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# Functional Principal Component Analysis via Regularized Gaussian Basis Expansions and Its Application to Unbalanced Data

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### SUMMARY

This paper introduces regularized functional principal component analysis for multidimensional functional data sets, utilizing Gaussian basis functions. An essential point in a functional approach via basis expansions is the evaluation of the matrix for the integral of the product of any two bases (cross product matrix). Advantages of the use of the Gaussian type of basis functions in the functional approach are that its cross product matrix can be easily calculated, and it creates a much more flexible instrument for transforming each individual's observation into a functional form. The proposed method is applied to the analysis of three-dimensional (3D) protein structural data that can be referred to as unbalanced data. It is shown that our method extracts useful information from unbalanced data. Numerical experiments are conducted to investigate the effectiveness of our method via Gaussian basis functions, comparing to the method based on $B$-splines. On performing regularized functional principal component analysis with $B$-splines, we also derive the exact form of its cross product matrix. The numerical results show that our methodology is superior to that based on $B$-splines for unbalanced data.

KEY WORDS: functional data analysis, model selection, protein structure, radial basis functions, regularization, smoothing parameter, spline.

## 1. Introduction

Multivariate analysis deals with observations on more than one variable, where there is some inherent interdependence between the variables (Mardia, Kent and Bibby (1979)),

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and principal component analysis (PCA) is one of the most widely used multivariate analysis techniques in various fields of natural and social sciences (see, e.g., Jolliffe (2002)). The concepts of PCA are the dimension reduction and visualization of data. However, there are some problems with applying conventional PCA to the longitudinal type of data. For example, if the observational points are not equally spaced and differ among subjects, PCA cannot be directly applied. Accordingly, a number of recent papers have investigated functional principal component analysis (functional PCA) and its regularization methods that reformulate PCA in terms of the functions rather than the discrete observations (Besse and Ramsay (1986), Rice and Silverman (1991), Silverman (1996)).

These functional approaches are referred to as functional data analysis (FDA; Ramsay and Silverman (2002, 2005), Ferraty and Vieu (2006), Mizuta (2006)). The basic idea behind FDA is the conversion of observational discrete data to functional data by a smoothing method and then extracting information from the obtained functional data set by applying concepts from traditional multivariate analysis. In modeling with FDA, many studies employ a basis expansion which assumes that functional data and coefficient functions may be expressed as linear combinations of known basis functions. Fourier series are useful if the observations are periodic and have sinusoidal features, whereas splines (Green and Silverman (1994)) and $B$-splines (De Boor (2001), Eilers and Marx (1996), Imoto and Konishi (2003)) are utilized to non-periodic data.

An essential point for FDA via basis expansions is the evaluation of the matrix for the integral of the product of any two bases (cross product matrix). The orthonormal property of Fourier series yields the identity cross product matrix, and then we need not evaluate the cross product matrix for Fourier series. In contrast, spline types of bases do not have the orthonormal property, and in consequence the cross-product matrix must be calculated. Previous works, however, utilized discrete approximation to evaluate the cross product matrix for spline types of bases (see e.g., Ramsay and Silverman (2002, §2)). In this paper, we provide the exact form for the integral of the product of any two $B$-spline bases.

The main aim of this paper is to introduce regularized functional PCA for multidimensional (multivariate) functional data sets, utilizing Gaussian basis functions. Advantages of the use of the Gaussian type of basis functions are that its cross product matrix can be easily calculated, and it creates a much more flexible instrument for transforming each individual's observation into a functional form. Numerical experiments are conducted to investigate the effectiveness of our method via Gaussian basis functions. In addition, the proposed method is applied to functionalized three-dimensional (3D) protein structural data that determine the 3D arrangement of amino-acids in individual protein and also de-

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termine proteins that have special structures. An objective of the analysis of the protein structural data is to characterize any features of proteins without relying on their sequence information and physicochemical properties. Our functionalization method permits a low-dimensional visualization of proteins, and provides a useful information concerning to biological view points.

This paper is organized as follows. Section 2 describes observational discrete data and their functinalization to multidimensional functional data. Section 3 introduces a regularized functional principal component procedure based on multidimensional functional data sets and gives an outline of its implementation. In Section 4, Monte Carlo simulations are conducted to investigate the effectiveness of the proposed regularized functional PCA based on Gaussian basis functions, in which we compare our procedure to that based on $B$-splines with the derived exact cross product matrix. Section 5 describes an application of the proposed method to the 3D protein structural data. Finally, some concluding remarks are presented in Section 6.

## 2. Discrete and functional data

Suppose we have $N$ independent discrete observations $\{t_{ij}, (x_{i1j}, \cdots, x_{ipj}) \, ; \, j = 1, \cdots, n_i\}$ $(i = 1, \cdots, N)$, where each $t_{ij}$ $(\in \mathcal{T} \subset \mathbb{R})$ is the $j$-th observational point of the $i$-th individual and $(x_{i1j}, \cdots, x_{ipj})$ $(\in \mathbb{R}^p)$ is the discrete data observed at $t_{ij}$ for $p$ variables $X_1, \cdots, X_p$. In particular, the $i$-th discrete data set observed at $t_{ij}$ for $X_l$ is represented by $\{(t_{ij}, x_{ilj}) \, ; \, j = 1, \cdots, n_i\}$. It may be noted that we have the discrete data observed at possibly different observational points $t_{i1}, \cdots, t_{in_i}$ for each subject, and then the discrete observations can be referred to as unbalanced data. For example, $\{t_{ij}, (x_{i1j}, x_{i2j}, x_{i3j}) \, ; \, j = 1, \cdots, n_i\}$ $(i = 1, \cdots, 12)$ are the measurements in XYZ coordinates of 3D protein structures, where $t_{ij}$ are the positions in $i$-th amino-acid sequence and $(x_{i1j}, x_{i2j}, x_{i3j})$ are the XYZ coordinates values of amino acids which compose $i$-th 3D protein structure. Fig1 (upper) shows an example of discretized 3D protein structural data with $p = 3$ and $n_i = 186$.

