

Principal Component Analysis for Functional Data

Yoshihiro YAMANISHI*

Yutaka TANAKA†

(Received October 31, 2000)

In functional principal component analysis (PCA), we treat the data that consist of functions not of vectors (Ramsay and Silverman, 1997). It is an attractive methodology, because we often meet the cases where we wish to apply PCA to such data. But, to make this method widely useful, it is desirable to study advantages and disadvantages in actual applications. As alternatives to functional PCA, we may consider multivariate PCA applied to 1) original observation data, 2) sampled functional data with appropriate intervals, and 3) coefficients of basis function expansion. Theoretical and numerical comparison is made among ordinary functional PCA, penalized functional PCA and the above three multivariate PCA.

Keywords: Functional data, Multivariate data, Principal component analysis, Eigenvalue, Eigenvecotor

1 INTRODUCTION

In functional data analysis, we can analyze the data that look like curves (Ramsay and Silverman, 1997). We often confront the case in which it is better to treat such data as functions or curves rather than as multivariate observations. For example, we have growth curves, brain waves or electrocardiographic waves function. In such cases we sometimes take samples at time points t_1, t_2, \dots and regard $\{x(t_j), j = 1, 2, \dots\}$ as a multivariate observation vector. In this sense the original function $x(t)$ can be regarded as the limit of $\{x(t_j)\}$ as the sampling interval tends to zero and the dimension of the vectors tends to infinity. Here we focus our attention to the principal component analysis (PCA) in functional context. The purpose of this study is to see how the functional (or multivariate) PCA works in actual data analysis. After

confirming the behavior, we try to investigate the relationship between multivariate PCA and functional PCA.

2 FUNCTIONAL DATA

In practice we usually obtain sampled data. So at the first stage of functional data analysis we must transform the data into functional form. That is, we have to estimate a function on the basis of sampled observations with noise by using an appropriate smoothing method.

2.1 Roughness penalty smoothing method

Here we introduce the idea of roughness penalty in estimating a function x from observations $y_j = x(t_j) + \epsilon_j$. We use the roughness penalty method to smooth a function x which has a considerable roughness. A popular measure of the roughness of a function is defined as its integrated squared

*Graduate School of Natural Science and Technology, Okayama University, Tsushima, Okayama 700-8530, Japan.

†Department of Environmental and Mathematical Science, Okayama University, Tsushima, Okayama 700-8530, Japan.

second derivative, i.e.,

$$PEN_2(x) = \|D^2x\|^2 = \int \{D^2x(s)\}^2 ds. \quad (1)$$

This measure assesses the total curvature in x , or in other words, the degree to which x departs from a straight line. Then we can define the penalized residual sum of squares as

$$PENSSSE_\lambda(x|y) = \sum_j \{y_j - x(t_j)\}^2 + \lambda PEN_2(x). \quad (2)$$

The smooth function is estimated by minimizing PENSSE over the space of function x for which PEN is defined. The parameter λ is a smoothing parameter that represents the rate of exchange between the fit to the data, which is measured by the residual sum of squares, and the roughness of the function x , which is quantified by PEN.

2.2 Basic statistics in functional context

Suppose we have N data functions, which are denoted by $x_1(t), x_2(t), \dots, x_N(t)$. In the similar manner as in ordinary statistical theory, the basic statistics in functional context are defined as follows:

Mean function:

$$\bar{x}(t) = N^{-1} \sum_{i=1}^N x_i(t) \quad (3)$$

Variance function:

$$Var(x(t)) = N^{-1} \sum_{i=1}^N [x_i(t) - \bar{x}(t)]^2 \quad (4)$$

Covariance function:

$$v(s, t) = N^{-1} \sum_{i=1}^N (x_i(s) - \bar{x}(s))(x_i(t) - \bar{x}(t)) \quad (5)$$

Inner product of two functions:

$$\langle x_i(t), x_j(t) \rangle = \int x_i(t)x_j(t)dt. \quad (6)$$

3 FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS

3.1 Ordinary functional principal component analysis

Suppose we have a set of functional data $x(s)$. Weight function $\xi(s)$ is chosen in such a way that it maximizes the variance

$$PCASV = \int \int v(s, t)\xi(s)\xi(t)dsdt, \quad (7)$$

where $v(s, t)$ indicates a variance-covariance function based on the functional data set. The maximization of PCASV under the constraints

$$\int \xi_k(t)^2 dt = 1, \quad \int \xi_k(t)\xi_m(t)dt = 0 \quad (k < m) \quad (8)$$

leads to an integral eigenequation as follows:

