# Supplementary Material to "Additive Nonlinear Functional Concurrent Model"

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This Supplementary Material contains six sections. Section A discusses modifications required by the proposed estimation procedure when responses and/or covariates are observed on a sparse and irregular grid of points. Section B describes the transformation of the functional covariates required by our estimation procedure. Section C details the evaluation criteria used in our simulation experiment. Additional simulation results are in Section D. Additional results from data applications are in Section E. Section F presents the implementation details.

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### A Model Estimation for Irregular and Sparse Design

The proposed method easily accommodates more realistic situations where the covariates or the responses are observed on a sparse sampling design. Here we discuss the modifications required by the proposed estimation procedure to accommodate such sparseness. This approach was used in the simulation study as well as in the analysis of the dietary calcium absorption data.

Suppose for  $i = 1, ..., n$  we observe the functional covariates  $X_{1,i}(t_{1ij})$  for  $j =$  $1, \ldots, m_{1i}$  and  $X_{2,i}(t_{2ij})$  for  $j = 1, \ldots, m_{2i}$ . Also, for  $i = 1, \ldots, n$  we observe the functional response  $Y_i(t_{ik})$  for  $k = 1, ..., m_{Y,i}$ . Our goal is to estimate the unknown model components,  $\mu_Y(\cdot)$ ,  $F_1(\cdot, \cdot)$  and  $F_2(\cdot, \cdot)$ , of additive nonlinear functional concurrent model (ANFCM),  $Y_i(t) = \mu_Y(t) + F_1\{X_{1,i}(t), t\} + F_2\{X_{2,i}(t), t\} + \epsilon_i(t)$ . Using basis expansions, an equivalent form of the model can be found as  $Y_i(t) = \mathbf{B}_{\mu}^T(t)\mathbf{\Theta}_{\mu} + \mathbf{Z}_{1,i}^T(t)\mathbf{\Theta}_1 +$  $\mathbf{Z}_{2,i}^T(t)\mathbf{\Theta}_2+\epsilon_i(t)$ ; here,  $\mathbf{B}_{\mu}(t)$  and  $\mathbf{Z}_{q,i}(t)$   $(q=1,2)$  are defined using pre-specified B-spline basis functions, as detailed in Section 2.2 of the main article.

When the responses and the covariates have different observation points, we first smooth the covariates  $X_{q,i}(\cdot)$  to obtain the estimated smooth curve  $\widehat{X}_{q,i}(\cdot)$  of  $X_{q,i}(\cdot)$ , and we evaluate the smooth curve  $\widehat{X}_{q,i}(\cdot)$  at the points  $t_{ik}$  - the points at which the response is observed. Then we approximate the penalized sum of squares by

$$
\sum_{i=1}^n \Big[ \sum_{k=1}^{m_{Y,i}} \{ Y_i(t_{ik}) - \mathbf{B}_{\mu}(t_{ik})^T \mathbf{\Theta}_{\mu} - \mathbf{Z}_{1,i}^T(t_{ik}) \mathbf{\Theta}_1 - \mathbf{Z}_{2,i}^T(t_{ik}) \mathbf{\Theta}_2 \}^2 / m_{Y,i} \Big] +
$$
  

$$
\mathbf{\Theta}_{\mu}^T \mathbb{P}_{\mu} \mathbf{\Theta}_{\mu} + \mathbf{\Theta}_1^T \mathbb{P}_1 \mathbf{\Theta}_1 + \mathbf{\Theta}_2^T \mathbb{P}_2 \mathbf{\Theta}_2,
$$

where  $\mathbb{P}_{\mu}$ ,  $\mathbb{P}_{1}$  and  $\mathbb{P}_{2}$  are the penalty matrices defined in Section 2.2 of the main article using  $\widehat{X}_{q,i}(\cdot)$  in place of  $X_{q,i}(\cdot)$  ( $q = 1, 2$ ). To estimate the unknown parameters  $\Theta_{\mu}$ ,  $\Theta_{1}$ and  $\Theta_2$ , we minimize the above penalized criterion. For a simple illustration, let  $Y_i =$  $[Y_i(t_{i1}), \ldots, Y_i(t_{im_{Y,i}})]^T$  and  $\mathbf{E}_i = [\epsilon_i(t_{i1}), \ldots, \epsilon_i(t_{im_{Y,i}})]^T$  be the  $m_{Y,i}$ -dimensional vector of response and random errors for subject *i*. Define  $\mathbb{B}_{\mu}$  as  $m_{Y,i} \times K_{\mu}$ -dimensional matrix with the j-th row given by  $\mathbf{B}_{\mu}^{T}(t_{ik})$  and  $\mathbb{Z}_{q,i}$  as  $m_{Y,i}\times K_{xq}K_{tq}$ -dimensional matrix with the j-th row given by  $\mathbf{Z}_{q,i}^T(t_{ik})$ . We further denote  $\mathbb{Z}_i = [\mathbb{B}_{\mu} | \mathbb{Z}_{1,i} | \mathbb{Z}_{2,i}], \ \mathbf{\Theta}^T = [\mathbf{\Theta}_{\mu}^T, \mathbf{\Theta}_1^T, \mathbf{\Theta}_2^T]^T$ 

and  $\mathbb{P} = \text{diag}(\mathbb{P}_{\mu}, \mathbb{P}_{1}, \mathbb{P}_{2})$ . Then, the solution of  $\Theta$  is found as

$$
\widehat{\mathbf{\Theta}} = \mathbb{H}\{\textstyle{\sum_{i=1}^{n}}\mathbb{Z}_i^T\mathbf{Y}_i\}
$$

with  $\mathbb{H} = \{\sum_{i=1}^n \mathbb{Z}_i^T \mathbb{Z}_i + \mathbb{P}\}^{-1}$ . Furthermore, the variance of  $\widehat{\Theta}$  can be derived, following the same procedure described in Section 2.3 of the main article:

$$
\text{var}(\widehat{\boldsymbol{\Theta}}) = \mathbb{H}\{\sum_{i=1}^n \mathbb{Z}_i^T \mathbb{G}_i \mathbb{Z}_i\} \mathbb{H}^T,
$$

where  $\mathbb{G}_i = \text{cov}(\mathbf{E}_i) = [G(t_{ij}, t_{ik})]_{1 \leq j,k \leq m_{Y,i}}$  with dimension  $m_{Y,i} \times m_{Y,i}$  for each i.

