Principle Component

Goal: Specify a few values, *principle component*, in order to reconstruct almost the entire outcome of the full vector.

Given random vector $\mathbf{x} = (x_1, \cdots, x_n)^\top$ with mean zero and covariance matrix $\Sigma = \mathbb{E}(xx^\top)$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n > 0$ and orthonormal eigen vectors p_k.

With these assumptions, we want to find random variables $z_1, \cdots, z_n$ with mean zero and covariance matrix $\mathbf{I}_n$. The specific expression of z_k is

$$z_k = \frac{1}{\sqrt{\lambda_k}} \mathbf{p}_k' \mathbf{x}$$

The **principle component** of $\mathbf{x}$ is $y_k = \sqrt{\lambda_k} z_k$, or $\mathbf{y} = \mathbf{PX}$. It analogies to the eigenvector in the linear algebra.

Similarly, the original x-variables can be expressed as a linear combination of the uncorrelated variables y_k and z_k:

$$x_k = \mathbf{p}_k' \mathbf{y} = \sum_{j=1}^{n} \sqrt{\lambda_j} p_{jk} z_j$$

Expansion along eigenfunctions

Comparison with Finite Dimension

Here, we generalize the orthogonormality and eigenvectors in functional space.

	FINITE DIMENSION	INFINITE DIMENSION
orthogonal	$\sum p_i \overline{q_i} = 0$	$\int_a^b c(t)\overline{d(t)} dt = 0$
normal	$\sum \lvert p_i \rvert^2 = 1$	$\int_a^b \lvert c(t) \rvert^2 dt = 1$
eigen component	$\mathbf{\Sigma p} = \lambda \mathbf{p}$	$\int_a^b r(s,t)c(t)\mathrm{d}t = \lambda c(s)$

Decomposition

Consider an one continuous parameter stochastic process $x(t), t \in [a, b]$. Similarly, we want to find the orthonormal basis for $\mathcal{H}(x)$, which satisfies

$$x(t) = \sum_k c_k(t) z_k$$
$$r(s,t) = \sum_k c_k(s) \overline{c_k(t)}$$

To achieve this,

- Firstly, find eigen functions $c_k(t)$ according to covariance function $r(s,t)$.
- Then, z_k's are obtained by $z_k = \frac{1}{\lambda_k}\int_a^b \overline{c_k(t)} x(t) \mathrm{d}t$
- The orthonormal eigenfunctions are $\phi_j(t) = \frac{1}{\sqrt{\lambda_j}} c_j(t)$

The optimal choice is minimizing integrated approximation error

$$\int_a^b E\left(e_n^2(t)\right) \mathrm{d}t = \int_a^b E\left(x^2(t)\right) \mathrm{d}t - \sum_0^n \lambda_k$$

Actually, we wish it converges to zero uniformly.

The Karhunen-Loève theorem

The Karhunen-Loève theorem

Let $\{x(t), a \leq t \leq b\}$ be continuous in quadratic mean with mean zero and covariance function $r(s,t) = E(x(s)\overline{x(t)})$. Then there exist orthonormal eigenfunctions $\phi_k(t), k = 0, 1, \ldots, N \leq \infty$, for $a \leq t \leq b$, with eigenvalues $\lambda_0 \geq \lambda_1 \geq \ldots$, to the equation

$$\int_a^b r(s,t)\phi(t)\mathrm{d}t = \lambda\phi(s)$$

such that the random variables $z_k = \frac{1}{\sqrt{\lambda_k}} \int_a^b \overline{\phi_k(t)} x(t) dt$ are uncorrelated, $V(z_k) = 1$, and can represent $x(t)$ as

$$x(t) = \sum_0^\infty \sqrt{\lambda_k}\phi_k(t) z_k$$

Note: We can also express $x(t)$ as this $x(t) = \sum_0^\infty \sqrt{\lambda_k}\phi_k(t) z_k = \sum_0^\infty \int_a^b \overline{\phi_k(t)} x(t) dt \; \phi_k(t)$. In this way, the orthonormal term is $\phi_k(t)$.

Optimality of the Karhunen-Loève expansion

If $\psi_k(t), k = 0, 1, \ldots$, is any sequence of functions and $y_k \in \mathscr{H}(x)$ are uncorrelated random variables, then, for each n

$$\int_a^b E\left(\left|x(t) - \sum_0^n \sqrt{\lambda_k}\phi_k(t) z_k\right|^2\right) \mathrm{d}t \leq \int_a^b E\left(\left|x(t) - \sum_0^n \psi_k(t) y_k\right|^2\right) \mathrm{d}t$$

Reference

- Stationary Stochastic Processes: Theory and Applications