Stat 992: Lecture 11
Karhunen-Loève Expansion.

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1. *Orthogonal expansion for fields* Let $\mathcal{G} = L^2(G(\Omega))$ be the space of zero mean Gaussian random fields in $\Omega \subset \mathbb{R}^n$ with inner product

$$\langle X, Y \rangle = \mathbb{E} \int_\Omega X(x)Y(x)\, dx$$

with $\|X\| < \infty$. This is basically the integral of cross-covariance function between fields X and Y. $\mathcal{G}$ can be shown to be a separable Hilbert space. This can be shown by finding countable orthonormal basis in $\mathcal{G}$. See Random Fields and Their Geometry by R.J. Adler and J.E. Taylor.

Let ψ_i be basis for $L^2(\Omega)$ and Z_i be i.i.d. $N(0, \sigma_i^2)$. We will construct orthonormal expansion in the following fashion. Suppose for any $X \in \mathcal{G}$,

$$X(x) = \sum_{i=0}^{\infty} Z_i \psi_i(x).$$

Note that $\mathbb{E}X(x) = 0$ while the covariance function is

$$\begin{aligned} R(x,y) &= \mathbb{E} \sum_{i,j=0}^{\infty} Z_i \psi_i(x) Z_j \psi_i(y) \\ &= \sum_{i=0}^{\infty} \sigma_i^2 \psi_i(x) \psi_i(y). \end{aligned}$$

The covariance function of zero mean Gaussian field completely characterizes the field itself so we need to know if any covariance function can be expressed this way. Obviously R has to be symmetric to be expressible this way.

2. *Degenerate kernels.* We follow the argument of R. Courant and D. Hilbert (Methods of Mathematical Physics, Vol I. 1953). Suppose we fix y. Then from the Weierstrass's approximation theorem, for continuous function, $R(x, \cdot) = \sum_{i=0}^{\infty} \alpha_i(x)$ for some basis functions α_i uniformly. Now fix x and we have

$$\begin{aligned} R(x,y) &= \sum_{i=0}^{\infty} \alpha_i(x) \sum_{j=0}^{\infty} \beta_j(x) \\ &= \sum_{i,j=0}^{\infty} \alpha_i(x) \beta_j(x) \end{aligned}$$

Again, β_j are basis functions. Courant and Hilbert termed such the kernel degenerate. For finite number of basis $\alpha_1, \cdots, \alpha_p$ and $\beta_1, \cdots, \beta_p$, it can be representable as a linear combination of orthogonal basis ψ using the Gram-Schmidt orthogonalization. So we have

$$R(x,y) = \sum_{i,j=0}^{\infty} c_{ij} \psi_i(x) \psi_j(x).$$

Assume further that the kernel is symmetric then

$$\sum_{i,j=0}^{p} (c_{ij} - c_{ji}) \psi_i(x) \psi_j(x) = 0$$

for $p \to \infty$. Since ψ_i and ψ_j are independent, $c_{ij} = c_{ji}$. We can do a better job than this via Mercer's theorem (Read Riesz and Sz.-Nagy, 1956; Courant and Hilbert. 1953; Adler and Taylor, 2004).

3. *Mercer's theorem.* For continuous symmetric kernel R, define linear operator $\mathcal{R} : L^2(\Omega) \to L^2(\Omega)$ as

$$\mathcal{R}f(x) = \int_\Omega R(x,y) f(y)\, dy.$$

This is a compact self-adjoint operator[1] which yields unique countable eigenvalues λ_i and orthonormal eigenfunctions ϕ_i such that $\mathcal{R}\phi_i =$

[1] R is compact if the closure of R(close ball) is compact and it is self-adjoint if $\langle \mathcal{R}f, g \rangle = \langle f, \mathcal{R}g \rangle$. See J.B. Conway's A Course in Functional Analysis, 2nd edition (1990) for the discussion of compact operators on Hilbert space. S.C. Joshi's PhD thesis (1998) Large Deformation Diffeomorphisms and Gaussian Random Fields for Statistical Characterization of Brain Sub-manifolds for it's use in actual image analysis.

$\lambda_i {\phi_i}^2$ with $\lambda_\infty = 0$. We will order them such that $\lambda_0 > \lambda_1 > \lambda_2 > \cdots$.

The compact self-adjoint operator $\mathcal{R}$ has a spectral representation $\mathcal{R}f = \sum_{i=0}^{\infty} \lambda_i \langle \phi_i, f \rangle \phi_i$.[3] Mercer's theorem stats that

$$R(s,t) = \sum_{i=0}^{\infty} \lambda_i \phi_i(x) \phi_i(y).$$

Hence identifying $\lambda_i = \sigma_i^2$ and $\phi_i = \psi_i$, we have the desired orthonormal expansion and it is called the Karhunen-Loève expansion.

To prove the theorem, note that $\phi_i(x)\phi_j(y)$ forms basis in $\Omega \otimes \Omega$. This is how you expand basis function in 1 dimension to higher dimension in Euclidean space. Assuming $R(x,y) \in L^2(\Omega \otimes \Omega)$,

$$R(x,y) = \sum_{i,j=0}^{\infty} c_{ij} \phi_i(x) \phi_j(y).$$

Then

$$\begin{aligned} \int_\Omega R(x,y)\phi_k(y)\, dy &= \sum_{i,j=0}^{\infty} c_{ij} \int_\Omega \phi_k(y)\phi_i(x)\phi_j(y)\, dy \\ \lambda_k \phi_k(x) &= \sum_{i,j=0}^{\infty} c_{ij}\phi_i(x)\delta_{jk} = \sum_{i=0}^{\infty} d_i \phi_i(x) \end{aligned}$$

where $d_i = \sum_{k=0}^{\infty} c_{ik}$. Since they are linearly independent, $c_j = \lambda_j$.

Problem 21. Let X be a Brownian motion with covariance function given by $R(x,y) = \min(x,y)$. Find the eigenvalues and eigenfunctions. Based on this eigensystem, expand the Brownian motion via the Karhunen-Loève expansion. Based on the Karhunen-Loève expansion, simulate Brownian motion in `MATLAB`.

Problem 22. Without using the property of compact self-adjoint operator in Hilbert space, prove Mercer's theorem. Follow Riesz and Sz.-Nagy's classical derivation.

[2] This eigenequation is called a Fredholm equation of the first kind. Given covariance function, there is a numerical technique for estimating λ_i and ϕ_i numerically.

[3] See Conway Theorem 7.6.