We convert each discrete data set $\{(t_{ij}, x_{ilj}) \, ; \, j = 1, \cdots, n_i\}$ to functional data $x_{il}^*(t)$ using a smoothing method, as follows. It is assumed that each discrete data $\{(t_{ij}, x_{ilj}); j = 1, \cdots, n_i\}$ is generated from the nonlinear regression models

$$x_{ilj} = u_{il}(t_{ij}) + \varepsilon_{ilj} \qquad (j = 1, \cdots, n_i) \, ,$$

where the errors $\varepsilon_{ilj}$ are independently normally distributed with mean 0 and variance $\sigma_{il}^2$. The nonlinear functions $u_{il}(t)$ are assumed to be given by linear combinations of Gaussian
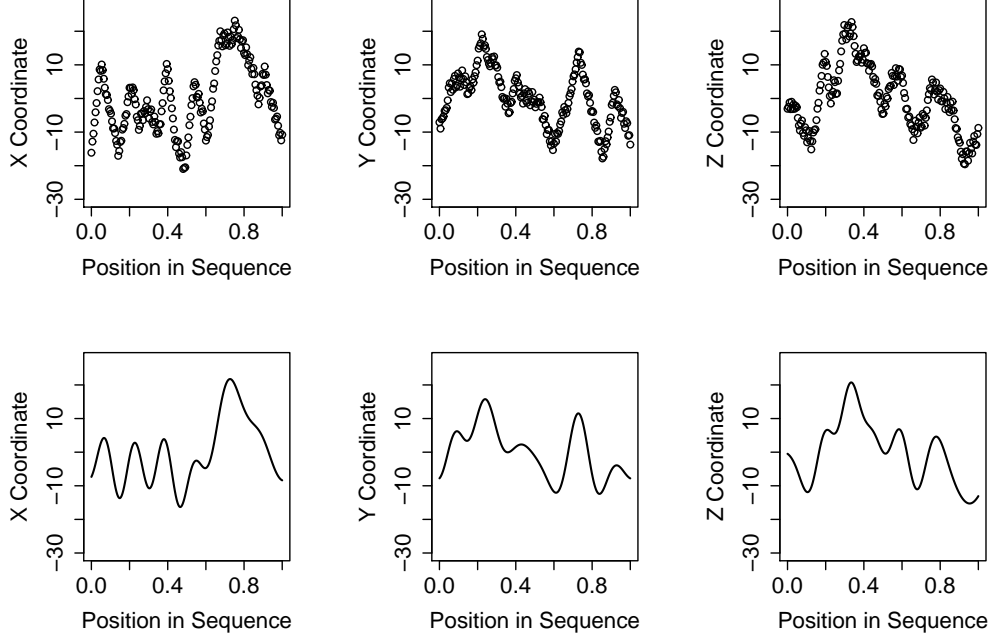
Fig. 1: An example of discrete data (upper) and corresponding three-dimensional functional data (lower) for a 3D protein structure ($p = 3$, $n_i = 186$).

basis functions $\{\phi_m(t) = \phi_m(t; \nu, \mu_m, \tau_m^2)\}$ with parameters $\mu_m$, $\tau_m$ and $\nu$,

$$u_{il}(t) = \sum_{m=1}^{M} c_{ilm}\phi_m(t) \ ,$$

where the $m$-th Gaussian basis function $\phi_m(t)$ has the form

$$\phi_m(t) = \phi_m(t; \ \nu, \mu_m, \tau_m^2) = \exp\left\{-\frac{(t-\mu_m)^2}{2\nu\tau_m^2}\right\} \qquad (m = 1, \cdots, M) \ . \qquad (1)$$

The parameters $\mu_m$ and $\tau_m$ express the position and width of the $m$-th basis function and $\nu$ is a hyper-parameter that adjusts the degree of overlapping among the basis functions (Ando *et al.* (2005)).

Each non-linear function $u_{il}(t)$ is estimated in two steps. First, the parameters $\mu_m$ and $\tau_m$ are estimated applying the $k$-means clustering method to $\sum_i n_i$ observational points $\{t_{ij} \ ; \ j = 1, \cdots, n_i, \ i = 1, \cdots, N\}$. The estimated parameters $\hat{\mu}_m$ and $\hat{\tau}_m^2$ are given by the sample mean and variance of $\{t_{ij} \in C_m\}$, where $C_m$ is the $m$-th cluster given by the $k$-means method. Let $\phi_m^\nu(t) = \phi_m(t; \ \nu, \hat{\mu}_m, \hat{\tau}_m^2)$ be the estimated $m$-th basis function. Next, the coefficient parameters $c_{il1}, \cdots, c_{ilM}$ and variance $\sigma_{il}^2$ are estimated by maximizing the penalized log-likelihood function with a smoothing parameter $\beta_{il} \ (> 0)$ that controls the smoothness of the nonlinear function $u_{il}(t)$. The estimators $\hat{\boldsymbol{c}}_{il}$ and

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$\hat{\sigma}_{il}^2$ depend on the number of basis functions $M$, hyper-parameter $\nu$ in Gaussian basis functions and smoothing parameter $\beta_{il}$ for each $i$ and $l$. The parameters are selected by minimizing the generalized information criterion (GIC), given by Konishi and Kitagawa (1996) (see also, Konishi and Kitagawa (2008)).

