Supplementary Document for the Manuscript entitled "Sparse Functional Principal Component Analysis in a New Regression Framework"

S1 Theoretical Results

We show the proof of Proposition 1 and Proposition 2 in Section 2 of the main manuscript in details. These two propositions shows that the empirical FPCs can be obtained by minimizing the mean L^2 errors to the observed function data $x_i(t)$. We start with only the first leading FPC in Proposition 1 and extend to the first J leading FPCs in Proposition 2.

Proposition 1. *For any $\tau > 0$, let*

$$\hat{\beta}(t) = \arg\min \frac{1}{n}\sum_{i=1}^{n} \left|\left| x_i - \alpha\langle \beta, x_i\rangle \right|\right|^2 + \tau \int \beta^2(t)dt, \tag{S1}$$

subject to $||\alpha||^2 = 1$, then $\hat{\beta} = c\hat{\phi}_1$, where $\hat{\phi}_1$ is the first empirical eigenfunctions of the sample covariance function $g(s,t) = \frac{1}{n}\sum_{i=1}^{n} x_i(s)x_i(t)$ and c is a constant scale factor.

Proof. For given $\alpha(t)$, each $x_i(t)$ can be expressed as $x_i(t) = \langle \alpha, x_i\rangle\alpha(t) + \eta_i(t)$, in which $\eta_i \perp \alpha$, then the loss function

$$\begin{aligned}
&\frac{1}{n}\sum_{i=1}^{n} ||x_i - \alpha\langle\beta, x_i\rangle||^2 + \tau\int \beta^2(t)dt \\
=&\frac{1}{n}\sum_{i=1}^{n} ||\big(\langle\alpha, x_i\rangle - \langle\beta, x_i\rangle\big)\alpha||^2 + \tau\int\beta^2(t)dt + \sum_{i=1}^{n}||\eta_i||^2 \\
=&\frac{1}{n}\sum_{i=1}^{n}\langle(\alpha-\beta), x_i\rangle^2 + \tau\int\beta^2(t)dt + \sum_{i=1}^{n}||\eta_i||^2,
\end{aligned} \tag{S2}$$

Note that the last term in (S2) does not depend on $\beta(t)$. Therefore, minimizing (S2) is equivalent to minimizing the sum of those first two terms. In addition, we can express both $\alpha(t)$ and $\beta(t)$ using the functional principal components $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_K)$ obtained by decomposing the sample covariance function $g(s,t) = \frac{1}{n}\sum_{i=1}^{n} x_i(s)x_i(t)$ of the functional data. To show that α and β can be expanded using $\boldsymbol{\phi}$, we denote $\alpha = \alpha_1 + \alpha_2$ and $\beta = \beta_1 + \beta_2$, in which $\alpha_1 = \mathbf{a}_1^T\boldsymbol{\phi}$, $\alpha_2 \perp \text{span}\{\phi_1, \ldots, \phi_K\}$, $\beta_1 = \mathbf{b}_1^T\boldsymbol{\phi}$, and $\beta_2 \perp \text{span}\{\phi_1, \ldots, \phi_K\}$. Then $\alpha_2 \perp x_i$ and $\beta_2 \perp x_i$. The loss function

$$\begin{aligned}
&\frac{1}{n}\sum_{i=1}^{n}\langle(\alpha-\beta), x_i\rangle^2 + \tau\int\beta^2(t)dt \\
=&\frac{1}{n}\sum_{i=1}^{n}\langle(\alpha-\beta), x_i\rangle^2 + \tau\int\beta_1^2(t)dt + \tau\int\beta_2^2(t)dt \\
=&\frac{1}{n}\sum_{i=1}^{n}||\mathbf{a}_1^T\mathbf{s}_i - \mathbf{b}_1^T\mathbf{s}_i||^2 + \tau||\mathbf{b}_1||^2 + \tau||\boldsymbol{\beta}_2||^2 \\
=&\frac{1}{n}||\mathbf{S}\mathbf{a}_1 - \mathbf{S}\mathbf{b}_1||^2 + \tau||\mathbf{b}_1||^2 + \tau||\boldsymbol{\beta}_2||^2,
\end{aligned}$$

where $\mathbf{s}_i = (\int x_i(t)\phi_1(t)dt, \ldots, \int x_i(t)\phi_K(t)dt)^T$, and $\mathbf{S} = (\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n)^T$ is an $n \times K$ score matrix. Then the above loss function becomes a ridge regression problem with the solution

$$\widehat{\mathbf{b}}_1 = (\mathbf{S}^T\mathbf{S} + n\tau\mathbf{I})^{-1}\mathbf{S}^T\mathbf{S}\mathbf{a}_1, \text{ and } \hat{\beta}_2(t) \equiv 0.$$

