Restricted Likelihood Ratio Tests for Functional Effects in the Functional Linear Model

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Modeling Framework

Consider $\{Y_i, \boldsymbol{X}_i, W_i\}$ modeled with a Functional Linear Model (FLM)

$$E[Y_i] = \alpha + \boldsymbol{X}_i\boldsymbol{\beta} + \int W_i(s)\gamma(s)ds \quad (1)$$

- Y_i: Continuous, scalar response for the i-th subject
- $\boldsymbol{X}_i$: Non-functional covariates with coefficients $\boldsymbol{\beta}$
- $W_i(s)$: Functional predictor for $s \in [0, 1]$
- α: Mean parameter
- $\gamma(s)$: Coefficient function of interest

Objective: Determine if a functional predictor should be included in FLM.

1. Test of functional form

$$\begin{aligned} H_0 &: E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \bar{W}_i\beta_W \\ H_A &: E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_i(s)\gamma(s)ds \end{aligned} \quad (2)$$

Does $\gamma(s)$ need to be written as a function, or is the mean sufficient?

Equivalently, $H_0 : \gamma(s) = c$ vs $H_A : \gamma(s) \neq c$ for all $c \in \mathbb{R}$.

2. Test of inclusion

$$\begin{aligned} H_0 &: E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds \\ H_A &: E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds + \int W_{i2}(s)\gamma_2(s)ds \end{aligned} \tag{3}$$

Is the second functional predictor necessary?

Equivalently, $H_0 : \gamma_2(s) = 0$ vs $H_A : \gamma_s \neq 0$.

Outline of Testing Procedure

The authors propose 2 testing procedures. The basic procedure is:

Step 1. Decompose the functional predictor $W_i(s)$ using functional principal components (FPC).

Step 2. Express the coefficient function, $\gamma(s)$, using basis functions.

Step 3. Rewrite the FLM as a linear model or linear mixed model.

Step 4. Test H_0 under the linear (mixed) model using a (restricted)-likelihood ratio test.

Method 1: Functional Principal Components Reg. (FPCR)

Step 1. Use FPC to decompose the functional predictor $W_i(s)$.

$$cov[W_i(s), W_i(s')] = \sum_{k=1}^{\infty} \lambda_k \psi_k(s) \psi_k(s')$$

By a truncated Karhunen-Loéve approximation:

$$W_i(s) = \mu(s) + \sum_{k=1}^{K_w} c_{ik} \psi_k(s)$$

- λ_k: (Non-decreasing) k-th eigenvalue
- ψ_k: k-th eigenfunction
- $\mu(s)$: Mean function
- $c_{ik} = \int \{W_i(s) - \mu(s)\} \psi_k(s) ds$; k-th score for i-th subject.
- K_w: Truncation parameter

Method 1: Functional Principal Components Reg. (FPCR)

Deviating from standard FPCR, subtract the subject-specific predictor means.

$$W_i(s) - \bar{W}_i = \sum_{k=1}^{K_g} c_{ik}^* \psi_k(s)$$

- $\bar{W}_i$: Predictor mean for i-th subject, defined as $\bar{W}_i = \int W_i(s)ds$
- $c_{ik}^* = \int \{W_i(s) - \bar{W}_i\}\psi_k(s)ds$

This is important for re-formulating the linear model to test H_0.

Step 2. Express $\gamma(s)$ using basis set $\boldsymbol{\phi}(s)$.

Define the PC basis $\boldsymbol{\phi}(s) = \{\phi_1(s), \ldots, \phi_{K_g}(s)\}$, and let

$$\gamma(s) = \boldsymbol{\phi}(s)\boldsymbol{\gamma} = \sum_{k=1}^{K_g} \gamma_k \phi_k(s)$$

Where $\boldsymbol{\gamma} = \{\gamma_1, \ldots, \gamma_{K_g}\}$ are fixed basis coefficients.

Step 3. Rewrite the FLM as a linear model.

$$\begin{aligned} E[Y_i] &= \alpha + X_i\beta + \int W_i(s)\gamma(s)ds \\ &= \alpha + X_i\beta + \bar{W}_i\gamma_0 + \int \boldsymbol{c}_i^{*T}\boldsymbol{\psi}^T(s)\boldsymbol{\phi}(s)\boldsymbol{\gamma}ds \\ &= \alpha + X_i\beta + \bar{W}_i\gamma_0 + \boldsymbol{c}_i^{*T}\boldsymbol{\gamma} \end{aligned}$$

Let $\boldsymbol{\beta}^T = [\alpha, \beta, \gamma_0, \boldsymbol{\gamma}]$ and $\boldsymbol{X}_{[i,]} = \begin{bmatrix} 1 & X_i & \boldsymbol{c}_i^{*T} \end{bmatrix}$ Then,

$$E(\boldsymbol{Y}) = \boldsymbol{X}\boldsymbol{\beta}$$

Step 4. Test under the linear model $E[Y_i] = \alpha + X_i\beta + \bar{W}_i\gamma_0 + \mathbf{c}_i^{*T}\boldsymbol{\gamma}$.