Thus, we have the estimated nonlinear functions $\hat{u}_{il}(t) = \sum_{m=1}^M \hat{c}_{ilm}\phi_m(t)$ (($i = 1, \cdots, N$, $l = 1, \cdots, p$), where $\phi_m(t) = \phi_m^\nu(t) = \phi_m(t;\, \nu, \hat{\mu}_m, \hat{\tau}_m^2)$ is the $m$-th basis function with the optimal hyper-parameter $\nu$ selected by minimizing GIC. The $p$-dimensional functional data sets $\{x_{i1}^*(t), \cdots, x_{ip}^*(t)\,;\, t \in \mathcal{T}\}$ are given by $x_{il}^*(t) = \hat{u}_{il}(t)$ for each $i$ and $l$. In the next section, we introduce regularized functional PCA for the $p$-dimensional functional data sets, using Gaussian basis functions. An example of multidimensional functional data is shown in Fig1 (lower), corresponding to the discretized 3D protein structural data in Fig1 (upper).

# 3. Functional Principal Component Analysis

## 3.1 Model

Let $\{(x_{i1}^*(t), \cdots, x_{ip}^*(t))\,;\, t \in \mathcal{T}\}$ ($i = 1, \cdots, N$) be the $p$-dimensional functional data sets obtained by smoothing the observational discrete data sets $\{t_{ij}, (x_{i1j}, \cdots, x_{ipj})\,;\, j = 1, \cdots, n_i\}$ ($i = 1, \cdots, N$). A functional principal component method is here applied to the $p$-dimensional functional data sets $\{(x_{i1}(t), \cdots, x_{ip}(t))\,;\, t \in \mathcal{T}\}$ ($i = 1, \cdots, N$), where $x_{il}(t) = x_{il}^*(t) - \bar{x}_l^*(t)$ and each $\bar{x}_l^*(t)$ is the mean function of the functional data $x_{i1}^*(t), \cdots, x_{ip}^*(t)$. It is assumed that each functional data element $x_{il}(t)$ can be expressed as a linear combination of Gaussian basis functions $\phi_m(t) = \phi_m^\nu(t) = \phi_m(t;\, \nu, \hat{\mu}_m, \hat{\tau}_m^2)$,

$$x_{il}(t) = \sum_{m=1}^M \tilde{c}_{ilm}\phi_m(t) = \tilde{\boldsymbol{c}}_{il}'\boldsymbol{\phi}(t) \qquad (i = 1, \cdots, N,\, l = 1, \cdots, p),$$

where $\tilde{\boldsymbol{c}}_{il} = (\tilde{c}_{il1}, \cdots, \tilde{c}_{ilM})'$ and $\boldsymbol{\phi}(t) = (\phi_1(t), \cdots, \phi_M(t))'$.

Let $f_i$ be an inner product for a $p$-dimensional weight function $\boldsymbol{\xi}(t) = (\xi_1(t), \cdots, \xi_p(t))'$ ($t \in \mathcal{T}$) and $i$-th $p$-dimensional functional data $\boldsymbol{x}_i(t) = (x_{i1}(t), \cdots, x_{ip}(t))'$,

$$f_i = \langle \boldsymbol{\xi}, \boldsymbol{x}_i \rangle_p = \sum_{l=1}^p \langle \xi_l, x_{il} \rangle = \sum_{l=1}^p \int_\mathcal{T} \xi_l(t)x_{il}(t)dt \qquad (i = 1, \cdots, N)\,.$$

We adopt a straightforward definition of an inner product between two $p$-dimensional functions. It is assumed that the weight functions $\xi_1(t), \cdots, \xi_p(t)$ can be expressed in terms of the same basis functions as the functional data sets $\{(x_{i1}(t), \cdots, x_{ip}(t))\}$,

$$\xi_l(t) = \sum_{m=1}^M \theta_{lm}\phi_m(t) = \boldsymbol{\theta}_l'\boldsymbol{\phi}(t) \qquad (l = 1, \cdots, p)$$

with $\boldsymbol{\theta}_l = (\boldsymbol{\theta}_{l1}, \cdots, \boldsymbol{\theta}_{lM})'$. A general functional principal component method maximizes the sample variance of the inner products subject to the orthonormal constraints, in order to estimate weight functions. It may be noted that the weight functions correspond to the weight vectors in conventional PCA. Ramsay and Silverman (2005, §8.5) describes the functional principal component method to the 2-dimensional functional data sets which include the hip and knee angles during a human gait cycle.

On the other hand, regularized (smoothed) functional principal component analysis (regularized functional PCA) proposed by Rice and Silverman (1991) and Silverman (1996) avoids ill-posed problems from functional PCA and maximizes the penalized sample variance (PSV) instead of the sample variance in functional PCA. In this paper, we estimate the $p$-dimensional weight function $\boldsymbol{\xi}(t)$ that maximizes the following penalized sample variance subject to penalized orthonormal constraints.

$$\mathrm{PSV}_\lambda(\boldsymbol{\xi}) = \frac{\mathrm{var}(f)}{\|\boldsymbol{\xi}\|_p^2 + \boldsymbol{\theta}' Q_\lambda \boldsymbol{\theta}} \;, \tag{2}$$

where $\boldsymbol{\theta} = (\boldsymbol{\theta}_1', \cdots, \boldsymbol{\theta}_p')'$, $\|\boldsymbol{\xi}\|_p^2 = \sum_l \|\xi_l\|^2 = \sum_l \int_{\mathcal{J}} \xi_l^2(t)\,dt$ is the norm of a $p$-dimensional weight function $\boldsymbol{\xi}(t)$ and $Q_\lambda = \mathrm{diag}(\lambda_1 Q^*, \cdots, \lambda_p Q^*)$ is a $pM \times pM$ positive-semidefinite block diagonal matrix with $M \times M$ positive-semidefinite matrix $Q^*$ and smoothing parameters $\lambda_l > 0$ which control the smoothness of the weight functions $\xi_l(t)$. The smoothing parameters $\lambda_l$ can be optimally selected by minimizing a cross validation score.