Substituting the estimate $\hat{\beta} = \widehat{\mathbf{b}}_1^T\boldsymbol{\phi}$ into the loss function, we have

$$\begin{aligned}
&\frac{1}{n}\sum_{i=1}^{n}||x_i - \alpha\langle\hat{\beta}, x_i\rangle||^2 + \tau\int\hat{\beta}^2(t)dt \\
=&\frac{1}{n}\sum_{i=1}^{n}||\mathbf{s}_i^T\boldsymbol{\phi} - (\mathbf{a}_1^T\boldsymbol{\phi} + \alpha_2)\widehat{\mathbf{b}}_1^T\mathbf{s}_i||^2 + \tau\hat{\mathbf{b}}_1^T\hat{\mathbf{b}}_1 \\
=&\frac{1}{n}\sum_{i=1}^{n}||\mathbf{s}_i^T\boldsymbol{\phi} - \widehat{\mathbf{b}}_1^T\mathbf{s}_i\mathbf{a}_1^T\boldsymbol{\phi}||^2 + \tau\hat{\mathbf{b}}_1^T\hat{\mathbf{b}}_1 + \frac{1}{n}\sum_{i=1}^{n}||\alpha_2\hat{\mathbf{b}}_1^T\mathbf{s}_i||^2 \\
=&\frac{1}{n}\sum_{i=1}^{n}||\mathbf{s}_i - \mathbf{a}_1\hat{\mathbf{b}}_1^T\mathbf{s}_i||^2 + \tau\hat{\mathbf{b}}_1^T\hat{\mathbf{b}}_1 + \frac{1}{n}\sum_{i=1}^{n}||\alpha_2\hat{\mathbf{b}}_1^T\mathbf{s}_i||^2 \\
=&Tr(\mathbf{S}^T\mathbf{S}) - 2\mathbf{a}_1^T\mathbf{S}^T\mathbf{S}\hat{\mathbf{b}}_1 + \hat{\mathbf{b}}_1^T(n\tau\mathbf{I} + \mathbf{S}^T\mathbf{S})\hat{\mathbf{b}}_1 + \frac{1}{n}\sum_{i=1}^{n}||\alpha_2\hat{\mathbf{b}}_1^T\mathbf{s}_i||^2 \\
=&Tr(\mathbf{S}^T\mathbf{S}) - \mathbf{a}_1^T\mathbf{S}^T\mathbf{S}(n\tau\mathbf{I} + \mathbf{S}^T\mathbf{S})^{-1}\mathbf{S}^T\mathbf{S}\mathbf{a}_1 + \frac{1}{n}\sum_{i=1}^{n}||\alpha_2\hat{\mathbf{b}}_1^T\mathbf{s}_i||^2. \qquad \text{(S3)}
\end{aligned}$$

The last term in (S3) is reduced to zero only when $\alpha_2(t) = 0$. In addition, since

$$\mathbf{S}^T\mathbf{S}(n\tau\mathbf{I} + \mathbf{S}^T\mathbf{S})^{-1}\mathbf{S}^T\mathbf{S} = \text{diag}(\frac{\lambda_1^2}{n\tau + \lambda_1}, \ldots, \frac{\lambda_K^2}{n\tau + \lambda_K}),$$

the second term in (S3) is maximized when $\widehat{\mathbf{a}}_1 = (1, 0, 0, \ldots, 0)$, due to the fact that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_K$. Therefore, $\hat{\alpha} = \phi_1$ and $\widehat{\beta} = \frac{\lambda_1}{n\tau + \lambda_1}\phi_1$. $\square$

The next theorem extends Proposition 1 into the first J leading FPCs.