1. Test of Functional form

$$H_0 : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \bar{W}_i\beta_W \qquad \Leftrightarrow \boldsymbol{\gamma} = \mathbf{0}$$

$$H_A : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_i(s)\gamma(s)ds \qquad \Leftrightarrow \boldsymbol{\gamma} \neq \mathbf{0}$$

2.Test of Inclusion

$$H_0 : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds$$

$$\Leftrightarrow \gamma_0 = 0 \text{ and } \boldsymbol{\gamma} = \mathbf{0}$$

$$H_A : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds + \int W_{i2}(s)\gamma_2(s)ds$$

$$\Leftrightarrow \gamma_0 \neq 0 \text{ or } \boldsymbol{\gamma} \neq \mathbf{0}$$

Method 2: Penalized Functional Regression (PFR)

Step 1. Use FPC to decompose the functional predictor $W_i(s)$.

$$cov[W_i(s), W_i(s')] = \sum_{k=1}^{\infty} \lambda_k \psi_k(s) \psi_k(s')$$

By a truncated Karhunen-Loéve approximation:

$$W_i(s) = \mu(s) + \sum_{k=1}^{K_w} c_{ik} \psi_k(s)$$

- λ_k: (Non-decreasing) k-th eigenvalue
- ψ_k: k-th eigenfunction
- $\mu(s)$: Smooth mean function
- $c_{ik} = \int \{W_i(s) - \mu(s)\} \psi_k(s) ds$; k-th score for i-th subject.
- K_w: Truncation parameter

Method 2: Penalized Functional Regression (PFR)

Step 2. Express $\gamma(s)$ using basis $\phi(s)$.

Define the B-spline basis $\phi(s) = \{\phi_1(s) = 1, \phi_2(s), \ldots, \phi_{K_g}(s)\}$, and let

$$\gamma(s) = \phi(s)\boldsymbol{g} = \gamma_0 + \sum_{k=1}^{K_g} g_k \phi_k(s)$$

Where $\boldsymbol{g} = \{\gamma_0, g_1, \ldots, g_{K_g}\}$ are basis coefficients, γ_0 is fixed, and g_k are random (from mixed models).

Use a modified first-order random walk prior for g_k, where $g_1 \sim N(0, \sigma_g^2)$ and $g_l \sim N(g_{l-1}, \sigma_g^2)$.

Step 3. Rewrite the FLM as a linear mixed model.

$$
\begin{aligned}
E[Y_i] &= \alpha + X_i\beta + \int W_i(s)\gamma(s)ds \\
&= \alpha + X_i\beta + a + \int \boldsymbol{c}_i^{*T} \boldsymbol{\psi}^T(s)\boldsymbol{\phi}(s)\boldsymbol{\gamma} ds \\
&= \alpha + X_i\beta + a + \boldsymbol{c}_i^{*T} \boldsymbol{Mg}
\end{aligned}
$$

Where $\boldsymbol{M}_{[m,n]} = \int \psi_m(s)\phi_n(s)ds$ and $a = \int \mu(s)\gamma(s)ds$.

In matrix notation, let

- $\boldsymbol{\beta}^T = [\alpha + a, \beta, \gamma_0]$
- $\boldsymbol{X}_{[i,]} = \begin{bmatrix} 1 & X_i & (\boldsymbol{c_i^*}^T \boldsymbol{M})_{[1]} \end{bmatrix}$
- $\boldsymbol{Z}_{[i,]} = (\boldsymbol{c_i^*}^T \boldsymbol{M})_{[2:K_g]}$
- $\boldsymbol{u}^T = \{g_k\}_{k=1}^{K_g}$

Then,

$$E[\boldsymbol{Y}|\boldsymbol{X}, \boldsymbol{u}] = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u}$$
$$\boldsymbol{u} \sim N(\mathbf{0}, \sigma_g^2 \boldsymbol{D})$$

Where $\boldsymbol{D}$ is the penalty matrix induced by the random walk prior.

Step 4. Test under the linear mixed model
$E[\boldsymbol{Y}|\boldsymbol{X}, \boldsymbol{u}] = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u}, \boldsymbol{u} \sim N(\boldsymbol{0}, \sigma_g^2 \boldsymbol{D}), \boldsymbol{\beta}^T = [\alpha, \beta, \gamma_0, \boldsymbol{\gamma}]$

1. Test of Functional form

$$H_0 : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \bar{W}_i\beta_W \qquad \Leftrightarrow \sigma_g^2 = 0$$
$$H_A : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_i(s)\gamma(s)ds \qquad \Leftrightarrow \sigma_g^2 \neq 0$$

2.Test of Inclusion

$$H_0 : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds$$
$$\Leftrightarrow \gamma_0 = 0 \text{ and } \sigma_g^2 = 0$$
$$H_A : E(Y_i) = \alpha + \boldsymbol{X}_i\beta + \int W_{i1}(s)\gamma_1(s)ds + \int W_{i2}(s)\gamma_2(s)ds$$
$$\Leftrightarrow \gamma_0 \neq 0 \text{ or } \sigma_g^2 \neq 0$$

Comparison of Approaches

Method 1: Functional Principal Components Regression (FPCR)

- Testing is done with standard likelihood-ratio tests of fixed effects.
- Selection of K_g controls the smoothness of $\gamma(s)$ and is very important. The authors suggested using cross-validation.
- Overall, simpler and more straightforward than PFR to implement.

Method 2: Penalized Functional Regression (PFR)

- Testing is done with non-standard likelihood-ratio test for random and fixed effects (Crainiceanu and Ruppert (2004), Greven et al. (2008).
- Smoothness of $\gamma(s)$ is induced through the mixed model framework for $\boldsymbol{g}$, for sufficiently large $\#$ of PCs.
- Overall, more flexible than FPCR but more complex to implement.