The principal component (PC) curves are defined by the $p$-dimensional weight function $\boldsymbol{\xi}(t)$ that maximizes the penalized sample variance $\mathrm{PSV}_\lambda(\boldsymbol{\xi})$ given by (2) subject to the penalized orthonormal constraints.

First PC Curve $\boldsymbol{\xi}_1^\lambda(t) = (\xi_{11}^\lambda(t), \cdots, \xi_{1p}^\lambda(t))'$ :
    the $p$-dimensional weight function $\boldsymbol{\xi}(t)$ that maximizes $\mathrm{PSV}_\lambda(\boldsymbol{\xi})$
                        subject to $\|\boldsymbol{\xi}\|_p^2 = 1$,

$k\ (\geq 2)$-th PC Curve $\boldsymbol{\xi}_k^\lambda(t) = (\xi_{k1}^\lambda(t), \cdots, \xi_{kp}^\lambda(t))'$ :
    the $p$-dimensional weight function $\boldsymbol{\xi}(t)$ that maximizes $\mathrm{PSV}_\lambda(\boldsymbol{\xi})$
        subject to $\|\boldsymbol{\xi}\|_p^2 = 1$ and $\langle \boldsymbol{\xi}, \boldsymbol{\xi}_r^\lambda \rangle_p + \boldsymbol{\theta}' Q_\lambda \boldsymbol{\theta}_r^\lambda = 0\ (r < k)$,

where the $l$-th element $\xi_{kl}^\lambda(t)$ of $\boldsymbol{\xi}_k^\lambda(t)$ may be expressed as the basis expansion $\xi_{kl}^\lambda(t) = \sum_m \theta_{klm}^\lambda \phi_m(t) = (\boldsymbol{\theta}_{kl}^\lambda)' \boldsymbol{\phi}(t)$, and $\boldsymbol{\theta}_k^\lambda = ((\boldsymbol{\theta}_{k1}^\lambda)', \cdots, (\boldsymbol{\theta}_{kp}^\lambda)')'$. The $k$-th principal component score is defined by $\{ f_{ki}^\lambda = \langle \boldsymbol{\xi}_k^\lambda, \boldsymbol{x}_i \rangle_p ; i = 1, \cdots, N \}\ (k = 1, \cdots, pM)$. We note that there are $pM$ principal components by the assumption of basis expansions.

## 3.2 Eigenvalue Problem

The PC curves $\boldsymbol{\xi}_k^\lambda(t) = (\xi_{k1}^\lambda(t), \cdots, \xi_{kp}^\lambda(t))'$ can be estimated by solving an eigenvalue problem. The inner product $f_i = \langle \boldsymbol{\xi}, \boldsymbol{x}_i \rangle_p$ for a $p$-dimensional weight function $\boldsymbol{\xi}(t)$ and $i$-th $p$-dimensional functional data $\boldsymbol{x}_i(t)$ can be written as

$$f_i = \langle \boldsymbol{\xi}, \boldsymbol{x}_i \rangle_p = \sum_{l=1}^{p} \langle \xi_l, x_{il} \rangle = \sum_{l=1}^{p} \int_{\mathfrak{J}} \boldsymbol{\theta}_l' \boldsymbol{\phi}(t) \boldsymbol{\phi}(t)' \tilde{\boldsymbol{c}}_{il} \, dt = \sum_{l=1}^{p} \boldsymbol{\theta}_l' W^* \tilde{\boldsymbol{c}}_{il} = \boldsymbol{\theta}' W \tilde{\boldsymbol{c}}_i,$$

where $\tilde{\boldsymbol{c}}_i = (\tilde{\boldsymbol{c}}_{i1}', \cdots, \tilde{\boldsymbol{c}}_{iM}')'$, each $\boldsymbol{\theta}_l$ is the coefficient vectors of $\xi_l(t)$, the $M \times M$ cross-product matrix $W^* = \int_{\mathfrak{J}} \boldsymbol{\phi}(t) \boldsymbol{\phi}(t)' dt$ has the $(m,n)$-th element $W_{mn}^* = \int_{\mathfrak{J}} \phi_m(t) \phi_n(t) \, dt$, and the $pM \times pM$ matrix $W = \mathrm{diag}(W^*, \cdots, W^*)$ is the block diagonal matrix formed from $W^*$.

The $(m,n)$-th components of the cross-product matrix $W^*$ for Gaussian basis functions $\phi_l(t) = \phi_l^\nu(t) = \phi_l(t; \nu, \hat{\mu}_l, \hat{\tau}_l^2)$ are given by

$$W_{mn}^* = \frac{\sqrt{2\pi\nu\hat{\tau}_m^2\hat{\tau}_n^2}}{\sqrt{\hat{\tau}_m^2 + \hat{\tau}_n^2}} \exp\left\{ -\frac{(\hat{\mu}_m - \hat{\mu}_n)^2}{2\nu(\hat{\tau}_m^2 + \hat{\tau}_n^2)} \right\} \qquad (m, n = 1, \cdots, M).$$

We assume that the cross-product matrix $W^*$ of Gaussian basis functions is positive definite. From this assumption, it follows that the condition for a norm is satisfied and regularized functional PCA can be applied. In addition, to satisfy the assumption, we employ Gaussian basis functions except constant term (1), which are as flexible as common Gaussian RBF.

