On the estimation of the number of components in multivariate functional principal component analysis

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Abstract

Happ and Greven [2018] developed a methodology for principal components analysis of multivariate functional data for data observed on different dimensional domains. Their approach relies on an estimation of univariate functional principal components for each univariate functional feature. In this paper, we present extensive simulations to investigate choosing the number of principal components to retain. We show empirically that the conventional approach of using a percentage of variance explained threshold for each univariate functional feature may be unreliable when aiming to explain an overall percentage of variance in the multivariate functional data, and thus we advise practitioners to be careful when using it.

Keywords— Functional principal components analysis; Multivariate functional data; Simulation; Variance explained

1 Introduction

Happ and Greven [2018] develop innovative theory and methodology for the dimension reduction of multivariate functional data on possibly different dimensional domains (e.g., curves and images), which extends existing methods that were limited to either univariate functional data or multivariate functional data on a common one-dimensional domain. Recent research has shown a growing presence of data defined on different dimensional domains in diverse fields such as biomechanics, e.g., Warmenhoven et al. [2019] and neuroscience, e.g., Song and Kim [2022], so we expect the work to have significant practical impact. We aim to provide commentary on the estimation of the number of principal components utilising the methodology proposed in Happ and Greven [2018]. Note that Happ and Greven [2018, Online Supplement, Section 2.3] briefly comment about it. To achieve this, we conduct an extensive simulation study and subsequently propose practical guidelines for practitioners to adeptly choose the appropriate number of components for multivariate functional datasets. For ease of presentation, we use the same notation as in Happ and Greven [2018]. Code to reproduce the simulation study and data analysis in this discussion is available at `https://github.com/FAST-ULxNUIG/variance_mfpca`.

2 Model

Happ and Greven [2018] proposed an extension of functional principal components analysis (FPCA, Ramsay and Silverman [2005]) to multivariate functional data defined on different dimensional domains, named multivariate functional principal components analysis (MFPCA). We briefly present the estimation procedure of the principal components given a sample $x_1, \ldots, x_N$ of multivariate functional data. The detailed estimation procedure is given in Happ and Greven [2018], Section 3. For all $n = 1, \ldots, N$, the observation x_n is a vector of p functions, each defined on a domain with possibly different dimensions. We denote by $x_n^{(j)}$ the jth entry of the vector x_n, referred to as the jth feature. The first step is to perform a univariate FPCA for each individual feature j using $x_1^{(j)}, \ldots, x_N^{(j)}$. We estimate M_j univariate functional principal components for each feature j. The

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total number of components that have been estimated over all p features is thus $M_+ = \sum_{j=1}^{p} M_j$. We also define $M_- = \min_{j=1,\dots,p} M_j$ to be the minimum number of univariate components estimated across all univariate features j. The univariate FPCA scores are estimated by projecting the (mean-centered) univariate functional observations onto the estimated eigenfunctions. The univariate scores from the p features are then concatenated in a matrix of size $N \times M_+$. An eigenanalysis of this matrix is performed resulting in eigenvalues ν_m and eigenvectors $\mathbf{c}_m$. Finally, the multivariate eigenfunctions and scores are estimated as a linear combination of the univariate eigenfunctions and scores weighted by the eigenvectors $\mathbf{c}_m$. The multivariate eigenvalues are the same as the eigenvalues of the matrix of the concatenated scores ν_m. In this context, our focus lies in investigating how the selection of the parameter M_j impacts the estimation of the eigenvalues ν_m.

Using this methodology, the maximum number of multivariate eigenvalues that can be estimated is M_+. Let $\{\nu_m\}_{1\leq m\leq M_+}$ be the set of true eigenvalues and $\{\widehat{\nu}_m\}_{1\leq m\leq M_+}$ be the set of estimated eigenvalues. We use the relative errors $\text{Err}(\widehat{\nu}_m) = (\nu_m - \widehat{\nu}_m)^2/\nu_m^2$ to assess the accuracy of the estimates. The authors also propose to estimate the number of multivariate components using the percentage of variance explained. For that, they first select M_j univariate components that explain $\alpha\%$ of the variance for each univariate features [Ramsay and Silverman, 2005, Chapter 8.2] and they claim that this number of components is enough to estimate the number of multivariate components that explain $\alpha\%$ of the variance in the multivariate functional data [Happ and Greven, 2018, Section 3.2]. The percentage of variance explained by the mth component and the cumulative percentage of variance explained by the first m components are defined as

