1}{2}\right) \pi t\right) dt \\ &= A^2/2. \end{aligned}$$

Therefore, $A = \sqrt{2}$. Thus, the KL expansion is

$$B(t) = \sqrt{2} \sum_{i \geq 1} \frac{2\xi_i}{(2i-1)\pi} \sin\left(\left(i - \frac{1}{2}\right) \pi t\right), \quad \xi_i \stackrel{iid}{\sim} N(0, 1).$$

Analytic example: Brownian bridge on $\mathcal{T} = [0, 1]$

Let $B(t)$ be a standard Brownian motion and define the Brownian bridge $X(t)$ as

$$X(t) = B(t) - tB(1).$$

The covariance function is $K(s, t) = \min(s, t) - st$. To see this, let $s \leq t$:

$$\begin{aligned} K(s, t) &= E(X(s)X(t)) = E((B_s - sB_1)(B_t - tB_1)) \\ &= E(B_s B_t) - sE(B_1 B_t) - tE(B_s B_1) + stE(B_1^2) \\ &= s - st - st + st = s - st. \end{aligned}$$

So the integral equation is

$$\int (\min(s, t) - st) \phi(s) ds = \lambda \phi(t)$$

Analytic example: Brownian bridge on $\mathcal{T} = [0, 1]$

Differentiating the integral equation

$$\int_0^1 (\min(s, t) - st) \phi(s) ds = \lambda \phi(t)$$

w.r.t. t gives

$$\int_t^1 \phi(s) ds - \int_0^1 s\phi(s) ds = \lambda \frac{d}{dt} \phi(t),$$

and differentiating again gives

$$-\phi(t) = \lambda \frac{d^2}{dt^2} \phi(t).$$

Just as with the standard Brownian motion, assuming $\phi(0) = 0$ results in $\phi(t) = A \sin(t/\sqrt{\lambda})$.

Analytic example: Brownian bridge on $\mathcal{T} = [0, 1]$

Substituting $\phi(t) = A \sin(t/\sqrt{\lambda})$ into the first derivative equation

$$\int_t^1 \phi(s) ds - \int_0^1 s \phi(s) = \lambda \frac{d}{dt} \phi(t)$$

gives

$$\begin{aligned} A \int_t^1 \sin(s/\sqrt{\lambda}) ds - A \int_0^1 s \sin(s/\sqrt{\lambda}) ds &= A \lambda \cos(t/\sqrt{\lambda}) / \sqrt{\lambda} \\ \sqrt{\lambda} \left(\cos(t/\sqrt{\lambda}) - \cos(1/\sqrt{\lambda}) \right) - \\ \lambda \sin(1/\sqrt{\lambda}) + \sqrt{\lambda} \cos(1/\sqrt{\lambda}) &= \sqrt{\lambda} \cos(t/\sqrt{\lambda}) \\ \sin(1/\sqrt{\lambda}) &= 0 \\ \lambda_i &= \frac{1}{i^2 \pi^2}, \quad i \geq 1. \end{aligned}$$

Analytic example: Brownian bridge on $\mathcal{T} = [0, 1]$

Again, we use orthonormality of ϕ_i to solve for A :

$$1 = A^2 \int_0^1 \sin^2(s/\sqrt{\lambda_i}) ds = A^2 \int_0^1 \sin^2(i\pi s) ds = \frac{A^2}{2}.$$

Again, we have $A = \sqrt{2}$, and the KL expansion for the Brownian bridge may be written

$$\begin{aligned} X(t) &= \sum_{i \geq 1} \sqrt{\lambda_i} \phi_i(t) \xi_i \\ &= \sqrt{2} \sum_{i \geq 1} \frac{\xi_i}{\pi i} \sin(i\pi t), \quad \xi_i \stackrel{iid}{\sim} N(0, 1). \end{aligned}$$