Now, let $V = N^{-1} \sum_i \tilde{\boldsymbol{c}}_i \tilde{\boldsymbol{c}}_i'$ be the $pM \times pM$ sample variance-covariance matrix of the estimated coefficient vectors $\tilde{\boldsymbol{c}}_i$ of the $p$-dimensional functional data $\boldsymbol{x}_i(t)$. The sample variance $\mathrm{var}(f)$ of $\{f_i \, ; \, i = 1, \cdots, N\}$ can be written as

$$\mathrm{var}(f) = \frac{1}{N} \sum_{i=1}^{N} f_i^2 = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{\theta}' W \tilde{\boldsymbol{c}}_i \tilde{\boldsymbol{c}}_i' W \boldsymbol{\theta} = \boldsymbol{\theta}' W V W \boldsymbol{\theta} \,.$$

The penalized sample variance $\mathrm{PSV}_\lambda(\boldsymbol{\xi})$ in (2) can then be written as

$$\mathrm{PSV}_\lambda(\boldsymbol{\theta}) = \frac{\boldsymbol{\theta}' W V W \boldsymbol{\theta}}{\boldsymbol{\theta}'(W + Q_\lambda)\boldsymbol{\theta}} \,,$$

since the norm of the $p$-dimensional weight function $\boldsymbol{\xi}(t)$ is expressed as

$$\|\boldsymbol{\xi}\|_p^2 = \sum_{l=1}^{p} \|\xi_l\|^2 = \sum_{l=1}^{p} \boldsymbol{\theta}_l' W^* \boldsymbol{\theta}_l = \boldsymbol{\theta}' W \boldsymbol{\theta} \,.$$

Also let $\boldsymbol{u} = U_\lambda \boldsymbol{\theta}$ and $S_\lambda = U_\lambda^{-1}$, where the $pM \times pM$ non-singular upper triangular matrix $U_\lambda$ satisfies $W + Q_\lambda = U_\lambda' U_\lambda$. We then have

$$\mathrm{PSV}_\lambda(\boldsymbol{u}) = \frac{\boldsymbol{u}' S_\lambda' W V W S_\lambda \boldsymbol{u}}{\boldsymbol{u}' \boldsymbol{u}} \,. \tag{3}$$

Thus, the maximum problem of the penalized sample variance $\text{PSV}_\lambda(\boldsymbol{\xi})$ is equivalent to the maximum problem of the above quadratic form (3). Therefore we need to solve the eigenvalue problem for the $pM \times pM$ matrix $S'_\lambda WVWS_\lambda$.

Let $\rho_1 \geq \cdots \geq \rho_{pM}$ be the eigenvalues of $S'_\lambda WVWS_\lambda$ and $\boldsymbol{e}_1, \cdots, \boldsymbol{e}_{pM}$ be the orthonormal eigenvectors corresponding to the eigenvalues $\rho_1, \cdots, \rho_{pM}$, respectively. The estimated coefficient parameter vectors $\hat{\boldsymbol{\theta}}_k^\lambda = ((\hat{\boldsymbol{\theta}}_{k1}^\lambda)', \cdots, (\hat{\boldsymbol{\theta}}_{kp}^\lambda)')'$ are given by

$$\hat{\boldsymbol{\theta}}_k^\lambda = \frac{1}{\sqrt{\boldsymbol{e}'_k S'_\lambda W S_\lambda \boldsymbol{e}_k}} S_\lambda \boldsymbol{e}_k \qquad (k = 1, \cdots, pM) .$$

The $p$-dimensional $k$-th PC curves $\boldsymbol{\xi}_k^\lambda(t)$ and PC scores $\{f_{ki}^\lambda = \langle \boldsymbol{\xi}_k^\lambda, \boldsymbol{x}_i \rangle_p \; ; \; i = 1, \cdots, N\}$ can then be obtained by using $\hat{\boldsymbol{\theta}}_k^\lambda$. Furthermore, we can express the $p$-dimensional functional data sets $\{x_{i1}(t), \cdots, x_{ip}(t) \; ; \; i = 1, \cdots, N\}$ as uncorrelated scores, since the sample covariance of the $k$-th and $k' (\neq k)$-th PC scores is 0.

## 3.3 Smoothing Parameter Selection

The smoothing parameters $\lambda_l$ in regularized functional PCA can be optimally selected, as follows. Rice and Silverman (1991) and Silverman (1996) selected the optimal smoothing parameter using a cross validation (CV) method.