$$\text{PVE}_m = 100 \times \nu_m \times \left(\sum_{l=1}^{M_+} \nu_l\right)^{-1} \quad \text{and} \quad \text{PVE}_{1:m} = \sum_{l=1}^{m} \text{PVE}_l, \quad m = 1, \dots, M_+.$$

If we fix the percentage of variance explained to be $\alpha\%$, the number of components needed to explain $\alpha\%$ of the variance is given by

$$\text{NPC}_\alpha = \sum_{m=1}^{M_+} \mathbf{1}\left\{\text{PVE}_{1:m} < \alpha\right\} + 1. \tag{1}$$

3 Simulation

We perform a simulation study based on the first setting in the simulation in Happ and Greven [2018]. The data-generating process is based on a truncated version of the Karhunen-Loève decomposition. First, we generate a large orthonormal basis $\{\psi_m\}_{1\leq k\leq M}$ of $\mathcal{L}^2(\mathcal{T})$ on an interval $\mathcal{T} = [0, T] \subset \mathbb{R}$. We fix $T_1 = 0$ and $T_{p+1} = T$ and we generate $p-1$ cut points $T_2, \dots, T_p$ uniformly in $\mathcal{T}$ such that $0 = T_1 < \cdots < T_p < T_{p+1} = T$. Let $s_1, \dots, s_p \in \{-1, 1\}$ be coefficients that randomly flip the eigenfunctions with probability 0.5, generated according to a Bernoulli distribution. The univariate components of the eigenfunctions are then defined as

$$\psi_m^{(j)}(t_j) = s_j \psi_m\big|_{[T_j, T_{j+1}]}\left(\frac{t_j - T_j}{T_{j+1} - T_j}\right), \quad m = 1, \dots, M, \quad j = 1, \dots, p.$$

The notation $\psi_m\big|_{[T_j, T_{j+1}]}$ is the restriction of the function ψ_m to the set $[T_j, T_{j+1}]$. The set of multivariate functions $\{\psi_m\}_{1\leq m\leq M}$ is an orthonormal system in $\mathcal{H} := \mathcal{L}^2(\mathcal{T}_1) \times \cdots \times \mathcal{L}^2(\mathcal{T}_p)$ with $\mathcal{T}_j = [0, 1]$. Each curve is then simulated using the truncated multivariate Karhunen-Loève expansion,

$$x_i(\mathbf{t}) = \sum_{m=1}^{M} \rho_{i,m} \psi_m(\mathbf{t}), \quad \mathbf{t} \in \mathcal{T}, \quad i = 1, \dots, N,$$

where the scores $\rho_{i,m}$ are sampled as Gaussian random variables with mean 0 and variance ν_m. The eigenvalues ν_m are defined with an exponential decrease, $\nu_m = \exp(-(m+1)/2)$. We simulate $N = 25, 50$ and 100 observations for each replication of the simulation. Similarly, each component is sampled on a regular grid of $S = 25, 50$ and 100 sampling points. We use $p = 5$ features and we set $M = 50$. This estimation procedure consists of densely observed multivariate functional data defined on different one-dimensional domains. The parameters are chosen to reflect the sample size and observation points typically found in real-world datasets. The estimation is done using the R package `MFPCA` (Happ-Kurz [2020]). For each univariate feature j, we estimate M_j principal