# B Preprocessing of the Functional Covariates

One challenge of our estimation approach is that some B-spline basis functions might not have observed data on its support. This problem is more likely to arise when the covariate  $X(\cdot)$  is observed on sparse and irregular gird of points, and realizations of the function,  $X(t_j)$ , are not dense over R. To bypass this limitation, we propose to apply a point-wise centering and scaling transformation of the covariates; it is worthwhile to note that this problem is addressed by [2] with a different approach.

We define point-wise center/scaling transformation of  $X(t)$  by

$$
X^*(t) = \{X(t) - \mu_X(t)\}/\sigma_X(t),
$$

where  $\mu_X(t)$  and  $\sigma_X(t)$  denote the mean and the standard deviation of  $X(t)$ , respectively. One can interpret the transformed covariate  $X^*(t)$  as the amount of standard deviations  $X(t)$  is away from the mean at time t. In practice, we estimate the mean and the standard deviation by the sample mean  $\hat{\mu}_X(t)$  and the sample standard deviation  $\hat{\sigma}_X(t)$  of the covariate. Thus for a fixed point  $t_j$  we will obtain realizations of the transformed covariates  ${X_i^*(t_j)}_{i=1}^n$  based on the sample mean  $\hat{\mu}_X(t_j)$  and the sample standard deviation  $\hat{\sigma}_X(t_j)$ at the same point. The prediction procedure described in Section 2.4 of the main article proceeds as before with the understanding that one now uses the transformed version of the new covariates,  $X^*_{\text{new}}(t)$ 

$$
X_{\text{new}}^*(t) = \{X_{\text{new}}(t) - \mu_X(t)\}/\sigma_X(t),
$$

where we estimate the mean  $\mu_X(t)$  and the standard deviation  $\sigma_X(t)$  using the sample mean and the sample standard deviation obtained from the training data. Our empirical study has shown that the above transformation technique effectively controls the numerical stability issues while still preserving predictive accuracy.

### C Evaluation Criteria

In Section 5.2.1 of the main article, we studied prediction performance of the proposed method using 1000 Monte Carlo simulations. Estimation and prediction accuracy were assessed using in-sample and out-of-sample root mean squared prediction error (RMSPE). The performance of variance estimation was measured through integrated coverage probability (ICP) and integrated width (IW) of the point-wise prediction intervals. We now describe how we define the above measures.

We define the in-sample RMSPE by

RMSPE<sup>in</sup> = 
$$
\frac{1}{1000 \cdot n} \sum_{r=1}^{1000} \left[ \sum_{i=1}^{n} \frac{1}{m_i} \sum_{k=1}^{m_i} \left\{ Y_i^{(r)}(t_{ik}) - \widehat{Y}_i^{(r)}(t_{ik}) \right\}^2 \right]^{\frac{1}{2}},
$$

where  $Y_i^{(r)}$  $\hat{Y}_i^{(r)}(t_{ik})$  and its estimate  $\hat{Y}_i^{(r)}(t_{ik})$  are from the r-th Monte Carlo simulation. The out-of-sample RMSPE, denoted by RMSPE<sup>out</sup>, is defined similarly.

We construct  $(1 - \alpha)100\%$  point-wise prediction intervals to observe coverage probabilities at the nominal level. The ICP at the  $(1 - \alpha)$  level is given by

$$
\text{ICP}(1-\alpha) = \frac{1}{1000 \cdot n} \sum_{r=1}^{1000} \sum_{i=1}^{n} \int_{0}^{1} I\{Y_{\text{new},i}^{(r)}(t) \in C_{1-\alpha,i}^{(r)}(t)\} dt,
$$

where  $C_{1-\alpha,i}^{(r)}(t)$  is the point-wise prediction interval from the r-th Monte Carlo simulation and  $I(\cdot)$  is the indicator function. The prediction interval  $C_{1-\alpha,i}^{(r)}(t)$  is as previously defined in Section 2.4 of the main article.

The IW of the  $(1 - \alpha)$  level prediction intervals is defined by

$$
IW(1 - \alpha) = \frac{1}{1000 \cdot n} \sum_{r=1}^{1000} \sum_{i=1}^{n} \int_{0}^{1} 2MOE_{1-\alpha,i}^{(r)}(t)dt,
$$

where  $\text{MOE}_{1-\alpha,i}^{(r)}(t) = \Phi^{-1}(1-\alpha/2) \times [\widehat{\text{var}}\{Y_{\text{new}}^{(r)}\}]$  $\hat{P}_{\text{new},i}^{(r)}(t) - \widehat{Y}_{\text{new},i}^{(r)}(t)\}]^{-\frac{1}{2}}, \text{ and } \Phi(\cdot) \text{ is the standard}$ Gaussian cumulative distribution function.

The prediction bands may fluctuate dramatically at some points, and such cases may not be captured by the IW. Therefore, we examine the range of the estimated standard errors (SE). For  $(1 - \alpha)100\%$  prediction intervals, we define the minimum SE by

$$
\min(\text{SE}) = \frac{1}{1000 \cdot n} \sum_{r=1}^{1000} \sum_{i=1}^{n} \min_{t} \{2\text{MOE}_{1-\alpha,i}^{(r)}(t)\}.
$$

The maximum SE, denoted by max(SE), is defined similarly. Then we define  $R(SE)$ =  $\lceil \min(\text{SE}), \max(\text{SE}) \rceil$ , which gives the range of SE at the  $(1 - \alpha)$  level.

