Functional regression paper review

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1 Functional Principal Components Analysis

1.1 Connection to the conventional PCA

There are two approaches to PCA: SVA and eigendecomposition of the covariance matrix. These are equivalent after centering the columns of design matrix X. The centering is essential because $(n-1)^{-1} X^\top X$ is not the covariance matrix otherwise. SVD states the identity $X = U\Sigma V^\top$. Then, $X^\top X = V\Sigma U^\top U \Sigma V^\top$. U and V are orthogonal matrices, forcing $U^\top$ and U to cancel each other out. Hence, $X^\top X = V\Sigma^2 V^\top$, which resembles the eigendecomposition of $X^\top X$.

The functional analog of PCA uses the covariance function instead and defines the covariance function $v(s,t)$ by

$$v(s,t) = \frac{1}{n-1} \sum_{i=1}^{n} x_i(s)\, x_i(t)\,. \tag{1}$$

The eigenequation $A\vec{v} = \lambda \vec{v}$ becomes an integral

$$\int v(s,t)\, \xi(t)\; dt = \rho \xi(s) \tag{2}$$

where $\xi(\cdot)$ works as the eigenvector; hence the name *eigenfunction*. It corresponds to an *integral transform* and is often written with the operator notation

$$V\xi = \rho\xi \tag{3}$$

making it seem identical to the matrix eigenequation.

1.2 Computation

The above introduction is useful in facilitating the understanding of fPCA. However, it does not tell us how to actually do it. The most intuitive way of doing it is to discretize the design function $X_i(t)$ into a design matrix. However in Jeff Goldsmith's paper, basis function expansion technique was adopted to address the computation. Suppose each design function $X_i(t)$ has basis expansion

$$X_i(t) = \sum_{k=1}^{K} c_{ik} \phi_k(t)\,. \tag{4}$$

The notation simplies upon defining vector-valued functions $\boldsymbol{X}(t)$ and $\boldsymbol{\phi}(t)$ as

$$\boldsymbol{X} = \boldsymbol{C}\boldsymbol{\phi}, \tag{5}$$

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where the coefficient matrix $\boldsymbol{C}$ is $n \times K$. Then the covariance matrix is

$$v(s,t) = \frac{1}{n-1} \boldsymbol{\phi}(s)^\top \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{\phi}(t). \tag{6}$$

Introducing another matrix $\boldsymbol{W} = \int \boldsymbol{\phi}\boldsymbol{\phi}^\top$, we can now say that

$$\int v(s,t)\,\xi(t)\,dt = \frac{1}{n-1} \int \boldsymbol{\phi}(s)^\top \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{\phi}(t)\,\boldsymbol{\phi}(t)^\top \boldsymbol{b}\,dt \tag{7}$$

$$= \boldsymbol{\phi}(s)^\top \frac{1}{n-1} \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{W} \boldsymbol{b} \tag{8}$$

where the vector $\boldsymbol{b}$ comes from the expansion of the eigenfunction $\xi(s)$:

$$\xi(s) = \sum_{k=1}^{K} b_k \phi_k(s) \tag{9}$$

$$= \boldsymbol{\phi}(s)^\top \boldsymbol{b}. \tag{10}$$

The eigenequation 2 reduces to a matrix equation

$$\boldsymbol{\phi}(s)^\top \frac{1}{n-1} \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{W} \boldsymbol{b} = \rho \boldsymbol{\phi}(s)^\top \boldsymbol{b}. \tag{11}$$

We can do without $\boldsymbol{\phi}$ since the equation must hold for all s:

$$\frac{1}{n-1} \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{W} \boldsymbol{b} = \rho \boldsymbol{b}. \tag{12}$$

However, $\|\xi\| = 1$ indicates $\boldsymbol{b}^\top \boldsymbol{W} \boldsymbol{b} = 1$. Furthermore, by the definition of *orthogonality* of functions, ξ_1 and ξ_2 are orthogonal if and only if $\boldsymbol{b}^\top \boldsymbol{W} \boldsymbol{b}_2 = 0$. Since the equation is not straightforward and does not look like an eigenequation, we define $\boldsymbol{u} = \boldsymbol{W}^{1/2} \boldsymbol{b}$ and solve

$$\frac{1}{n-1} \boldsymbol{W}^{1/2} \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{W}^{1/2} \boldsymbol{u} = \rho \boldsymbol{u} \tag{13}$$

and revert it by $\boldsymbol{b} = \boldsymbol{W}^{-1/2} \boldsymbol{u}$. Note that if the basis functions are orthonormal, $\boldsymbol{W}$ reduces to an identity matrix.