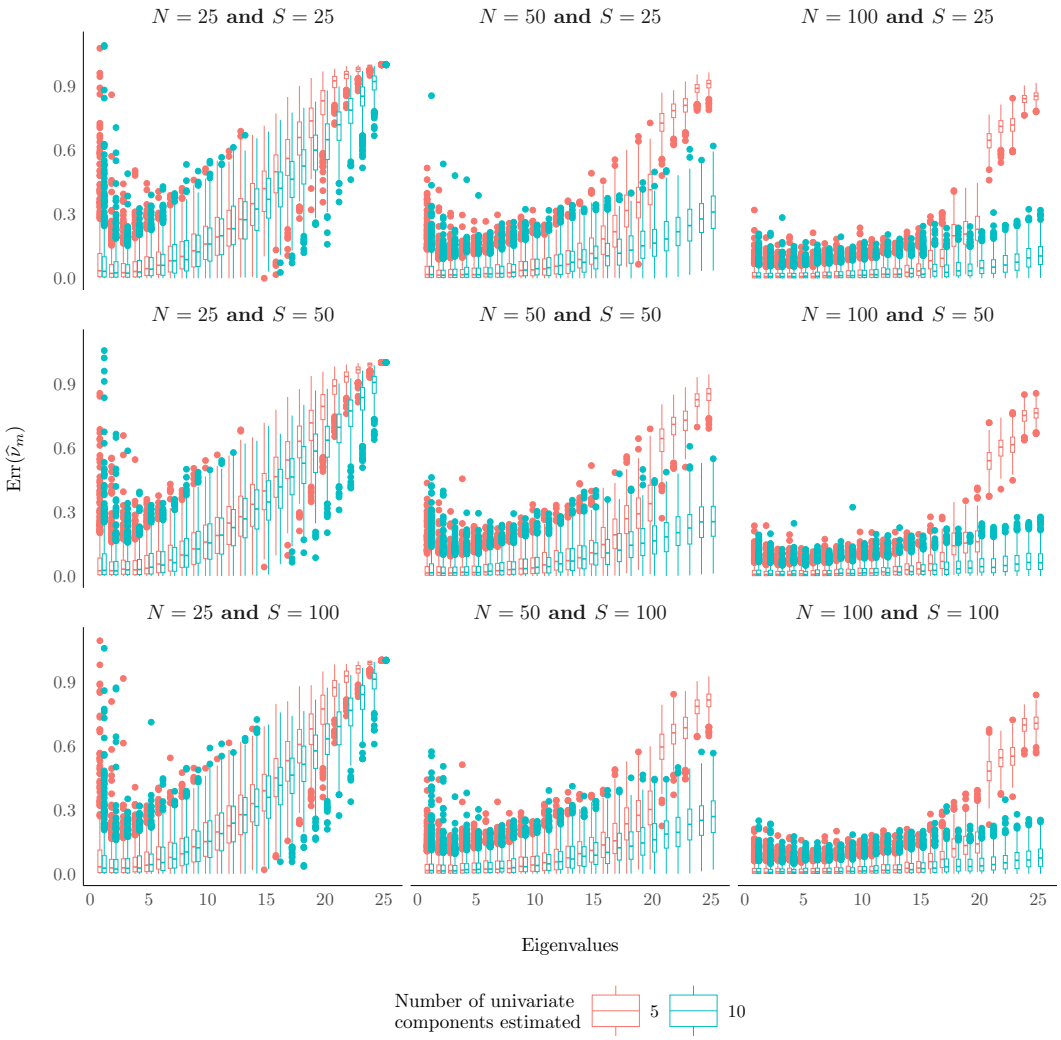


Figure 1: Boxplots of the estimation errors of the eigenvalues. We estimated $M_j = 5$ (red boxplots) and $M_j = 10$ (blue boxplots) univariate functional components for $j = 1, \ldots, p$. The number of multivariate eigencomponents that are estimated is 25. N is the number of observations, S is the number of sampling points per curve. We run 500 simulations.

components. Then, following the multivariate components estimation procedure, we can estimate $M_+ = \sum_{j=1}^{p} M_j$ multivariate components. The simulations are replicated 500 times.