$$\int v(s, t)\xi(t)dt = \rho\xi(t). \quad (9)$$

3.2 Penalized functional principal component analysis

Here penalty function is introduced to incorporate smoothing into the principal components (PCs). Suppose the function ξ has square-integrable derivatives up to degree four, and also that ξ satisfies one of the following conditions: 1) either $D^2\xi$ and $D^3\xi$ are zero at the ends of the interval \mathcal{T} , or 2) the second and third derivatives of ξ satisfy periodic boundary conditions on \mathcal{T} . Then the most popular form of the penalty for ξ is given by

$$PEN_2(\xi) = \|D^2\xi\|^2 = \int \xi(t)D^4\xi(t)dt. \quad (10)$$

In this case the penalized variance can be expressed by

$$PCAPSV = \frac{PCASV}{\|\xi\|^2 + \lambda \times PEN_2(\xi)}, \quad (11)$$

where λ is a smoothing parameter. This expression means that the trade-off between maximizing the sample variance and smoothing ξ is controlled

by parameter λ . The solution ξ is obtained as the eigenfunction associated with the largest eigenvalue of the following penalized eigenequation

$$\int v(s, t)\xi(t)dt = \rho(I + \lambda D^4)\xi(s). \quad (12)$$

3.3 Choice of the smoothing parameter λ by cross-validation

Let M be the number of PCs, and define the cross-validation score as

$$CV(\lambda) = \sum_{i=1}^N \|x_i(s) - \sum_{m=1}^M \sum_{l=1}^M (\mathbf{G}^{-1})_{ml} \left(\int \xi_m^{[i]}(t)x_i(t)dt \right) \xi_l^{[i]}(s)\|^2, \quad (13)$$

where \mathbf{G} is the $M \times M$ matrix whose (m, l) element is the inner product $\int \xi_m(t)\xi_l(t)dt$ and the subscript $[i]$ means the omission of the i -th observation. Choose λ which minimizes $CV(\lambda)$.

3.4 Numerical algorithm

Suppose we use a set of basis functions $\phi(s) = (\phi_1(s), \dots, \phi_K(s))^T$. Then a functional observation $x(s)$ and a weight function $\xi(s)$ can be expanded as

$$x(s) = \sum_{k=1}^K c_k \phi_k(s) = c^T \phi(s), \quad (14)$$

$$\xi(s) = \sum_{k=1}^K y_k \phi_k(s) = y^T \phi(s), \quad (15)$$

where $x(s)$ is a centered function and K is the number of basis functions. Define \mathbf{V} as the covariance matrix of c_i and let $\mathbf{J} = \int \phi\phi^T$, $\mathbf{K} = \int (D^2\phi)(D^2\phi)^T$, $\mathbf{L}\mathbf{L}^T = \mathbf{J} + \lambda\mathbf{K}$, and $\mathbf{S} = \mathbf{L}^{-1}$. Then the functional eigenequation (9) is transformed to an eigenvalue problem of a symmetric matrix defined as

$$(\mathbf{S}\mathbf{J}\mathbf{V}\mathbf{S}^T)((\mathbf{S}^{-1})^T y) = \rho((\mathbf{S}^{-1})^T y). \quad (16)$$