# D Additional Simulation Results

In this section, we report results from additional simulation studies. Section D.1 reports simulation results corresponding to another level of sparseness. Section D.2 compares the prediction results using other competitive approaches for covariance estimation. Section D.3 presents additional results for larger measurement error variance in functional covariates as well as a smaller sample size  $(n = 40)$  in addition to  $n = 100$  and 300. Section D.4 investigates the effect of different choices of number of basis functions. Section D.5 investigates the model performance with up to five functional covariates through a numerical study. Section D.6 presents power curves for a densely sampled scenario.

#### D.1 Further Investigation of Prediction Error

#### D.1.1 Additional Simulations for Irregular and Sparse Design

We provide additional simulation results corresponding to another level of sparseness. Specifically, we consider a scenario with a lower level of sparseness compared to that of the sparse design considered in Section 5.1 of the main article; the new setting uses  $m_i \stackrel{iid}{\sim} Unif(29, 41)$  points for the functional response and covariates, and thereby this sampling design is called *moderately sparse design*. As before, the setting used in the main article is called sparse design. We compared the predictive accuracy of our method for both scenarios (moderately sparse and sparse designs) using the evaluation criteria defined in Section C, and results are presented in Table 1. The moderately sparse setting improved both in-sample and out-of-sample prediction accuracy, compared to the results corresponding to the sparse design.

#### D.1.2 Additional Simulations for Complicated Error Structure

Next, we further discuss prediction accuracy investigated in Section 5.2.1 of the main article. In Table 2 of the main article, the value of RMSPE<sup>in</sup> corresponding to non-stationary error covariance  $(\mathbf{E}_{i}^{3})$  slightly increases with the larger sample size. For further investigation, one needs to compare the values of  $RMSPE^{in}$  with the true standard deviation of the error process. The true standard deviation (averaged over  $t$ ) of the error process used in the simulation study can be computed as:

$$
sd(\mathbf{E}_i^1) = \sqrt{0.8} \approx 0.89.
$$
  
\n
$$
sd(\mathbf{E}_i^2) = \sqrt{0.8 + 0.8} \approx 1.26.
$$
  
\n
$$
sd(\mathbf{E}_i^3) = \sqrt{2 + 0.75^2 + 0.8} \approx 1.83.
$$

Table 2 shows the RMSPE<sup>in</sup> with the estimated standard errors in the parentheses for different sampling scenarios and for the error process corresponding to  $\mathbf{E}_i = \mathbf{E}_i^3$ . As expected, the performance of the proposed estimation is slightly affected by the different sampling designs (e.g., dense/sparse design) and the model complexity. With the smaller number of observations per curve (e.g., sparse design) and/or with the increased model complexity (e.g., Scenario C), the values of  $RMSPE<sup>in</sup>$  are more different from the true standard deviation of the error process, compared to the results corresponding to the different simulation settings. Nevertheless, the results indicate that the target values (true standard deviation of the error process) are within two standard deviations of the estimated values, and therefore the results are still valid for the different model complexity as well as for the dense/sparse sampling designs.



		dense design	moderately sparse design	sparse design
Scenario	n	$m=81$	$m_i \stackrel{iid}{\sim} Unif(29, 41)$	$m_i \stackrel{iid}{\sim} Unif(20,31)$
Α	100	1.80(0.08)	1.81(0.08)	1.81(0.08)
	300	1.83(0.05)	1.83(0.05)	1.84(0.05)
В	100	1.84(0.08)	1.90(0.09)	1.94(0.09)
	300	1.87(0.05)	1.92(0.05)	1.96(0.05)
C	100	1.80(0.08)	1.86(0.08)	1.91(0.09)
	300	1.85(0.05)	1.90(0.05)	1.94(0.05)

Table 2: Summary of RMSPE<sup>in</sup> and the estimated standard errors (in parentheses) obtained by fitting the ANFCM based on 1000 simulations. The simulation settings correspond to the case where  $\mathbf{E}_i = \mathbf{E}_i^3$ .

# D.2 Further Investigation of Different Covariance Estimation Methods

In the literature, there are various approaches to estimate the covariance of the residual process: using local polynomial smoothing and using global smoothing via B-spline basis functions. So far the latter approach is implemented in R, whereas the former one is implemented in Matlab. The proposed method in Section 2.3 of the main article is implemented by fpca.sc function in refund R package, which uses the tensor product bi-variate P-splines. In this section, we further consider two alternative approaches: (i)  $|5|$  which is implemented using the Matlab toolbox PACE and (ii)  $|4|$  implemented in R using fpca.face function of the refund package [1]. We carried out additional simulation studies to compare the performance of variance estimation for two cases when the functional covariates are observed densely or sparsely and with measurement error. In the interest of space, we only considered the situations where we have a single functional covariate (see Scenario A and B defined in Section 5.1 of the main article). Table 3 shows the results for the  $n = 100$  and  $\mathbf{E}_i = \mathbf{E}_i^3$  obtained by fitting the ANFCM. Evidently, the results are quite robust to the methods.

# D.3 Additional Simulations for Larger Measurement Error in Functional Covariates and Small Sample Size

In Table 2 of the main article, the covariates are generated with measurement error with variance 0.6<sup>2</sup>. Now, we consider two different error variances:  $\tau^2 = 1$  and 2. We also