When we have smoothing parameters $\lambda_l$ and $k \in \{1, 2, \cdots, pM\}$, then $i$-th $p$-dimensional functional data $\boldsymbol{x}_i(t)$ is projected into the space spanned by the PC curves $\{\boldsymbol{\xi}_r^{\lambda, -i}(t) \; ; \; r = 1, \cdots, k\}$, where each $\boldsymbol{\xi}_r^{\lambda, -i}(t)$ denotes the $r$-th PC curve estimated from the functional data set excluding $\boldsymbol{x}_i(t)$. The projected (reconstructed) functional data $\hat{\boldsymbol{x}}_{ik}^{\lambda, -i}(t)$ are given by

$$\hat{\boldsymbol{x}}_{i,k}^{\lambda, -i}(t) = \sum_{r=1}^k \sum_{q=1}^k \left( G_k^{\lambda, -i} \right)_{rq}^{-1} \langle \boldsymbol{\xi}_q^{\lambda, -i}, \boldsymbol{x}_i \rangle_p \; \boldsymbol{\xi}_r^{\lambda, -i}(t) \qquad (i = 1, \cdots, N) ,$$

where the $k \times k$ matrix $G_k^{\lambda, -i}$ has $(r, q)$-th components $G_{k,rq}^{\lambda, -i} = \langle \boldsymbol{\xi}_r^{\lambda, -i}, \boldsymbol{\xi}_q^{\lambda, -i} \rangle_p$. The cross validation scores $CV_k(\lambda)$ and $CV(\lambda)$ are defined by

$$CV_k(\lambda) = \sum_{i=1}^N \left\| \boldsymbol{x}_i - \hat{\boldsymbol{x}}_{i,k}^{\lambda, -i} \right\|_p^2 , \qquad CV(\lambda) = \sum_{k=1}^{pM} CV_k(\lambda) .$$

The set of optimal smoothing parameters is obtained by minimizing $CV(\lambda)$.

# 4. Numerical experiments

In this section, Monte Carlo experiments are conducted to compare the effectiveness of the proposed method via Gaussian basis functions and cubic $B$-splines with equidistant

knots. We refer to De Boor (2001) and Imoto and Konishi (2003) for $B$-splines. We note that Fourier series are orthonormal, while Gaussian basis functions and $B$-splines are not. The evaluation of the cross product matrix for Gaussian basis functions was described in the subsection 3.2. Then if we perform regularized functional PCA via $B$-splines, its cross-product matrix $W^*$ must be evaluated. We derived the integral of the product of any two $B$-spline bases. An outline of the evaluation is shown in Appendix.

A true functional data set $\{x_i(t); t \in [0,1], i = 1, \cdots, 15\}$ was generated in each trial of Monte Carlo experiments. However this data set $x_i(t)$ could not be expressed in terms of a basis expansion, so a discrete data set was generated from $\{x_i(t)\}$, and a new functional data set $\{\tilde{x}_i(t); i = 1, \cdots, 15\}$ was then obtained by smoothing the generated discrete data set. Applying regularized functional PCA to $\tilde{x}_i(t)$, we calculated the mean square error (MSE) between the true functional data $x_i(t)$ and the that reconstructed by estimated PC curves. More precisely, we performed the Monte Carlo experiment using the following procedure.

**Step 1.** Generate a true functional data set $\{x_i(t); i = 1, \cdots, 15\}$ from mixed effects models (see, e.g., James *et al.* (2000)),

$$x_i(t) = \mu(t) + \sum_{m=1}^{4} \alpha_{im} \xi_m(t) \qquad (t \in [0,1], \; i = 1, \cdots, 15),$$

where the mean function $\mu(t)$ is assumed to be the following functions

1.  $\mu(t) = e^{-3t} \sin(3\pi t)$,

2.  $\mu(t) = 1 - 48t + 218t^2 - 315t^3 + 145t^4$,

and $\xi_{2r-1}(t) = \sin(2\pi r t)$, $\xi_{2r}(t) = \cos(2\pi r t)$ $(r = 1, 2)$. The random components $\alpha_{im}$ are assumed to be independently normally distributed with $\alpha_{im} \overset{iid}{\sim} N(0, (0.03R_x)^2)$, where $R_x$ is the range of $\mu(t)$ over $t \in [0,1]$.

**Step 2.** Generate discrete data $\{x_{ij}; j = 1, \cdots, n_i\}$ from the nonlinear regression models with the true functions $x_i(t)$,

$$x_{ij} = x_i(t_{ij}) + \varepsilon_{ij} \qquad (j = 1, \cdots, n_i \; i = 1, \cdots, 15),$$

where the errors $\varepsilon_{ij}$ are assumed to be independently normally distributed with $\varepsilon_{ij} \overset{iid}{\sim} N(0, \sigma_\varepsilon^2)$, where standard deviation $\sigma_\varepsilon$ is taken as $0.05R_x$, $0.1R_x$, $0.2R_x$. A set of observational points $t_{ij}$ is generated from the uniform distribution on $[0,1]$. The numbers $n_i$ of observational points are taken as $n_i = 100$ or generated from the normal distribution

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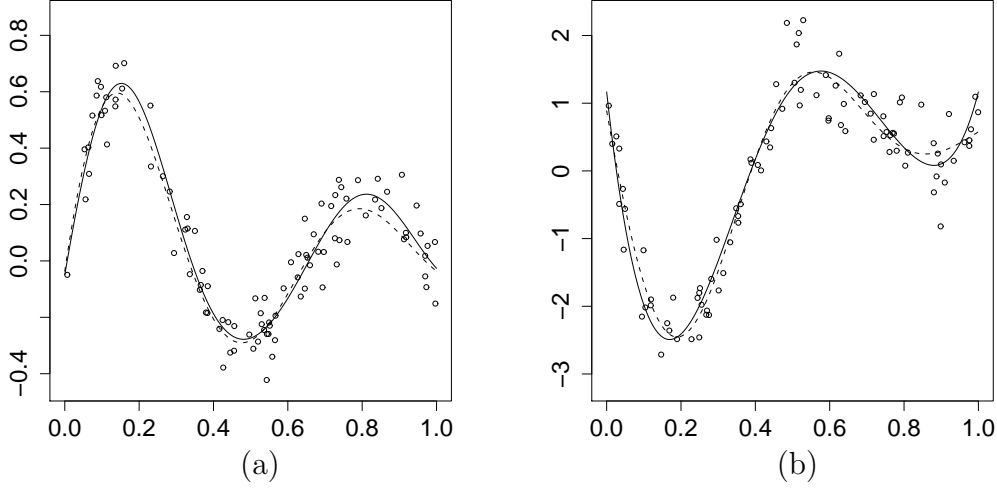
Fig. 2: Examples of simulated data: The dashed lines are the true functional data, while the solid lines are the estimated functional data. $\mu(t) =$ (a) $e^{-3t}\sin(3\pi t)$ and (b) $1 - 48t + 218t^2 - 315t^3 + 145t^4$.