To illustrate the effect of M_j on the estimation of the eigenvalues ν_m, Figure 1 displays a comparison of the errors for the first 25 estimated eigenvalues $\widehat{\nu}_m$ when using $M_j = 5$ and $M_j = 10$. The accuracy of the estimation of the multivariate eigenvalue $\widehat{\nu}_m$ declines with m in all scenarios. However, the decreasing of the accuracy is faster when $M_j = 5$ than when $M_j = 10$. We observe in particular a notable drop in accuracy for the estimated eigenvalues $\widehat{\nu}_m, m = 21, \ldots, 25$ when $M_j = 5$ in most scenarios, while this drop does not appear when $M_j = 10$. The dependence of the eigenvalue estimates $\widehat{\nu}_m$ on the number of univariate functional principal components retained M_j is clear, but establishing a general rule based on these observations is challenging. Increasing the number of univariate components estimated M_j improves the accuracy. Morover, for a given m, there is a required number of univariate eigencomponents that is needed to accurately estimate the multivariate eigenvalues. For example, the errors of the first five eigenvalues is similar with $M_j = 5$ and $M_j = 10$ for all scenarios. If this is reached, it is not useful to use larger M_j and will only results in a waste of computing power. We thus suggest to estimate at most M_- multivariate components using M_j univariate components; otherwise, the univariate components may not contain enough information to effectively recover their corresponding multivariate counterparts.

In a second setting, for each univariate feature j, we fix a percentage of variance to be explained $\alpha\%$ and choose M_j principal components accordingly. We then estimate M_+ multivariate components and replicate the simulations 500 times. Table 1 presents the estimation of the number of multivariate components $\widehat{\mathrm{NPC}}_\alpha$ retained across 500 simulation scenarios for a fixed percentage of

N	S	$\widehat{\text{NPC}}_\alpha$ 1	2
25	25	**301**	199
25	50	**276**	224
25	100	**270**	230
50	25	235	**265**
50	50	208	**292**
50	100	254	**246**
100	25	158	**342**
100	50	165	**335**
100	100	178	**322**

(a) $\alpha = 50\%$ ($\text{NPC}_\alpha = 2$)

N	S	$\widehat{\text{NPC}}_\alpha$ 1	2	3
25	25	1	**464**	35
25	50	1	**456**	43
25	100	1	**461**	38
50	25	0	**459**	41
50	50	0	**461**	39
50	100	1	**450**	49
100	25	0	**467**	33
100	50	0	**469**	31
100	100	0	**471**	29

(b) $\alpha = 70\%$ ($\text{NPC}_\alpha = 3$)

N	S	$\widehat{\text{NPC}}_\alpha$ 3	4	5
25	25	15	**400**	85
25	50	18	**375**	107
25	100	12	**379**	109
50	25	0	**322**	178
50	50	0	**271**	229
50	100	0	**268**	232
100	25	0	212	**288**
100	50	0	157	**343**
100	100	0	136	**364**

(c) $\alpha = 90\%$ ($\text{NPC}_\alpha = 5$)

N	S	$\widehat{\text{NPC}}_\alpha$ 4	5	6	7
25	25	6	**379**	115	0
25	50	5	**376**	118	1
25	100	1	**357**	142	0
50	25	0	**288**	212	0
50	50	0	232	**267**	1
50	100	0	210	**289**	1
100	25	0	172	**328**	0
100	50	0	110	**390**	0
100	100	0	84	**416**	0

(d) $\alpha = 95\%$ ($\text{NPC}_\alpha = 6$)

N	S	$\widehat{\text{NPC}}_\alpha$ 7	8	9	10
25	25	10	**365**	125	0
25	50	2	**362**	136	0
25	100	2	**338**	160	0
50	25	0	117	**383**	0
50	50	0	86	**413**	1
50	100	0	52	**448**	0
100	25	0	8	**492**	0
100	50	0	0	**499**	1
100	100	0	2	**497**	1

(e) $\alpha = 99\%$ ($\text{NPC}_\alpha = 10$)