Scenario B (true relationship is nonlinear)									
	$1 - \alpha = 0.95$			$1 - \alpha = 0.90$		$1 - \alpha = 0.85$			
Method	ICP	IW	R(SE)	ICP	IW	ICP	IW		
$m = 81$ (dense design)									
fpca.sc	0.946	7.34	[5.53, 9.84]	0.895	6.16	0.844	5.39		
fpca.face	0.940	7.22	[5.49, 9.82]	0.886	6.06	0.835	5.30		
PACE	0.943	7.29	[5.43, 9.73]	0.889	6.12	0.839	5.35		
$m_i \stackrel{iid}{\sim} Unif(29, 41)$ (moderately sparse design)									
fpca.sc	0.948	7.55	[5.69, 10.67]	0.899	6.34	0.849	5.55		
fpca.face	0.943	7.37	[5.64, 10.24]	0.890	6.18	0.841	5.41		
PACE	0.948	7.62	[5.65, 11.12]	0.897	6.40	0.849	5.60		
iid $m_i \stackrel{ua}{\sim} Unif(20,31)$ (sparse design)									
fpca.sc	0.949	7.69	[5.82, 11.09]	0.900	6.46	0.852	5.65		
fpca.face	0.939	7.38	[5.59, 11.38]	0.885	6.19	0.834	5.42		
PACE	0.950	7.85	[5.84, 11.78]	0.902	6.59	0.855	5.77		
Scenario $\overline{A}$ (true relationship is linear)									
$1 - \alpha = 0.95$ $1 - \alpha = 0.90$ $1 - \alpha = 0.85$									
Method	ICP	IW	R(SE)	ICP	IW	ICP	IW		
			$m = 81$ (dense design)						
fpca.sc	0.943	7.16	[5.41, 9.10]	0.891	6.01	0.839	5.26		
fpca.face	0.936	7.06	[5.37, 9.37]	0.880	$5.92\,$	0.828	5.18		
PACE	0.939	7.13	[5.31, 9.08]	0.884	5.98	0.833	5.24		
fpca.sc	0.943	7.14	$\overline{m_i \overset{iid}{\sim} Unif(29, 41)}$ (moderately sparse design) [5.37, 9.36]	0.891	5.99	0.840	5.24		
fpca.face	0.935	7.03	[5.37, 9.24]	0.879	5.90	0.828	5.16		
PACE	0.941	7.21	[5.31, 9.76]	0.887	6.05	0.837	5.29		
fpca.sc	0.943	7.14	$\overline{m_i \overset{iid}{\sim} Unif(20, 31)}$ (sparse design) [5.38, 9.56]	0.891	6.00	0.840	$\overline{5.25}$		
fpca.face	0.925	6.87	[4.94, 10.19]	0.866	5.76	0.812	5.04		

Table 3: Summary of ICP, IW, and R(SE) for sample size 100 and  $\mathbf{E}_i = \mathbf{E}_i^3$  based on 1000 simulations. Results are obtained by fitting the ANFCM.

investigate a smaller sample size  $n = 40$  in addition to 100 and 300.

We start by investigating the case with a single functional covariate. The results are presented in Table 4 for error variance  $\tau^2 = 1$  and in Table 5 for  $\tau^2 = 2$ . It is evident that for larger measurement error in covariates, the prediction errors become larger as expected. However, the overall conclusions drawn in the main article remain same.

Next, simulation results from two functional covariates are summarized below. The covariates are generated based on the two scenarios:(i)  $W_{1i} = X_{1i}(t) + WN(0, 1)$  and  $W_{2i} = X_{2i}(t) + WN(0,1)$  (see Table 6) and (ii)  $W_{1i} = X_{1i}(t) + WN(0,2)$  and  $W_{2i} =$  $X_{2i}(t) + WN(0, 2)$  (see Table 7). Again, similar conclusions can be drawn from these results as in the main article.

#### D.4 Choice of Number of Basis Functions

We conducted additional simulation study to investigate the effect of different choices of number of basis functions. The simulation settings are same as those in the main article, with differing number of basis functions. The results are displayed in Table 8.

#### D.5 Further Investigation for More than Two Covariates

We conducted a numerical study to investigate the finite sample performance of the proposed method based on 200 Monte-Carlo repeats with  $1 \sim 5$  covariates. In this study, the true covariates are given by  $X_q(t) = a_{q0} + a_{q1}$ √  $2\sin(\pi t) + a_{q2}$ √  $2\cos(\pi t)$ , where  $a_{q0} \sim$  $N(0, \{2^{-0.5(q-1)}\}^2)$ ,  $a_{q1} \sim N(0, \{0.85 \times 2^{-0.5(q-1)}\}^2)$  and  $a_{q2} \sim N(0, \{0.70 \times 2^{-0.5(q-1)}\}^2)$  for  $q = 1, \ldots, 5$ . Throughout the study, it is assumed that the covariates  $X_{q,i}(t)$  are not observed directly. Instead we observe  $W_{q,i} = X_{1,i}(t) + \text{WN}(0, 0.6^2)$ . The response  $Y_i(\cdot)$  (*i* = 1..., 100) is generated based on models given by  $Y_i(t) = \sum_{q=1}^{Q} F_q\{X_{q,i}(t), t\} + \epsilon(t)$  with  $F_q\{X_{q,i}(t), t\} = qx^2t^2/5 - xt$  and  $[\epsilon_i(t_1), \ldots, \epsilon_i(t_m)]^T \sim \xi_{i1}$ √  $2\cos(\pi t) + \xi_{i2}$ √  $2\sin(\pi t) +$  $N(0, 0.9^2 \mathbb{I}_m)$ , where  $\xi_{i1} \stackrel{iid}{\sim} N(0, 2)$ ,  $\xi_{i2} \stackrel{iid}{\sim} N(0, 0.75^2)$  and  $Q$  is the number of covariates incorporated. We set  $Q = 1, 2, \ldots, 5$  in this simulation study. For the training set, we considered the dense design with  $m = 81$  equally spaced points in [0, 1] for all i. The test sets contain  $n = 100$  subjects and are obtained using the set of 81 equally spaced points in [0, 1] as well. Results from simulation studies are presented in Table 9. The average computation time increases with the number of covariates. We also see increasing trend