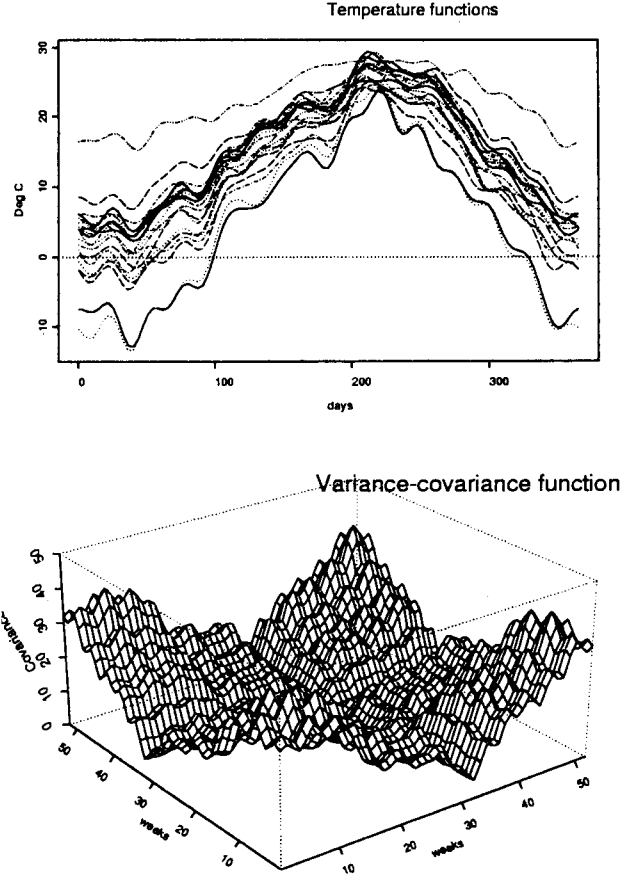


Figure 1: Daily temperature data and their variance-covariance function

4 NUMERICAL EXAMPLE

We shall apply the penalized functional PCA to the mean daily temperature data of the 20 weather stations in Japan in 1999. We use Fourier series as basis functions. Figure 1 shows the observed temperature curves and their variance-covariance function, where the number of basis functions is set as 30. The stations include Hokkaido, Tokyo, Kyoto, Osaka and so on.

4.1 Regularization by the number of basis functions

Consider to use the basis expansion algorithm discussed in Section 3.4. If we use the whole basis

functions whose number is equal to the total number of observation points (e.g., time points), the corresponding function has a lot of roughness and results in over-fitting. Not only to remove considerable roughness but also to avoid extraordinary computational burden, it is important to use the appropriate number of basis functions, where it is denoted by K . Here we investigate the effect of the number of basis functions on the obtained PCs by applying ordinary functional PCA with four different K to the temperature data. Figure 2 shows the weight functions for PC1 and PC2, where $K = 365, 50, 30$, and 10 , respectively. From these figures it is found that the effect of regularization becomes stronger as K decreases.

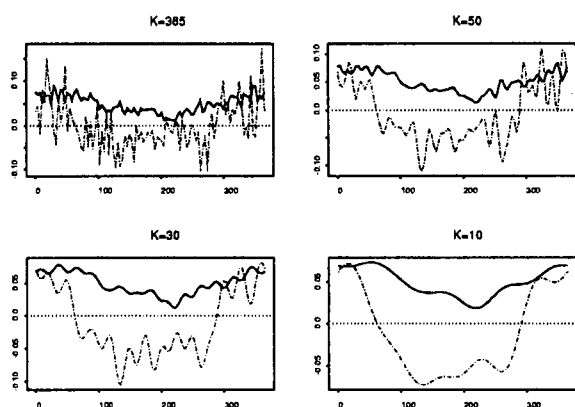


Figure 2: Weight functions for PC1 (solid) and PC2 (dashed) obtained by ordinary functional PCA for four K values ($K = 365, 50, 30$ and 10)

4.2 Regularization by a smoothing parameter λ

Here we study the performance of smoothing with roughness penalty. By applying penalized functional PCA discussed in Section 3.2 to the same data set, where the number of basis functions is fixed as $K = 365$. Figure 3 shows the penalized weight functions for PC1 and PC2, where $\lambda = 0, 10, 100$ and 1000 , respectively. From these figures it is found that we can remove the considerable roughness from the weight function as λ increases.

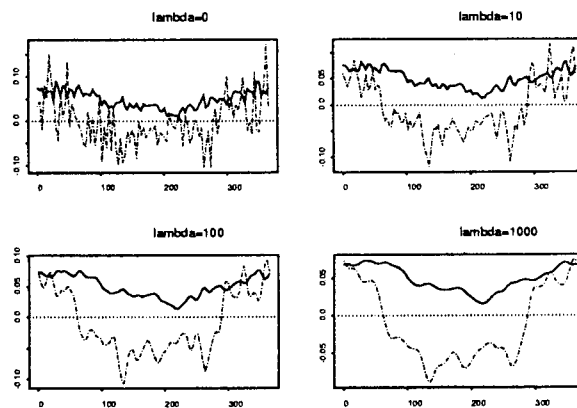


Figure 3: Weight functions for PC1 (solid) and PC2 (dashed) obtained by penalized functional PCA for four λ values ($\lambda = 0, 10, 100$ and 1000)

4.3 Cross-validation

So far, we have confirmed that we can regularize the weight function by using a smoothing parameter λ . To determine the value of smoothing parameter λ automatically, we apply cross-validation method discussed in Section 3.3. Figure 4 shows the cross-validation scores $CV(\lambda)$ computed by varying the value of λ with step 10. This figure shows that the optimum λ is given by $\lambda = 250$. Figure 5 shows the corresponding weight functions for PC1 and PC2 using the optimum λ value determined by cross-validation. Looking at these weight functions, we can interpret the PCs as follows: The PC1 is a measure of overall temperatures throughout the year, while the PC2 represents the contrast between the temperatures in summer and in winter.