with mean 100 and variance $2^2$. We note that the generated data can be referred to as high-dimensional and small sample-size data.

**Step 3.** Estimate a functional data set by smoothing the discrete data set $\{x_{ij} \,;\, j = 1, \cdots, n_i, \ i = 1, \cdots, 12\}$. It is assumed that each functional data $x_i(t)$ can be expressed as a linear combination of Gaussian basis functions or $B$-splines. The number $M$ of basis functions, hyper-parameter $\nu$ (for Gaussian basis functions) and smoothing parameters $\beta_i$ are optimally selected by minimizing GIC (Konishi and Kitagawa (1996, 2008)). Fig2 shows generated true functional data $x_1(t)$ (dashed line), discrete data $\{x_{1j}; j = 1, \cdots, n_i\}$ and estimated functional data $\tilde{x}_1(t)$ (solid line) for 2 mean functions with $\sigma_\varepsilon = 0.1 R_x$.

**Step 4.** Perform regularized functional PCA on the estimated functional data set $\{\tilde{x}_i(t) \,;\, i = 1, \cdots, 15\}$ and smoothing parameter selection based on the cross validation method.

**Step 5.** Calculate the mean square error for the $b$-th trial,

$$\text{MSE}_b = \frac{1}{15} \sum_{i=1}^{15} \|x_i - \hat{x}_i^\lambda\|^2 \,,$$

where $\lambda$ is the selected smoothing parameter using cross validation and $\hat{x}_i^\lambda(t) = \sum_{r=1}^{4} \sum_{q=1}^{4} (G_4^\lambda)_{rq}^{-1} \langle \xi_q^\lambda, \tilde{x}_i \rangle \xi_r^\lambda(t)$ are the reconstructed functional data with the $4 \times 4$ matrix $G_4^\lambda$ that has $(r, q)$-th element $G_{4,rq}^\lambda = \langle \xi_r^\lambda, \xi_q^\lambda \rangle$.

**Step 6.** Repeat **Steps 1** to **5** for each trial. Then the average mean square error (AMSE)

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Table1: Simulation results for 2 mean functions.

$$\mu(t) = e^{-3t}\sin(3\pi t)$$

|  | $\sigma_\varepsilon = 0.05R_x$ | | $\sigma_\varepsilon = 0.1R_x$ | | $\sigma_\varepsilon = 0.2R_x$ | |
|---|---|---|---|---|---|---|
|  | Gaussian | $B$-splines | Gaussian | $B$-splines | Gaussian | $B$-splines |
| $n_i = 100$ |  |  |  |  |  |  |
| AMSE $\times 10^2$ | 7.792 | 7.792 | 7.962 | 7.957 | 7.972 | 7.960 |
| SD(MSE) $\times 10^3$ | 9.17 | 9.16 | 9.77 | 9.76 | 9.23 | 9.26 |
| $n_i$ : normal |  |  |  |  |  |  |
| AMSE $\times 10^2$ | 7.682 | 9.197 | 7.802 | 9.230 | 7.987 | 9.312 |
| SD(MSE) $\times 10^3$ | 8.43 | 10.04 | 9.54 | 12.15 | 9.59 | 12.62 |

$$\mu(t) = 1 - 48t + 218t^2 - 315t^3 + 145t^4$$

|  | $\sigma_\varepsilon = 0.05R_x$ | | $\sigma_\varepsilon = 0.1R_x$ | | $\sigma_\varepsilon = 0.2R_x$ | |
|---|---|---|---|---|---|---|
|  | Gaussian | $B$-splines | Gaussian | $B$-splines | Gaussian | $B$-splines |
| $n_i = 100$ |  |  |  |  |  |  |
| AMSE | 1.472 | 1.471 | 1.508 | 1.504 | 1.520 | 1.509 |
| SD(MSE) $\times 10$ | 1.72 | 1.72 | 1.92 | 1.92 | 1.81 | 1.82 |
| $n_i$ : normal |  |  |  |  |  |  |
| AMSE | 1.468 | 1.786 | 1.504 | 1.790 | 1.518 | 1.793 |
| SD(MSE) $\times 10$ | 1.86 | 2.03 | 1.67 | 1.81 | 1.85 | 2.35 |

is given by AMSE $= 100^{-1}\sum_{b=1}^{100} \text{MSE}_b$.

Table1 shows the simulation results with the AMSE and standard deviation (SD) of MSE for Gaussian basis functions and $B$-splines. From this table, if the numbers $n_i$ of observational points were generated from the normal distribution, all AMSE and SD(MSE) for Gaussian basis functions were smaller than the corresponding values for $B$-splines. Moreover, most of results for Gaussian basis functions to the unbalanced data ($n_i$:normal) are better than the that to the equispaced data ($n_i = 100$), while the results for $B$-splines were not. In consequence, regularized functional PCA via Gaussian basis functions performs well to unbalanced data in the sense of minimizing AMSE and SD(MSE) through these simulations.