Proposition 2. *Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_J)$ and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_J)$. For any $\tau > 0$, let*

$$(\widehat{\boldsymbol{\alpha}}, \widehat{\boldsymbol{\beta}}) = \arg\min \frac{1}{n} \sum_{i=1}^{n} ||x_i - \sum_{j=1}^{J} \alpha_j \langle \beta_j, x_i \rangle||^2 + \tau \sum_{j=1}^{J} \int \beta_j^2(t) dt,$$

subject to $\langle \alpha_i, \alpha_j \rangle = \delta_{ij}$ and δ_{ij} is the Kronecker delta, then $\hat{\beta}_j = c_j \hat{\phi}_j, j = 1, \ldots, J$, where $\hat{\phi}_j(t)$ is the j-th empirical eigenfunctions of the sample covariance function $g(s,t) = \frac{1}{n}\sum_{i=1}^{n} x_i(s) x_i(t)$ and c_j is a scale factor.

Proof. For given $\boldsymbol{\alpha}$, each x_i can be expressed as $x_i(t) = \sum_{j=1}^{J} \langle x_i, \alpha_j \rangle \alpha_j(t) + \eta_i(t)$, in which $\eta_i \perp span\{\alpha_1, \ldots, \alpha_J\}$, then

$$\begin{aligned}
&\frac{1}{n} \sum_{i=1}^{n} ||x_i - \sum_{j=1}^{J} \alpha_j \langle \beta_j, x_i \rangle||^2 + \tau \sum_{j=1}^{J} \int \beta_j^2(t) dt \\
=&\frac{1}{n} \sum_{i=1}^{n} ||\Big(\langle \boldsymbol{\alpha}, x_i \rangle - \langle \boldsymbol{\beta}, x_i \rangle \Big)^T \boldsymbol{\alpha}||^2 + \tau ||\boldsymbol{\beta}||^2 + \sum_{i=1}^{n} ||\eta_i||^2 \\
=&\frac{1}{n} \sum_{i=1}^{n} ||\langle \boldsymbol{\alpha}, x_i \rangle - \langle \boldsymbol{\beta}, x_i \rangle||^2 + \tau ||\boldsymbol{\beta}||^2 + \sum_{i=1}^{n} ||\eta_i||^2.
\end{aligned}$$

Due to the fact that α_j is orthogonal to each other, we can maximize the above loss function for each $\beta_j, j = 1, \ldots, J$ separately. More specifically,

$$\hat{\beta}_j(t) = \arg\min \frac{1}{n} \sum_{i=1}^{n} ||\langle \alpha_j, x_i \rangle - \langle \beta_j, x_i \rangle||^2 + \tau ||\beta_j||^2.$$

Similarly, we can express both β_j and α_j using the FPCs $\boldsymbol{\phi}(t)$ as $\beta_j = \mathbf{b}_j^T \boldsymbol{\phi}$ and $\alpha_j = \mathbf{a}_j^T \boldsymbol{\phi}$. Then the solution is given as

$$\widehat{\mathbf{b}}_j = (\mathbf{S}^T\mathbf{S} + n\tau\mathbf{I})^{-1}\mathbf{S}^T\mathbf{S}\mathbf{a}_j,$$

in which $\mathbf{s}_i = (\int x_i(t)\phi_1(t)dt, \ldots, \int x_i(t)\phi_K(t)dt)^T$ and $\mathbf{S} = (\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n)^T$ is an $n \times K$ score matrix. Now substituting $\widehat{\mathbf{b}}_j$ into the loss function, we have

$$\begin{aligned}
&\frac{1}{n} \sum_{i=1}^{n} ||x_i - \sum_{j=1}^{J} \alpha_j \langle \beta_j, x_i \rangle||^2 + \tau \sum_{j=1}^{J} \int \beta_j^2(t) dt \\
=&Tr(\mathbf{S}^T\mathbf{S}) - 2Tr(\mathbf{a}^T\mathbf{S}^T\mathbf{S}\hat{\mathbf{b}}) + Tr(\hat{\mathbf{b}}^T(\mathbf{S}^T\mathbf{S} + n\tau\mathbf{I})\hat{\mathbf{b}} \\
=&Tr(\mathbf{S}^T\mathbf{S}) - 2\sum_{j=1}^{J} Tr(\mathbf{a}_j^T\mathbf{S}^T\mathbf{S}\hat{\mathbf{b}}_j) + \sum_{j=1}^{J} Tr(\hat{\mathbf{b}}_j^T(\mathbf{S}^T\mathbf{S} + n\tau\mathbf{I})\hat{\mathbf{b}}_j) \\
=&Tr(\mathbf{S}^T\mathbf{S}) - \sum_{j=1}^{J} Tr(\mathbf{a}_j^T\mathbf{S}^T\mathbf{S}(\mathbf{S}^T\mathbf{S} + n\tau\mathbf{I})^{-1}\mathbf{S}^T\mathbf{S}\mathbf{a}_j).
\end{aligned}$$