5 RELATIONSHIP BETWEEN MULTIVARIATE PCA AND FUNCTIONAL PCA

In practice, we usually obtain sampled data that takes the form of the vector. To apply functional data analysis, we must transform the original sampled data into functional form. In the process of transformation, we can get the coefficient vector

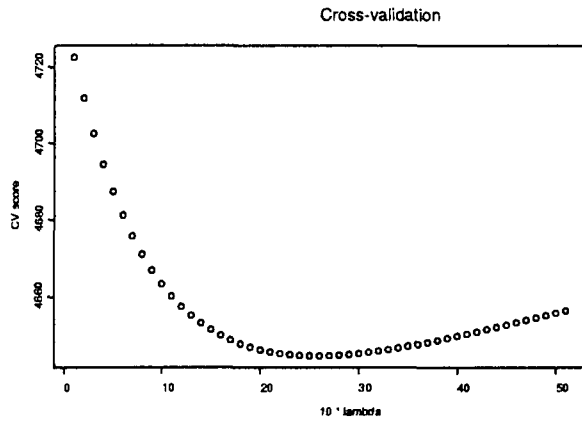


Figure 4: Cross-validation score ($\lambda = 0, 10, 20, \dots, 500$)

of the functional data. We are interested in the relationship among the three forms of the data, i.e., the original data, the coefficient data and the functional data. Moreover, we may consider the discrete functional data that is obtained by sampling from the functional data in appropriate time points. Now we shall apply PCA to the above four different forms of data and investigate numerically their mutual relationships and finally compare to the result of penalized functional PCA.

5.1 Theoretical comparison

Before making comparison of those PCA numerically, we shall discuss their relationships theoretically. The functional PCA is formulated as the integral eigenequation (9). If we perform sampling with interval h , then it is transformed to an eigenequation

$$\sum_k v(t_j, t_k) \xi(t_k) = (\rho/h) \xi(t_j), \quad (17)$$

of a symmetric matrix $V = (v(t_j, t_k))$. Comparing the two eigenequations (9) and (17), it is obvious that the eigenvalues are equal with each other up to a multiplying constant, and the eigenvectors of (17) are equal to the sampled values of the eigenfunction of (9) if an appropriate normalizing constant is multiplied. Next, as discussed in Ramsay

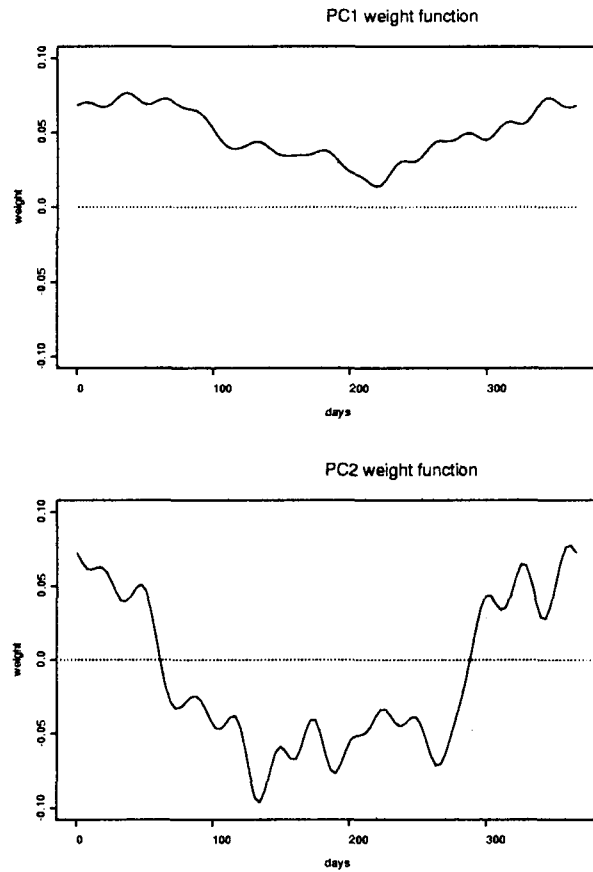


Figure 5: Weight functions for PC1 and PC2 determined by cross-validation

and Silverman (1997, P.101), eq.(9) can be transformed to

$$N^{-1} \mathbf{C}^T \mathbf{C} \mathbf{J} \mathbf{y} = \rho \mathbf{y}, \quad (18)$$

where \mathbf{C} is an $N \times K$ coefficient matrix of the data functions and \mathbf{y} is a $K \times 1$ coefficient vector of the eigenfunction. As $J = \int \phi \phi^T$ reduces to an identity matrix for Fourier series expansion, eq.(18) is just equal to the eigenequation of multivariate PCA of the coefficients for basis functions. The integral eigenequation for the penalized functional PCA is expressed as