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n  $\mathbb{E}_i$  RMSPE<sup>in</sup> RMSPE<sup>out</sup> ICP at ICP at ICP at  $1 - \alpha = 0.95 \quad 1 - \alpha = 0.90 \quad 1 - \alpha = 0.85$ Scenario B (model with single functional covariate),  $m = 81$  $\mathbf{E}^1_i$ 1.07 1.35 0.957 0.916 0.874 40  $\mathbf{E}_i^2$ 1.39 1.55 0.953 0.909 0.863  $\mathbf{E}_i^3$ 1.82 2.48 0.935 0.881 0.829  $\mathbf{E}_i^1$ 1.09 1.09 0.968 0.932 0.893 100  ${\bf E}_i^2$ 1.41 1.40 0.962 0.921 0.877  $\mathbb{E}^3_i$ 1.90 2.04 0.952 0.903 0.855  $\mathbf{E}_i^1$ 1.11 0.95 0.973 0.940 0.904  $300 E_i^2$ 1.43 1.31 0.966 0.927 0.884  $\mathbf{E}_i^3$ 1.94 1.89 0.958 0.913 0.866 Scenario B (model with single functional covariate),  $m_i \stackrel{iid}{\sim} Unif(20, 31)$  $\overline{\mathbf{E}^1_i}$ 1.41 1.94 0.955 0.924 0.891 40  $\mathbf{E}_i^2$ 1.67 2.07 0.953 0.915 0.876  $\mathbf{E}_i^3$ 2.06 2.68 0.937 0.889 0.842  $\mathbf{E}_i^1$ 1.43 1.43 0.974 0.949 0.920 100  $\mathbf{E}_i^2$ 1.68 1.66 0.968 0.936 0.900  $\mathbf{E}_i^3$ 2.11 2.21 0.958 0.916 0.873  $\mathbf{E}_i^1$ 1.44 1.10 0.984 0.963 0.937  $300 E_i^2$ 1.69 1.41 0.977 0.948 0.914  $\mathbf{E}_i^3$ 2.14 1.97 0.968 0.931 0.890 Scenario C (model with two functional covariates),  $m = 81$  $\overline{\mathbf{E}_i^1}$ 1.03 1.52 0.923 0.871 0.821 40  $\mathbf{E}_i^2$ 1.36 1.70 0.931 0.878 0.827  $\mathbf{E}_i^3$ 1.74 2.80 0.910 0.848 0.791  $\mathbf{E}_i^1$ 1.06 1.30 0.937 0.888 0.840 100  ${\bf E}_{i}^{2}$ 1.39 1.55 0.941 0.891 0.841  $\mathbf{E}_i^3$ 1.86 2.20 0.935 0.880 0.828  $\mathbf{E}_i^1$ 1.09 1.16 0.944 0.897 0.851 300  ${\bf E}_{i}^{2}$ 1.41 1.46 0.946 0.898 0.849  $\mathbf{E}_i^3$ 1.91 2.02 0.944 0.893 0.843 Scenario C (model with two functional covariates),  $m_i \stackrel{iid}{\sim} Unif(20,31)$  $\overline{\mathbf{E}_i^1}$ 1.32 1.98 0.932 0.890 0.848 40  $\mathbf{E}_i^2$ 1.60 2.07 0.936 0.890 0.844  $\mathbf{E}_i^3$ 1.94 2.75 0.914 0.857 0.804  $\mathbf{E}_i^1$ 1.37 1.56 0.955 0.918 0.880 100  ${\bf E}_{i}^{2}$ 1.63 1.76 0.953 0.912 0.869  $\mathbf{E}_i^3$ 2.05 2.31 0.944 0.895 0.847  $\mathbf{E}_i^1$ 1.40 1.29 0.967 0.935 0.900 300  ${\bf E}_{i}^{2}$ 1.66 1.56 0.963 0.925 0.885  $\mathbf{E}_i^3$ 2.11 2.08 0.957 0.913 0.868

Table 6: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, and ICP based on 1000 simulated data sets. The covariates are generated based on  $W_{1i} = X_{1i}(t) + WN(0, 1)$  and  $W_{2i} = X_{2i}(t) +$  $WN(0, 1)$ . The models are fitted by the estimation procedure of ANFCM.

n  $\mathbf{E}_i$  RMSPE<sup>in</sup> RMSPE<sup>out</sup> ICP at ICP at ICP at  $1 - \alpha = 0.95 \quad 1 - \alpha = 0.90 \quad 1 - \alpha = 0.85$ Scenario B (model with single functional covariate),  $m = 81$  $\mathbf{E}^1_i$ 1.21 1.73 0.960 0.925 0.888 40  $\mathbf{E}_i^2$ 1.50 1.84 0.956 0.916 0.874  $\mathbf{E}_i^3$ 1.91 2.70 0.940 0.888 0.838  $\mathbf{E}_i^1$ 1.24 1.27 0.974 0.945 0.911 100  ${\bf E}_i^2$ 1.53 1.53 0.967 0.931 0.892  $\mathbf{E}_i^3$ 1.99 2.15 0.957 0.913 0.866  $\mathbf{E}_i^1$ 1.27 1.02 0.980 0.955 0.924  $300 E_i^2$ 1.55 1.35 0.973 0.939 0.902  $\mathbf{E}_i^3$ 2.04 1.92 0.964 0.923 0.880 Scenario B (model with single functional covariate),  $m_i \stackrel{iid}{\sim} Unif(20, 31)$  $\overline{\mathbf{E}^1_i}$ 1.65 2.50 0.959 0.932 0.904 40  $\mathbf{E}_i^2$ 1.88 2.55 0.956 0.924 0.889  $\mathbf{E}_i^3$ 2.24 3.08 0.942 0.899 0.855  $\mathbf{E}_i^1$ 1.70 1.69 0.978 0.959 0.936 100  $\mathbf{E}_i^2$ 1.92 1.88 0.974 0.947 0.916  $\mathbf{E}_i^3$ 2.31 2.40 0.964 0.928 0.889  $\mathbf{E}_i^1$ 1.73 1.25 0.989 0.974 0.955  $300 E_i^2$ 1.95 1.53 0.983 0.960 0.934  $\mathbf{E}_i^3$ 2.35 2.06 0.975 0.944 0.909 Scenario C (model with two functional covariates),  $m = 81$  $\overline{\mathbf{E}_i^1}$ 1.14 2.00 0.914 0.863 0.814 40  $\mathbf{E}_i^2$ 1.45 2.09 0.923 0.871 0.821  $\mathbf{E}_i^3$ 1.81 3.04 0.906 0.844 0.789  $\mathbf{E}_i^1$ 1.20 1.63 0.932 0.885 0.839 100  ${\bf E}_{i}^{2}$ 1.49 1.79 0.937 0.888 0.840  $\mathbf{E}_i^3$ 1.94 2.37 0.933 0.879 0.827  $\mathbf{E}_i^1$ 1.24 1.37 0.942 0.897 0.853 300  ${\bf E}_{i}^{2}$ 1.53 1.63 0.944 0.897 0.850  $\mathbf{E}_i^3$ 2.01 2.14 0.943 0.893 0.844 Scenario C (model with two functional covariates),  $m_i \stackrel{iid}{\sim} Unif(20,31)$  $\overline{\mathbf{E}_i^1}$ 1.53 2.53 0.929 0.889 0.849 40  $\mathbf{E}_i^2$ 1.78 2.57 0.933 0.889 0.845  $\mathbf{E}_i^3$ 2.08 3.15 0.913 0.858 0.807  $\mathbf{E}_i^1$ 1.62 1.98 0.955 0.921 0.887 100  ${\bf E}_{i}^{2}$ 1.85 2.13 0.953 0.915 0.876  $\mathbf{E}_i^3$ 2.23 2.60 0.946 0.900 0.854  $\mathbf{E}_i^1$ 1.69 1.58 0.968 0.940 0.909 300  ${\bf E}_{i}^{2}$ 1.91 1.80 0.965 0.932 0.895  $\mathbf{E}_i^3$ 2.31 2.27 0.960 0.920 0.878