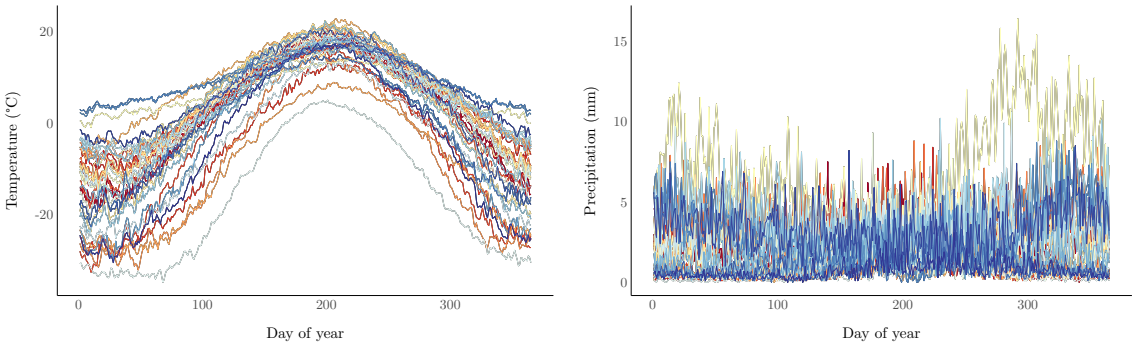
Table 1: Estimation of the number of components to explain $\alpha\%$ of the variance over 500 simulations. The true number of components that explain $\alpha\%$ of the variance is given in parenthesis. N is the number of observations, S is the number of sampling points per curve.

variance explained $\alpha\%$. The quantity NPC_α represents the number of multivariate components that would be needed to explain at least $\alpha\%$ of the variance ($50\%, 70\%, 90\%, 95\%$ and 99%), considering an exponential decay of the eigenvalues as defined in (1). Note that, we can compute the true number of multivariate components as we know the true eigenvalues. Each entry in Table 1 indicates the number of times each number of multivariate components has been selected over the 500 simulations. The number of components appears to be consistently underestimated for various combinations of the number of observations N, number of sampling points S, and desired percentage of variance explained $\alpha\%$. Therefore, this simulation scenario shows that using a percentage of variance explained of level $\alpha\%$ to choose the number of univariate components M_j is not sufficient to estimate the number of multivariate functional principal components that explain $\alpha\%$ of the variance in the multivariate functional data. These findings may hold considerable significance for practitioners as the percentage of variance explained by each eigencomponent is a popular method to determine the number of eigencomponents retained (see, e.g., James et al. [2021] for scalar data and Horváth and Kokoszka [2012] for functional data).

4 Application: Canadian weather dataset

To illustrate our simulation results, we apply the same idea on a real dataset, the Canadian weather dataset [Ramsay and Silverman, 2005], available in the `R` package `fda` [Ramsay et al., 2023]. The dataset contains daily measurements of temperature (in Celsius) and precipitation (in millimeters) for 35 Canadian weather stations, averaged over the years 1960 to 1994. The data are presented in Figure 2. This is an example of multivariate functional data with $p = 2$ defined on one dimensional domain, the temperature being the first feature $x^{(1)}$ and the precipitation being the second feature $x^{(2)}$. We aim to estimate M multivariate eigencomponents of the data using different number of univariate eigencomponents and compare the results. For that, we define two scenarios, one where $M = M_+$ and one where $M = M_-$.

We first expand the data in a B-splines basis with 10 functions. In the first scenario, for each feature, we estimate two univariate eigencomponents ($M_1 = 2$ and $M_2 = 2$). In the second scenario, for each feature, we estimate four univariate eigencomponents ($M_1 = 4$ and $M_2 = 4$). In



(a) Temperature (first component)

(b) Precipitation (second component)

Figure 2: The daily temperature and precipitation in 35 Canadian weather stations. Each curve represents one weather station.