Note that

$$\mathbf{S}^T\mathbf{S}(\mathbf{S}^T\mathbf{S}+\tau\mathbf{I})^{-1}\mathbf{S}^T\mathbf{S} = \text{diag}(\frac{\lambda_1^2}{n\tau+\lambda_1}, \ldots, \frac{\lambda_K^2}{n\tau+\lambda_K}),$$

is a diagonal matrix with decreasing value on the diagonal, since $\lambda_1 > \lambda_2 > \ldots > \lambda_K$. When $J \le K$, the second term in the above equation, $\sum_{j=1}^{J} Tr(\mathbf{a}_j^T\mathbf{S}^T\mathbf{S}(\mathbf{S}^T\mathbf{S}+n\tau\mathbf{I})^{-1}\mathbf{S}^T\mathbf{S}\mathbf{a}_j) \le \sum_{k=1}^{J}\frac{\lambda_1^2}{n\tau+\lambda_1}$. We can see that the second term is maximized when $a_j = (0, \ldots, j, \ldots, 0)$, in which the jth element is 1 and 0 elsewhere. Therefore the loss function is minimized when $\hat{\alpha} = \hat{\phi}_j$ and $\hat{\beta}_j = \frac{\lambda_j}{\lambda_j+n\tau}\hat{\phi}_j$.

□

S2 More Simulation Studies

S2.1 Effect of τ

The ridge type penalty term $\sum_{j=1}^{J}\int\beta_j^2(t)dt$ essentially ensures the identifiability of the primary parameter (i.e., β_j). The reason can be explained by the following example.

We assume that the functional data $x_i(t)$ can be expressed by K eigenfunctions:

$$x_i(t) = \sum_{k=1}^{K}\alpha_{ik}\phi_k(t).$$

There always exits a fixed function η such as $\eta \perp span(\phi_1, \ldots, \phi_K)$.

Now if the ridge penalty term is removed in equation (1), the objective function in Proposition 1 becomes

$$Q(\beta) = \frac{1}{n}\sum_{i=1}^{n}\left|\left|x_i - \alpha\langle\beta, x_i\rangle\right|\right|^2,$$

subject to $||\alpha||^2 = 1$. However, this objective function doesn't result in a single minimizer. For example, given α, for any $\beta = \sum_{k=1}^{K} b_k\phi_k$, there always exists a corresponding $\beta' = \beta+\eta$ such that these two objective functions equal.

On the other hand, with $\tau > 0$, the new objective function becomes

$$Q_\tau(\beta) = \frac{1}{n}\sum_{i=1}^{n}\left|\left|x_i - \alpha\langle\beta, x_i\rangle\right|\right|^2 + \tau\int\beta^2(t)dt,$$

it grantees that, for any η such that $\eta \perp span(\phi_1, \ldots, \phi_K)$ and for any $\beta = \sum_{k=1}^{K} b_k\phi_k$, if $\beta' = \beta+\eta$, then $Q_\tau(\beta') > Q_\tau(\beta)$. Therefore, it guarantees that the minimizor of $Q_\tau(\beta)$ is identifiable.

We conduct a simulation study to investigate the effect of τ. The simulation results show that the estimated sparse FPCs are almost the same with different values of τ, as Proposition 2 is valid for any positive value of τ.

We generate the true underlying functional curves in a similar as the simulation study in the main manuscript. That is,

$$X_i(t) = s_{i1}\xi_1(t) + s_{i2}\xi_2(t) + s_{i3}\xi_3(t) + s_{i4}\xi_4(t),$$

$t \in [1, 60]$, where $\xi_k(t), k = 1, 2, 3, 4$, are obtained from the real data application as shown in Figure 3 in the manuscript, and $(\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3, \mathbf{s}_4)$ are generated from multivariate normal distribution with mean zero and the variance-covariance matrix $\Sigma = \text{diag}(30, 20, 10, 3)$. The observed trajectories are generated by $Y_{ij} = X_i(t_j) + \epsilon_{ij}$ for $j = 1, \ldots, 60$, where t_j is the j-th observed point equally spaced in $[1, 60]$ and $\epsilon_{ij} \overset{i.i.d}{\sim} N(0, \sigma_0^2)$.