Table 7: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, and ICP based on 1000 simulated data sets. The covariates are generated based on  $W_{1i} = X_{1i}(t) + WN(0, 2)$  and  $W_{2i} = X_{2i}(t) +$  $WN(0, 2)$ . The models are fitted by the estimation procedure of ANFCM.

$(K_x, K_t)$		RMSPE <sup>in</sup> RMSPE <sup>out</sup>	ICP at	ICP at	ICP at				
				$1 - \alpha = 0.95$ $1 - \alpha = 0.90$ $1 - \alpha = 0.85$					
Scenario B (model with single functional covariate), $m = 81$									
(7, 7)	1.84	1.98	0.946	0.895	0.844				
(9, 9)	1.83	2.00	0.945	0.893	0.842				
(11, 11)	1.82	2.00	0.943	0.891	0.840				
Scenario B (model with single functional covariate), $m_i \stackrel{iid}{\sim} Unif(20,31)$									
(7, 7)	1.94	2.06	0.949	0.900	0.852				
(9,9)	1.93	2.06	0.947	0.899	0.850				
(11, 11)	1.92	2.06	0.946	0.896	0.847				
			Scenario C (model with two functional covariates), $m = 81$						
(7, 7)	1.80	1.96	0.937	0.882	0.831				
(9, 9)	1.78	2.13	0.934	0.879	0.825				
(11, 11)	1.77	2.15	0.932	0.875	0.821				
Scenario C (model with two functional covariates), $m_i \stackrel{iid}{\sim} Unif(20,31)$									
(7, 7)	1.91	2.01	0.942	0.891	0.840				
(9,9)	1.89	2.11	0.938	0.886	0.834				
(11, 11)	1.87	2.11	0.935	0.881	0.829				

Table 8: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, and ICP based on 1000 simulated data sets. The models are fitted by the estimation procedure of ANFCM. Results correspond to  $n = 100$  and covariance structure  $\mathbf{E}_i = \mathbf{E}_i^3$ .

Table 9: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, ICP, and average computation time (in seconds) based on 200 simulated data sets. The average computation times (in seconds) are obtained using bam function in mgcv R package.

			ີ			
$\#\text{covariates } (Q)$		RMSPEin RMSPEout	ICP at	ICP at	ICP at	computation
					$1 - \alpha = 0.95$ $1 - \alpha = 0.90$ $1 - \alpha = 0.85$	time (seconds)
	1.80	1.91	0.943	0.890	0.838	$1.56\,$
2	$1.76\,$	1.96	0.938	0.883	0.831	2.34
3	1.74	2.02	0.934	0.879	0.825	3.85
4	1.70	2.16	0.928	0.869	0.814	6.28
5	$1.68\,$	2.80	0.920	0.859	0.802	10.40

in the RMSPEout as the number of covariates increases; this is indicative of the fact that one would require larger sample sizes as the number of covariate increases.

#### D.6 Power Performance of the Tests

In Section 5.2.2 of the main article, we discussed power performance of the proposed tests for sparsely sampled data. When the sampling design is dense, power properties are very similar to power properties corresponding to the sparse design, and we show the results in Figure 1.



Figure 1: Power ( $\times$ 100) of the tests at significance level  $\alpha = 5\%$ . The top (bottom) panel displays the results from scenario A (scenario B) for the setting where sampling design is dense. The error process in the left, middle and right panels is assumed to be  $\mathbf{E}_i^1$ ,  $\mathbf{E}_i^2$ and  $\mathbf{E}_i^3$ , respectively.



Figure 2: Top plots are longitudinal measurements of the hip angle (left) and the knee angle (right) is obtained from 39 children while they go through a single gait cycle. Bottom plots are longitudinal measurements of calcium intake (left) and calcium absorption (right) obtained from 188 patients.

# E Further Investigation of Real Data Examples

### E.1 Additional Figures

We present plots of gait data and dietary calcium absorption data illustrated in Section 6 of the main article. The top plots displayed in Figure 2 are individual trajectories of the hip angle and the knee angle along the gait cycles in [0, 1] interval. The bottom plots in Figure 2 are observed individual trajectories of the calcium intake and absorption along the patient's age at the visit.