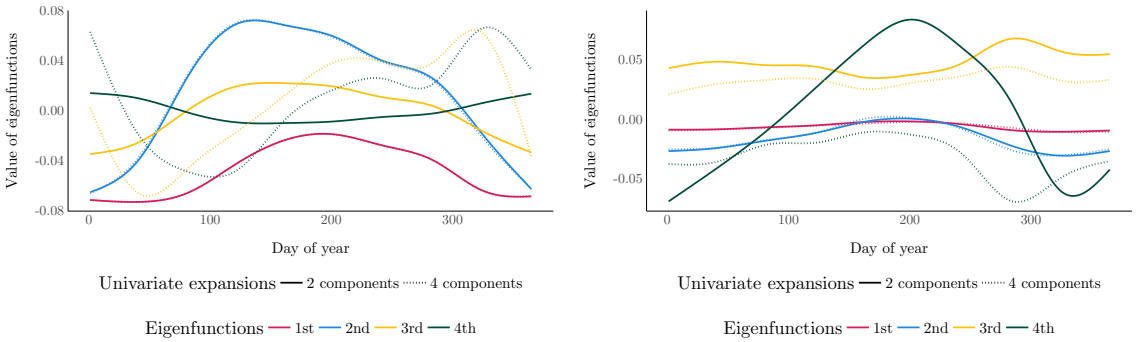
both scenarios, we then estimate $M = 4$ multivariate eigencomponents. So, for the first scenario, $M = M_+ = 4$ and for the second scenario, $M = M_- = 4$. Based on the simulation and Figure 1, we expect the first two multivariate eigencomponents to be similar and the other two to be unequal.

Table 2 presents the estimation of the eigenvalues for the Canadian weather dataset for both scenarios. We notice that the values are similar for the first two eigenvalues, but quite different for the other two. Figure 3 presents the estimation of the eigenfunctions for the Canadian weather

		Eigenvalues			
Scenario	Univariate expansions	1st	2nd	3rd	4th
1	2 components	15845	1675	308	45
2	4 components	15850	1679	438	213

Table 2: Estimation of the first four eigenvalues of the Canadian weather dataset using two and four univariate components for the univariate expansions.

dataset for both scenarios. As with the eigenvalues, we notice that the first two (multivariate) eigenfunctions are approximately the same, but the other two are not equal. The first two eigencomponents can be interpreted similarly in both scenarios. The first component is negative for both features, indicating that weather stations with positive scores have lower temperatures and less precipitation than average. While the first component for precipitation is relatively flat, the temperature component exhibits more variation at the beginning and end of the year. The second component contrasts winter and summer: stations with positive scores have higher temperatures and more precipitation in summer, and lower temperatures with less precipitation in winter compared to the average station. The third and fourth components differ between the scenarios. For univariate expansions with two components, the third multivariate component for temperature contrasts winter and summer, while with four univariate components, it contrasts spring and autumn. The third multivariate component for precipitation varies in magnitude depending on the number of univariate components. The fourth multivariate component for temperature is roughly flat when two univariate components are used but shows more variability with four components. For precipitation, the fourth component contrasts winter and summer when using two univariate components, but becomes flatter with a negative bump in autumn when four components are considered. These results highlight that the interpretation of the multivariate components depends on the number of univariate components used for the univariate decomposition. However, it would be preferable that the interpretation remains consistent and independent of the univariate decomposition. While we do not know the true eigenfunctions, based on simulation results, the estimated multivariate eigenfunctions from the second scenario should be closer to the truth than the estimation from the first scenario. We may explain this result as we have not estimated enough information in the univariate decomposition in the first scenario to effectively estimate the third and fourth multivariate eigencomponents. We reiterate the suggestion to estimate at most M_- multivariate eigencomponents (which will be $M_- = 2$ for the first scenario).



(a) Temperature (first component)

(b) Precipitation (second component)

Figure 3: Estimation of the first four eigenfunctions of the Canadian weather dataset using using two and four univariate components for the univariate expansions.

5 Conclusion

Happ and Greven [2018] present a general methodology to estimate principal components for a set of multivariate functional data defined on, possibly, different dimensional domains. Their approach, based on the decomposition of the covariance of each univariate feature, allows easy estimation of the components.

We have conducted a simulation study and an example on a real dataset, and the obtained results highlight two important findings. Firstly, although utilizing only a few univariate components may yield a substantial number of multivariate components, their accuracy is notably limited. Secondly, relying on the percentage of variance explained as a criterion for selecting the number of univariate components may result in an underestimation of the number of multivariate components. We, therefore, advise practitioners to exercise caution when determining the number of estimated components required in their analysis. We suggest to estimate at most M_- multivariate components. Additionally, we strongly recommend conducting simulations that closely resemble the characteristics of the actual data to select the appropriate number of components based on the percentage of variance explained criterion.

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