$$\int v(s, t) \xi(t) dt = \rho(1 + \lambda D^4) \xi(s). \quad (19)$$

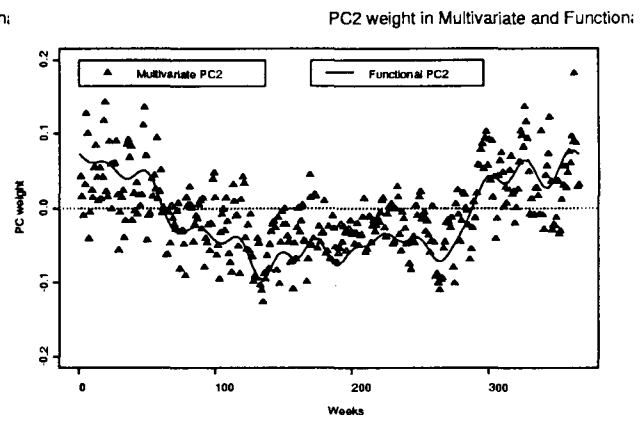
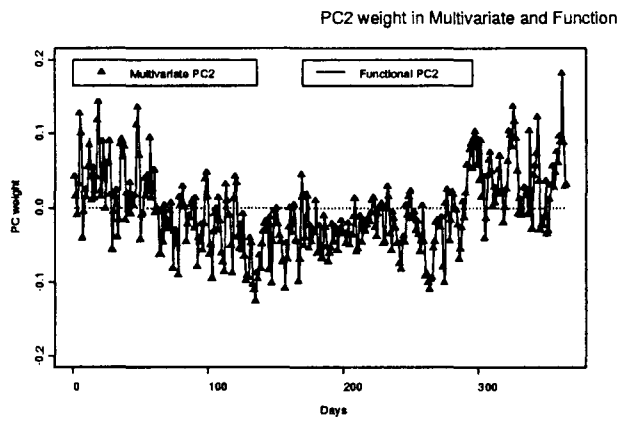
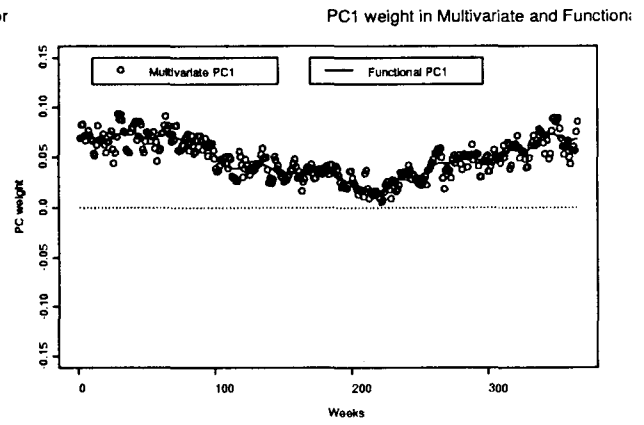
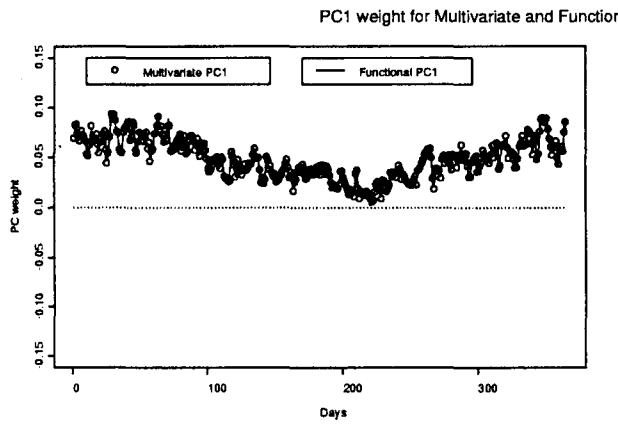


Figure 6: Comparison of PC weights (Multivariate PCA and Functional PCA)

Figure 7: Comparison of PC weights (Multivariate PCA and Penalized Functional PCA)

If we perform sampling with interval h , we obtain

$$\sum_k v(t_j, t_k) \xi(t_k) = \rho(1 + \lambda \Delta^4) \xi(t_j), \quad (20)$$

where Δ^4 indicates the fourth order difference operator. Obviously eq.(20) gives somewhat different eigenvalues and eigenvectors (eigenfunctions) from the other cases.

5.2 Multivariate PCA and ordinary functional PCA

Table 1 through 8 show the eigenvalues, the eigenvectors, PC1 scores and PC2 scores obtained as the results of PCA of the different data forms.