To propose a reasonable range for the candidate value of τ, we estimate first estimate the first 4 eigenvalues using conventional FPCA method. Then we specify various values of τ ranging from the smallest estimated eigenvalue $\hat{\lambda}_4$ to the largest eigenvalue $\hat{\lambda}_1$ with fixed value of $\gamma = 100$ and $\lambda = 40$ to compare estimated sparse FPCs.

Figure S1 above shows the estimated sparse FPCs when $\sigma_0 = 1$. In addition, τ is chosen from 10 different values equally spaced between 1 and 50. This range is select to include the smallest estimated eigenvalue, i.e., 14 and the largest eigenvalue, i.e.,38 using the conventional FPCA. As can be seen from Figure S1, different values of τ result in almost the same estimations of sparse FPC.

S2.2 Effect of Rank Misspecification

We conduct the following numerical study to investigate the effect of rank misspecification on the results of the proposed algorithm.

We generate the true underlying functional curves in a similar manner as the simulation study in the main manuscript. That is,

$$X_i(t) = s_{i1}\xi_1(t) + s_{i2}\xi_2(t) + s_{i3}\xi_3(t) + s_{i4}\xi_4(t),$$

$t \in [1, 60]$, where $\xi_k(t), k = 1, 2, 3, 4$, are obtained from the real data application as shown in Figure 3 in the manuscript, and $(\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3, \mathbf{s}_4)$ are generated from multivariate normal distribution with mean zero and the variance-covariance matrix $\Sigma = \text{diag}(30, 20, 10, 3)$. The observed trajectories are generated by $Y_{ij} = X_i(t_j) + \epsilon_{ij}$ for $j = 1, \ldots, 60$, where t_j is the j-th observed point equally spaced in $[1, 60]$ and $\epsilon_{ij} \overset{i.i.d}{\sim} N(0, \sigma_0^2)$.

We fix $\gamma = 100$, $\lambda = 40$, $\tau = 30$ and compare two models: the correct rank model with $K = 4$ and a mis-specified with ranking being 3.

In each simulation repetition, we compute the the squared integrated difference (SID) between those two estimates defined as follows:

$$\text{SID}_k = \frac{1}{T}\int_0^T (\hat{\xi}_k^{(3)}(t) - \hat{\xi}_k^{(4)}(t))^2 dt,$$

in which $\hat{\xi}_k^{(3)}(t)$ and $\hat{\xi}_k^{(4)}(t)$ represent the estimated k-th FPC under the misspecified rank-3 and the correctly specified rank-4 model, respectively. Table S1 shows the mean SID for 100 simulation repetitions. Figure S2 shows the estimated sparse FPCs under those two models.