#### E.2 Further Investigation of Gait Data Example

The curves in gait data are quite different from the ones used in the simulation studies, and furthermore the sample size is smaller. In this section, we confirm the results of the gait data analysis by investigating the performance of proposed method using a generating model that mimic the feature of the gait data. The purpose of the numerical study is to assess predictive accuracy based on the simulated data sets and to ensure that our method is reliable also for smaller sample sizes; in the gait data example, the sample size is 39.

The new simulation study generates the covariates  $X_i(t)$  from a process with the mean and covariance functions that equal their estimated counterparts from the data. For this purpose, we first apply the FPCA to the observed hip angles using the entire 39 subjects, and obtain a smoothed version of n curves by computing  $\widehat{X}_i^{\text{sim}}(t_j) = \widehat{\mu}_X(t) + \sum_{j=1}^K \xi_{ik} \widehat{\phi}_k(t)$ , where  $\xi_{ik}$   $(k = 1, ..., K)$  are normally distributed with zero-mean and variance  $\hat{\lambda}_k$   $(i =$  $1, \ldots, n$ ). The estimates  $\widehat{\mu}_X(t)$ ,  $\widehat{\phi}_k(t)$ , and  $\widehat{\lambda}_k$  are obtained from the observed data, and the finite truncation K is chosen by setting the percent variance to  $99\%$ . It is assumed that hip angles are observed with some noise, and we generate noisy covariate trajectories from  $W_{ij}^{\text{sim}} = \hat{X}_i^{\text{sim}}(t_{ij}) + \delta_{ij}$ . The noise  $\delta_{ij}$  are normally distributed with zero-mean, and the noise variance is estimated from the original data. For the training data, we consider  $n = 30$ , 100, and 300 subjects. For the test data, we consider 9 subjects. For evaluation points  $t$ , we use the same time points used in the data analysis.

The response  $Y_i(\cdot)$  is generated using two choices for true function  $F(\cdot, \cdot)$ : a linear version  $F^{\text{L,gait}}(x,t)$  and a nonlinear version  $F^{\text{NL,gait}}(x,t)$ . We define the linear version by  $F^{\text{L,gait}}(x,t) = \beta_0(t) + \beta_1(t)x$ , where  $\beta_0(t) = \hat{\beta}_0^*(t) - \hat{\beta}_1^*(t)\hat{\mu}_X(t)/\hat{\sigma}_X(t)$  and  $\beta_1(t) = \hat{\sigma}_0^*(t)$  $\hat{\beta}_1^*(t)/\hat{\sigma}_X(t)$ . Here,  $\hat{\beta}_0^*(t)$  and  $\hat{\beta}_1^*(t)$  are the intercept and the slope estimated from the gait data. Such formulation allows  $F^{\text{L,gait}}(x, t)$  to mimic the fitted curve of the gait data. We define the nonlinear version by  $F<sup>NL,gait</sup>(x,t) = \exp(xt/12) - x$ . To generate the random errors  $\epsilon_i(t)$ , we first obtain residuals from the fitted linear model of the gait data, and employ the FPCA methods to estimate the variance of the random errors. Figure 3 displays the simulated covariates  $\hat{X}_i^{\text{sim}}(t)$   $(i = 1, ..., 100)$  evaluated at the points  $t_i$  (leftmost panel) as well as the response curves  $Y_i(t)$  obtained from the models  $F^{\text{L,gait}}(x,t)$  (middle panel) and  $F^{\text{NL,gait}}(x,t)$  (right panel). In the plot, when the true



Figure 3: Displayed plots are curves for sample size 100 simulated based on the gait data. The smoothed version of covariate functions  $\hat{X}_i^{\text{sim}}$  are presented in the left. The middle and the rightmost panel present response curves  $Y_i(t)$  generated based on  $F^{\text{L,gait}}(x,t)$ and  $F<sup>NL,gait</sup>(x, t)$ , respectively. The last two subjects are highlighted in different colors.

function is  $F^{\text{L,gait}}(x,t)$ , patterns in the response curves are very similar to the ones from the original gait data.

Finally, we assess the prediction performance of the proposed method using 1000 samples, and compare its performance with the linear FCM. We fit the ANFCM using  $K_x = K_t = 11$  cubic B-splines for x and t. When the true function is  $F<sup>L,sait</sup>(x, t)$  (the top three panels in Table 10), the overall predictive performance of the ANFCM and the linear FCM is relatively similar. These results indicate that the underlying relationship between the covariate and the response is linear, as investigated in the main article. When the true function is  $F<sup>NL,gait</sup>(x,t)$  (the bottom three panels in Table 10), the ANFCM better captures the complex nonlinear relationships than the linear FCM in all scenarios. Other measures also confirm that when the underlying relationship is complex, the ANFCM outperforms the linear FCM.

#### E.3 Further Investigation of Calcium Data Example

For the calcium data example, we further investigated choices of different number of basis functions as well as different dependence structures in the model. Specifically, we considered  $K_x = K_t = 7, 9,$  and 11 for the number of basis functions. For the form of the relationships, we considered two types:  $(i)E[Absorb_i(t)|Intake_i(t), BMI_i] =$  $F\{Intake_i(t), t\} + \gamma(t)BMI_i$  where F and  $\gamma$  are unknown smooth functions; and (ii)



Table 10: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, ICP, IW, and R(SE) obtained from the simulation studies of the gait data example.<br>The models fitted by our method and the linear FCM are indicated by ANFCM and FCM, respectively. Table 10: Summary of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, ICP, IW, and R(SE) obtained from the simulation studies of the gait data example.