Figure 6 shows the weight vectors in multivariate PCA and the weight functions in functional PCA ($K = 365$) for PC1 and PC2, respectively. From these results, it is found that if we use the whole basis functions whose number is equal to that of the observation points, the results of functional PCA coincides with those of multivariate PCA, where it is analyzed by regarding the observation points as variables. It is also found that when we apply PCA to the original data matrix, the coefficient matrix, the sampled functional data matrix, and the functional data, their eigenvalues and PC scores one-to-one correspond one another. And Table 3 and 4 show that the eigenvectors of the coefficient matrix is different from the others, because the view of the calculation is different. By

Eigenvalue			
PC	Original	Discrete	Coefficient
1	6.53E+03	6.53E+03	6.53E+03
2	1.98E+02	1.98E+02	1.98E+02
3	1.25E+02	1.25E+02	1.25E+02
4	8.99E+01	8.99E+01	8.99E+01
5	7.18E+01	7.18E+01	7.18E+01
6	4.60E+01	4.60E+01	4.60E+01
7	4.04E+01	4.04E+01	4.04E+01
8	2.75E+01	2.75E+01	2.75E+01
9	2.40E+01	2.40E+01	2.40E+01
10	2.23E+01	2.23E+01	2.23E+01
11	1.76E+01	1.76E+01	1.76E+01
12	1.36E+01	1.36E+01	1.36E+01
13	1.24E+01	1.24E+01	1.24E+01
14	9.63E+00	9.63E+00	9.63E+00
15	9.04E+00	9.04E+00	9.04E+00
16	6.81E+00	6.81E+00	6.81E+00
17	6.68E+00	6.68E+00	6.68E+00
18	6.27E+00	6.27E+00	6.27E+00
19	4.01E+00	4.00E+00	4.00E+00
20	3.47E-12	2.92E-12	1.00E-11

Table 1: Eigenvalues (Multivariate PCA for original data, discrete functional data and coefficient data)

combining the coefficient-type eigenvectors with basis functions, eventually it will be transformed into the corresponding eigenfunctions in ordinary functional PCA.

5.3 Multivariate PCA and penalized functional PCA

Here we try to investigate the relationship between multivariate PCA and penalized functional PCA. Figure 7 shows the weight vectors in ordinary PCA and the weight functions in penalized functional PCA for PC1 and PC2, respectively. From Table 2, the eigenvalues in penalized functional PCA are smaller compared to those in unpenalized functional PCA. It is quite natural considering that the results are different between the cases when the penalty is taken into account and not taken into account. Comparing the result of functional PCA to that of ordinary PCA, it seems that the eigenfunctions obtained by the penalized

Eigenvalue		
PC	Functional	Penalized Func
1	6.53E+03	6.35E+03
2	1.98E+02	1.16E+02
3	1.25E+02	4.94E+01
4	8.99E+01	3.44E+01
5	7.18E+01	1.31E+01
6	4.60E+01	1.04E+01
7	4.04E+01	8.53E+00
8	2.75E+01	5.78E+00
9	2.40E+01	4.05E+00
10	2.23E+01	3.07E+00
11	1.76E+01	1.50E+00
12	1.36E+01	1.36E+00
13	1.24E+01	9.76E-01
14	9.63E+00	7.71E-01
15	9.04E+00	6.34E-01
16	6.81E+00	5.03E-01
17	6.68E+00	3.51E-01
18	6.27E+00	3.12E-01
19	4.00E+00	2.32E-01
20	1.08E-11	1.51E-13

Table 2: Eigenvalues (Functional PCA and Penalized Functional PCA)

functional PCA interpolate the eigenvectors obtained by the multivariate PCA. Looking at these figures, we can find that it is easier to interpret the result in functional PCA than ordinary PCA.

6 CONCLUDING REMARKS

In this study, we have seen how the functional PCA works in actual data analysis and investigated the relationship between ordinary PCA and functional PCA numerically. It is observed that, when we use the basis functions whose number is equal to the observation points, then functional PCA provides the same result with ordinary PCA applied by regarding the observation points as variables. Also it is found that it is easier to interpret functional PCs than ordinary PCs if an appropriate smoothing parameter is chosen. In order to obtain easy-to-interpret result, we need to choose an appropriate number of basis functions and an appropriate smoothing parameter λ carefully. In particular, the regularization should