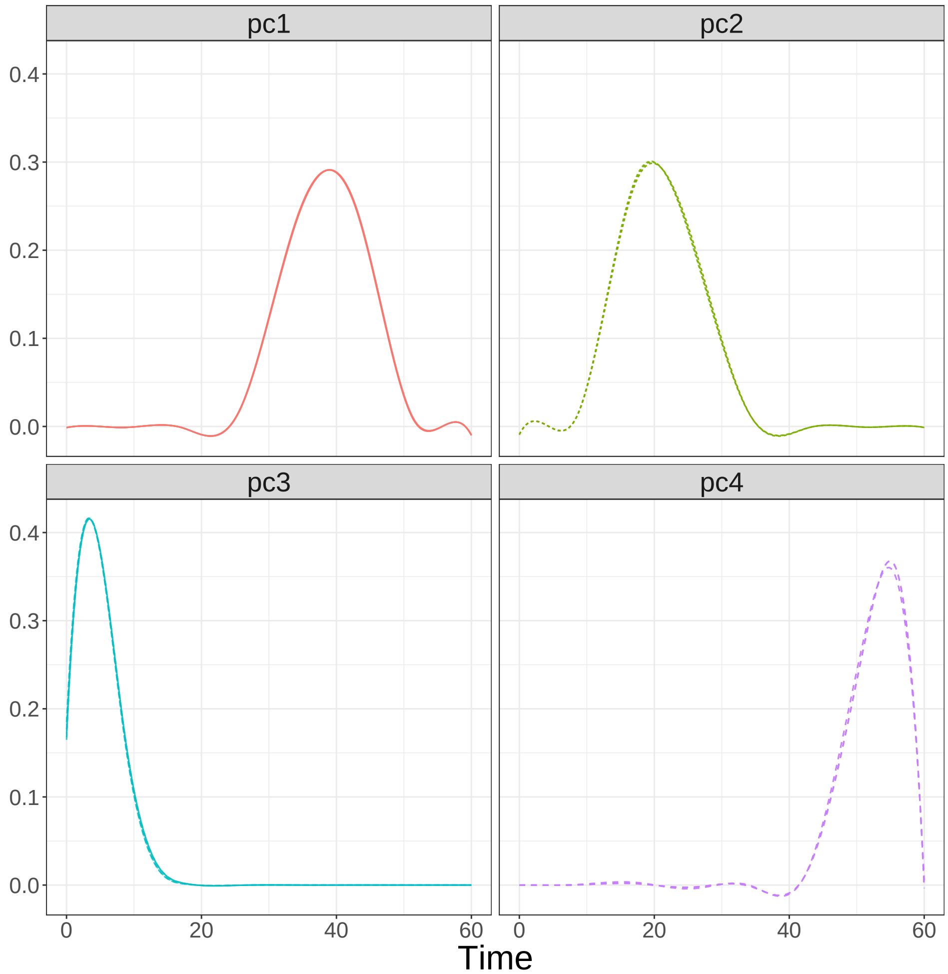

Figure S1: Estimated sparse FPCs with different values of ridge penalty parameter τ.

As can be seen from both the mean SID and Figure S2, when the rank is misspecified as 3, each estimated sparse FPC is almost the same as the corresponding estimated sparse FPC when the rank is correctly specified as 4.

Table S1: The average squared integrated difference (SID) for the first three estimated FPCs between rank-3 and rank-4 model.

	First FPC	Second FPC	Third FPC
Average SID	3.58e-03	1.58e-07	1.47e-05

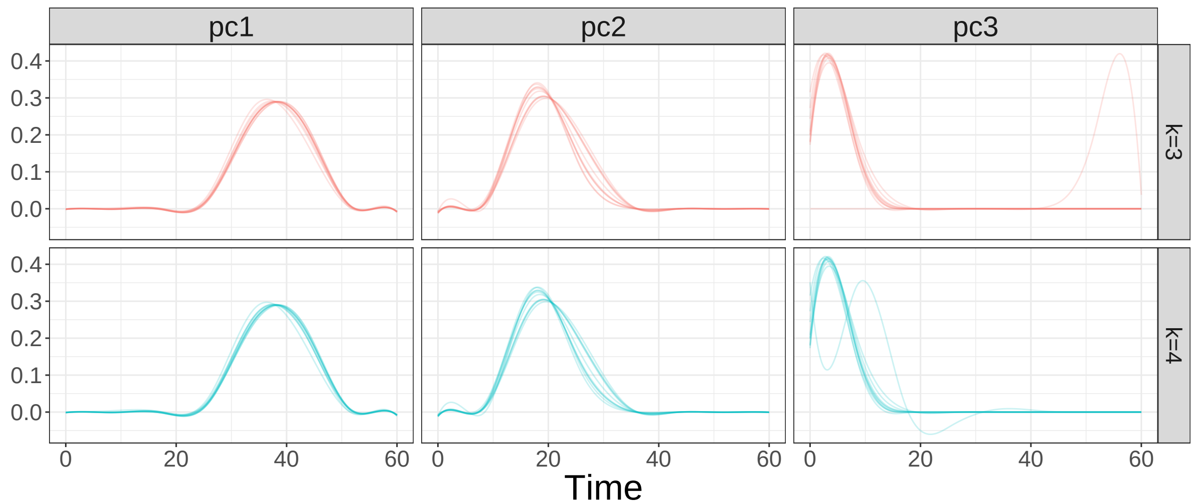

Figure S2: Estimated sparse FPCs with different values of rank specification: $k = 3$ and $k = 4$.