of regular $\mu$ , regular $\mu$ , regular $\mu$ , and $\mu$												
$\mathbf{E}[Absorb_i(t) Intake_i(t), BMI_i] = F\{Intake_i(t), t\} + \gamma(t)BMI_i(F, \gamma; unknown)$												
				$1-\alpha=0.95$			$1 - \alpha = 0.90$			$1 - \alpha = 0.85$		
$(K_x, K_t)$		$RMSPE^{in}$ RMSP $E^{out}$	ICP IW		R(SE)	ICP IW		R(SE)	ICP	IW	R(SE)	
(7, 7)	0.079	0.112			$0.950$ $0.35$ [0.32, 0.56]			$0.935$ $0.30$ $[0.27, 0.47]$			$0.919$ $0.26$ [0.23, 0.41]	
(9,9)	0.079	0.111			$0.951$ $0.35$ $[0.32, 0.56]$			$0.935$ $0.30$ $[0.26, 0.47]$			$0.921$ $0.26$ $[0.23, 0.41]$	
(11, 11)	0.079	0.111			$0.951$ $0.35$ $[0.32, 0.56]$			$0.934$ $0.29$ [0.26, 0.47]			$0.920$ $0.26$ $[0.23, 0.41]$	
$\mathbf{E}[Absorb_i(t) Intake_i(t), BMI_i] = F_1\{Intake_i(t), t\} + F_2(BMI_i, t)$ ( $F_1, F_2$ : unknown)												
					$1-\alpha=0.95$			$1 - \alpha = 0.90$			$1 - \alpha = 0.85$	
$(K_x, K_t)$		$\operatorname{RMSPE^{in}}$ $\operatorname{RMSPE^{out}}$	ICP IW		R(SE)	ICP IW		R(SE)	ICP IW		R(SE)	
(7, 7)	0.078	0.111			$0.955$ 0.36 [0.31, 0.60]			$0.940$ $0.30$ $[0.26, 0.50]$			$0.924$ 0.26 [0.23, 0.44]	
(9, 9)	0.078	0.102			$0.945$ 0.35 [0.30, 0.60]			$0.933$ $0.30$ $[0.25, 0.50]$			$0.918$ $0.26$ $[0.22, 0.44]$	
(11, 11)	0.078	0.097			$0.949$ $0.35$ [0.30, 0.58]			$0.931$ $0.29$ $[0.25, 0.49]$			$0.917$ $0.26$ [0.22, 0.43]	

Table 11: Results from calcium absorption data example. Displayed are the summaries of RMSPE<sup>in</sup>, RMSPE<sup>out</sup>, ICP, IW, and  $R(SE)$ .

 $E[Absorb_i(t)|Intake_i(t), BMI_i] = F_1\{Intake_i(t), t\} + F_2(BMI_i, t)$  where  $F_1$  and  $F_2$  are unknown smooth functions. Therefore, the former case assumed that the effect of  $BMI_i$ is linear, while the latter case assumed the effect is nonlinear. The results are included in Table 11.

# F Implementation Details

We implemented our proposed estimation and testing methodology using the R software. The model components of the ANFCM,  $Y_i(t) = \mu_Y(t) + F_1\{X_{1,i}(t), t\} + F_2\{X_{2,i}(t), t\} +$  $\epsilon_i(t)$ , can be estimated using the gam or the bam functions of mgcv package [3]. The smoothing parameter choice is automatic in both the functions; we use REML criteria to select the smoothing parameters. For the sparsely sampled design, we employ the R package refund to carry out FPCA. In the following, we illustrate how the R software codes can be used to implement our procedures.

We first pool all observed data. Let trep be the N-dimensional vector of evaluation points pooled from all subjects. Let  $y$ , vec be the N-dimensional vectors of response and transformed covariate, and let and x1.vec and x2.vec be the transformed covariates of dimension N, respectively, where the evaluation points of the functional correspond to the vector trep. The transformed covariate indicates that the point-wise center/scaling

transformation is applied. Then a simple command

fit  $\langle -\text{gam}(y.\text{vec} \sim \text{s}(\text{trep}, \text{bs}^{=\prime \prime} \text{ps'}) , \text{ k}^{=\text{Kmu}} \rangle + \text{te}(x1.\text{vec}, \text{trep}, \text{bs}^{=\prime \prime} \text{ps'})$  $k=c(Kx1, Kt1)) + te(x2.vec, trep, bs=''ps'', k=c(Kx2, Kt2)), method=''REM'')$ 

performs our estimation procedure. The function s() estimates the marginal smooth mean of response,  $\mu_Y(t)$ , and the number of basis functions for this term is indicated by Kmu. The function te() specifies the tensor product of basis functions. The bs argument selects the type of penalized splines. In our case, we set  $bs = '^\prime ps'$  to incorporate Bsplines with the second order difference penalties. The k argument specifies the number of basis functions; for example, when estimating the term  $F_2\{X_{1,i}(t), t\}$ , the number of basis functions is Kx1 for x1.vec and Kt1 for trep. Smoothing for the penalized splines is indicated by method=''REML''. The gam() function will automatically offer the parameter estimates  $\widehat{\Theta}$  as well as the estimated response y.vecEst at the points trep. For the large data sets, one can use bam() in place of gam().

To estimate  $G(\cdot, \cdot)$  at specific time points, one may use fpca.sc function of refund package in R. The model residuals are computed from res.vec=y.vec-y.vecEst; FPCA is then applied to the residuals using the function fpca.sc of R package refund as

fpc <- fpca.sc(matrix(res.vec, nrow=n, ncol=m, byrow=TRUE), pve, var=TRUE).

Note that the residuals must be transformed into a matrix format in fpca.sc. The pve argument specifies the percent of variance explained by the first few eigencomponents such as pve=0.9 or pve=0.95. We set var=TRUE to estimate the variance of measurement errors  $\sigma^2$ . This procedure offers the estimate of eigencomponents  $\{\phi_k(\cdot), \lambda_k\}$  and the estimate of  $\sigma^2$ , which will be used to reconstruct  $G = cov(\mathbb{E}_i)$ . For the case where the data are observed on a sparse grid of points, the  $n \times m$ -dimensional matrix of the residuals contains NAs as components, considered as missing values. Nevertheless, the fpca.sc() function can still estimate the underlying smooth curves and the eigencomponents.

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