1st Eigenvector			
vector	Ordinary	Discrete	Coefficient
1	0.06908894	0.06909035	-9.29E-01
2	0.08220368	0.08220291	-1.21E-01
3	0.0830903	0.0830905	-2.89E-01
4	0.07143334	0.07143336	-7.62E-05
5	0.06660804	0.0666083	4.19E-03
6	0.07230082	0.07230075	-2.62E-02
7	0.07656424	0.07656425	3.45E-02
8	0.07199331	0.0719933	4.86E-02
9	0.06820271	0.0682031	-3.56E-02
10	0.06624269	0.06624217	1.46E-02
11	0.05409188	0.05409244	1.61E-02
12	0.05187629	0.05187588	-1.06E-02
13	0.06233494	0.06233593	-3.40E-04
14	0.08146241	0.08146106	1.99E-02
15	0.06740007	0.06740126	3.01E-02
16	0.06689532	0.0668947	6.95E-03
17	0.06869738	0.06869796	-1.79E-02
18	0.07315014	0.07314972	1.66E-03
19	0.06269469	0.06269476	3.91E-03
20	0.05471905	0.05471962	5.55E-03
21	0.06505238	0.06505179	1.32E-02
22	0.06552827	0.06552874	-1.06E-02
23	0.07291382	0.07291386	-8.26E-03
24	0.0762496	0.07624936	-2.16E-02
25	0.05810713	0.05810712	-3.80E-06
26	0.04445394	0.04445451	-3.76E-02
27	0.05440026	0.0543997	1.33E-02
28	0.0703998	0.07040071	-1.84E-02
29	0.09334416	0.09334303	-2.27E-02
30	0.08765165	0.08765271	1.89E-02
31	0.09270653	0.09270611	7.78E-03
32	0.08690243	0.08690234	-7.24E-03
33	0.07599393	0.07599467	-3.05E-03
34	0.07464695	0.074646	-3.32E-02
35	0.05779601	0.05779706	-1.25E-02
36	0.05563449	0.05563355	-7.99E-03
37	0.05454821	0.05454936	-7.75E-03
38	0.07483257	0.0748317	-4.31E-03
39	0.07944731	0.07944779	1.50E-02
40	0.07872682	0.07872664	-2.20E-02
...
364	0.07508048	0.07508061	4.65E-04
365	0.08520142	0.08520043	5.30E-03

Table 3: 1st Eigenvectors (Multivariate PCA for original data, discrete functional data and coefficient data)

2nd Eigenvector			
vector	Ordinary	Discrete	Coefficient
1	0.043199562	0.043199167	-0.089238522
2	0.016455531	0.016454938	-0.107488772
3	-0.009046545	-0.009047895	0.58971268
4	0.03280157	0.032803885	0.00061051
5	0.127856922	0.127857836	0.165430202
6	0.10085961	0.100856568	-0.060575386
7	-0.039990744	-0.039985966	-0.098192826
8	-0.004721639	-0.004722962	0.125822062
9	0.025283388	0.025284231	-0.073961629
10	0.015405123	0.015407403	0.146646522
11	0.055766007	0.055767627	0.027207939
12	0.084849822	0.084852418	-0.119619921
13	0.042438587	0.042438075	0.065775966
14	0.010947198	0.010950926	0.008538453
15	0.054807513	0.054802859	0.057954734
16	0.013782898	0.013786466	0.044968133
17	0.042614463	0.042613954	-0.01055868
18	0.118058545	0.118063341	0.061992911
19	0.143535206	0.143532891	0.058941871
20	0.02363203	0.023638222	0.021080449
21	0.015977336	0.015978956	0.059359616
22	0.089993578	0.08999377	-0.067373909
23	0.059615585	0.059613361	-0.04566901
24	-0.00018376	-0.000180223	-0.126412032
25	0.060144852	0.060139713	0.018277551
26	0.06144119	0.061447954	-0.037243109
27	0.090464361	0.090463397	0.047468979
28	0.018949233	0.018950308	-0.074569412
29	-0.055483831	-0.055481166	-0.107881107
30	-0.004629095	-0.004632668	0.059414533
31	0.015658168	0.015660978	0.046704768
32	0.024711102	0.024707702	0.011914233
33	-0.038691817	-0.038690256	0.078940405
34	-0.015936751	-0.015935535	-0.158612387
35	0.086243635	0.08624431	0.047859055
36	0.092353797	0.092354233	-0.059995492
37	0.068678478	0.068685907	0.029130229
38	0.083631883	0.083625048	0.001109382
39	-0.015664878	-0.01565621	0.037187486
40	0.020996717	0.020988732	-0.079843979
...
364	0.029869332	0.029868798	0.035745595
365	0.032270868	0.032272753	-0.013045464

Table 4: 2nd Eigenvectors (Multivariate PCA for original data, discrete functional data and coefficient data)

