Functional Data

- $X(t)$: not equally-spaced data

  $\mu(t) = E(X(t))$

  Model: $Y(t) = \alpha(t) + \beta(t)X(t) + \varepsilon(t)$

- Functional Data Analysis
  - FPCA
  - Functional Linear Models

PCA

- $x \sim N(\mu, \Sigma)$, $u^T x \sim N(u^T\mu, u^T\Sigma u)$

- Objective $\max\ u^T \Sigma u$

  s.t. $u^T u = 1$

- Mechanics:

  1. $\Sigma = \frac{1}{n} \sum x_i x_i^T$
  2. $\Sigma = U D U^T$, $D = \mathrm{diag}\{d_1, d_2, \cdots, d_K\}$
  3. proportion of explained variance $= d_k / \sum_k d_k$
  4. Order U, D decreasingly by d_i
  5. $u_k \to$ k-th principle component, $x_i^T u_k \to$ k-th principle component score

FPCA

- Functional Principle Components (FPC) $w_1(t), w_2(t), \cdots, w_K(t)$ (Basis)
- FPCA → project sample curve $X_i(t), i=1,2,\cdots,n$ to FPCs

  $X_i(t) = \sum_{k=1}^{K} S_{ik} w_k(t)$

Preprocessing

1. Data curves: $X_1^*(t), X_2^*(t), \cdots, X_n^*(t)$
2. Pre-processing: $X_i(t) = X_i^*(t) - \mu(t)$, where $\mu(t) = \frac{1}{n}\sum_{i=1}^{n} X_i^*(t)$

Objectives:

1. $\forall$ FPC: $w_1(t)$, $S_{i1} = \int X_i(t) w_1(t)\, dt$

   $$\max \sum_{i=1}^{n} S_{i1}^2$$
   $$\text{s.t.} \int w_1^2(t)\, dt = 1$$

2. $\forall$ 2^{nd}-FPC: $w_2(t)$, $S_{i2} = \int X_i(t) w_2(t)\, dt$

   $$\max \sum_{i=1}^{n} S_{i2}^2$$
   $$\text{s.t.} \int w_2^2(t)\, dt = 1, \int [w_1(t) w_2(t)]\, dt = 0$$

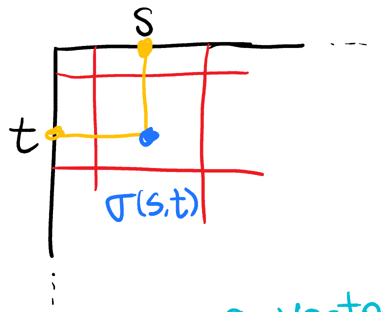
⋮

K. find $w_K(t)$

Therefore, we have K-top orthogonal FPCs.

FPCA v.s. PCA

- PCA: $Var(X) = \Sigma = U^T D U = \sum d_i u_i u_i^T$
- FPCA: $Var(X) = \sigma$ is a kernel



infinite dimension
infinite (s, t)

$$\sigma(s,t) = \sum_{j=1}^{\infty} d_j w_j(s) w_j(t)$$

← a vector with infinite dimension

$$\sigma(s,t) = E(X(s)X(t)) - E(X(s))E(X(t))$$

The variance of score on j-th FPC is d_j $\quad Var(s_j) = d_j$

$$s_{ij} = \int w_j(t) X_i(t)\, dt$$

r.v. X

$$s_{\cdot j} = \int w_j(t) \cdot X(t)\, dt, \quad E(s_{\cdot j}) = \int w_j(t) \underbrace{E\{X(t)\}}_{=\mu(t)=0} dt = 0$$

$$Var(s_{\cdot j}) = E(s_{\cdot j}^2) = E\left(\int w_j(t) X(t)\, dt\right)\left(\int w_j(s) X(s)\, ds\right)$$

$$= \iint w_j(t) E(X(t)X(s)) w_j(s)\, ds\, dt$$

$$= d_j \int w_j^2(t)\, dt \int w_j^2(s)\, ds = d_j$$

Proportion of variance explained $\dfrac{d_j}{\sum_{j=1}^{\infty} d_j}$

Computing FPCA:

- eigen-equation: $\int \sigma(s,t)\, w_i(s)\, ds = \lambda w_i(t)$

? Algebraic Interpretation: $\sigma(s,t) \sim A$

$A = (\alpha_t)_\infty \rightarrow \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_t \\ \vdots \end{pmatrix}$

$\sum \langle \alpha_t, q_s \rangle = \lambda q_t$

- Method 1:

$\hat{\sigma}(s,t) = \frac{1}{n} \sum_i X_i(s) X_i(t)$

grid the infinite dimensional space: $\Sigma = (\hat{\sigma}(t_i, t_j))_{n \times n}$

find vectors $u_1, u_2, \cdots, u_n = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$, interpolate $f(t_i) = x_i$

- Method 2:

  - $X(t) = (X_1(t), \cdots, X_n(t))^T$
    $\Phi(t) = (\phi_1(t), \cdots, \phi_J(t))^T$ $\Rightarrow$ $X(t) = C\, \Phi(t)$

  - $\sigma(s,t) = \frac{1}{n} X^T(s) X(t) = \frac{1}{n} \Phi^T(s) C^T C\, \Phi(t)$

    $w(t) = \Phi^T(t) b$ $\qquad \frac{1}{n} \int \cancel{\Phi^T(t)} C^T C\, \Phi(s)\, \Phi(s)^T b\, ds = \lambda \cdot \cancel{\Phi^T(t)}\, b$

  - $\max \int \sigma(s,t)\, w(s)\, ds = \lambda w(t)$
    s.t. $\int [w(t)]^2 dt = b^T \int \Phi(t) \Phi(t)^T dt \cdot b = 1$

  - $W = \mathrm{diag}(\int \Phi_i^2(t)\, dt)$
    $\frac{1}{n} C^T C W b = \lambda \cdot b$ $\qquad \frac{1}{n} W^{1/2} C^T C W^{1/2} u = \lambda W^{1/2} b$
    s.t. $b^T W b = 1$ $\quad \Rightarrow \quad$ s.t. $u^T u = 1$