PC1 score			
No.	Original	Discrete	Coefficient
1	-171.255921	-171.255669	-12.484194
2	-174.465445	-174.465229	-9.274634
3	-50.572018	-50.572008	-133.167853
4	-77.148632	-77.148611	-106.59125
5	-7.463038	-7.463015	-176.276845
6	36.902086	36.902103	-220.641962
7	-44.464158	-44.464222	-139.275639
8	41.294525	41.294535	-225.034394
9	-49.763224	-49.763263	-133.976598
10	4.942057	4.942025	-188.681884
11	49.216598	49.216547	-232.956405
12	12.457784	12.457715	-196.197574
13	34.129237	34.129192	-217.86905
14	-25.913217	-25.913282	-157.826579
15	29.862519	29.86245	-213.602309
16	22.838984	22.838964	-206.578823
17	34.563043	34.563022	-218.302881
18	54.468554	54.468527	-238.208386
19	87.658528	87.658465	-271.398322
20	192.711738	192.711754	-376.451609

Table 5: PC1 scores (Multivariate PCA for original data, coefficient data and discrete functional data)

PC2 score			
No.	Original	Discrete	Coefficient
1	16.60160571	16.60173691	-81.0193
2	3.27670984	3.27669324	-94.34434
3	30.25315204	30.2526252	-67.36841
4	8.34173234	8.34152632	-89.27951
5	-7.30532293	-7.30435282	-104.92539
6	-11.77505884	-11.77418222	-109.39522
7	-12.01393822	-12.01392783	-109.63496
8	-17.55555143	-17.555028	-115.17606
9	-16.29298649	-16.29270723	-113.91374
10	14.23676318	14.23593641	-83.3851
11	5.25584785	5.25542638	-92.36561
12	-16.19487262	-16.19456685	-113.8156
13	-15.14694071	-15.14639549	-112.76743
14	-9.34915908	-9.349376	-106.97041
15	9.87313244	9.87235317	-87.74868
16	-11.5528681	-11.55240177	-109.17344
17	0.07459628	0.07411778	-97.54692
18	-2.25411507	-2.25449731	-99.87553
19	4.67161286	4.67130154	-92.94973
20	26.85566095	26.85571859	-70.76532

Table 7: PC2 scores (Multivariate PCA for original data, coefficient data and discrete functional data)

PC1 score		
No.	Functional	Penalized Functional
1	-171.255666	-167.095349
2	-174.465225	-170.252668
3	-50.572007	-49.85052
4	-77.148609	-76.536393
5	-7.463015	-8.001284
6	36.902102	37.273276
7	-44.464221	-45.198728
8	41.294534	40.777838
9	-49.763262	-51.219215
10	4.942024	5.511518
11	49.216546	49.156567
12	12.457714	11.409134
13	34.129191	33.317169
14	-25.913281	-27.365068
15	29.862449	29.507093
16	22.838963	21.997128
17	34.563021	33.701597
18	54.468526	53.62796
19	87.658463	86.871977
20	192.71175	192.367967

Table 6: PC1 scores (Functional PCA and Penalized Functional PCA)

PC2 score		
No.	Functional	Penalized Functional
1	16.60173695	11.398121
2	3.27669332	-7.602013
3	30.25262516	27.67187
4	8.3415263	11.390834
5	-7.30435284	2.711583
6	-11.77418219	-10.3425
7	-12.01392783	-6.888396
8	-17.55502797	-17.478505
9	-16.29270725	-6.361094
10	14.23593642	8.529827
11	5.25542639	-1.260089
12	-16.19456685	-13.230451
13	-15.14639548	-12.106017
14	-9.34937604	-1.939452
15	9.87235315	7.153681
16	-11.55240178	-7.277027
17	0.07411776	2.538924
18	-2.25449732	-3.719148
19	4.67130154	-1.101829
20	26.85571857	17.911681

Table 8: PC2 scores (Functional PCA and Penalized Functional PCA)

be primarily controlled by the smoothing parameter λ , and truncating basis function should purely reduce computation without substantially altering the actual result. In this study, we have applied cross-validation in determining a smoothing parameter λ , although there is still room for improving the definition of cross-validation score and developing the efficient method to reduce the considerable computational burden. Moreover, functional data analysis has a lot of advantage. First it can be applied to the data set in which observation is made at different points (e.g., time points) for each individual. In addition, this method makes it possible to apply differential analysis easily as long as we use basis expansion method because all we have to do is to calculate the corresponding derivative of the basis functions. But there remains a problem of the lack of the theory to treat infinite dimensional data.

References

- [1] Besse, P. and Ramsay, J. O. (1986). Principal components analysis of sampled functions, *Psychometrika*, 51, 285-311.
- [2] Japan Meteorological Agency (1999). Annual report of Automated Meteorological Data Acquisition System, *Japan Meteorological Business Support Center (JMBSC)*.
- [3] Ramsay, J. O. and Silverman, B. W. (1996). *Functional Data Analysis, Springer*.