# 5. Real data example

We apply the proposed regularized functional PCA to 3D protein structures such as that shown in Fig3. There have been many studies that have analyzed proteins using statistical methods (Wu, Hastie and Schmidler (1998), Ding and Dubchak (2001), Green
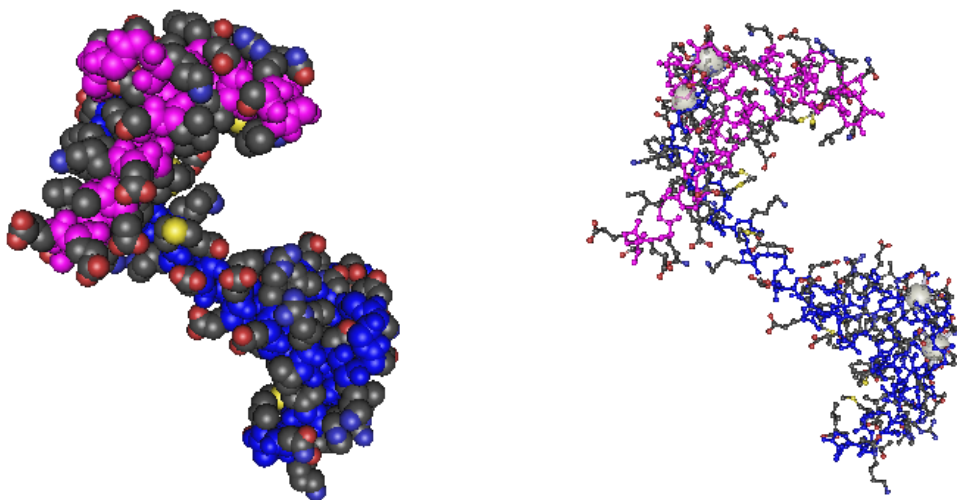
Fig. 3: Examples of 3D protein structures. The surface (left) and internal structures (right) of a protein.

Table 2: The 12 proteins from the 4 families.

| Family code | Family name | Protein code |
|---|---|---|
| adk | Nucleotide kinase | 1gky (186) 3adk (194) |
| aza | Azulin / plastocyanin | 1azu (125) 1plc (99) 7pcy (98) 1paz (120) 9pcy (92) |
| cbp | Calcium-binding protein (calmodulin-like) | 3cln (142) 4cln (148) 5cln (161) |
| dhfr | Dhydrofolate reductase | 3dfr (162) 8dfr (186) |

Each number in the parentheses shows the length of the amino-acid sequence.

and Mardia (2006), among others). Regularized functional PCA is applied here to 3-dimensional functional data sets representing 3D protein structures, in order to identify any features of the protein structures.

Proteins have been classified from a biological point of view, and a protein class is referred to as a family. A protein family is a group of evolutionarily related proteins. We treat 12 proteins from the 4 families given in Table 2. The 3D protein structural data set was obtained from the National Center of Biotechnology Information (NCBI, *http://www.ncbi.nlm.nih.gov/*). It should be noted that because the length of amino-acid sequence differs for each protein, the conventional multivariate analysis including PCA cannot be directly applied to this unbalanced data set. In what follows, it is assumed that we have the XYZ-coordinates values of all atoms for each protein in various coordinate systems.
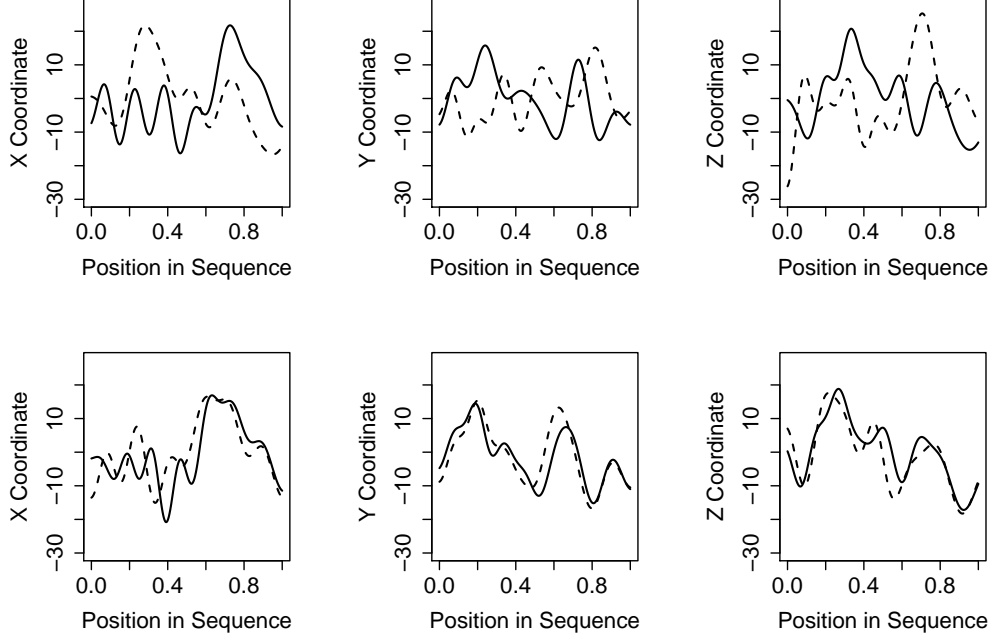
Fig. 4: An example of a rotation of proteins. The 3-dimensional functional data (upper) and rotated data (lower) of two proteins.

Firstly, the 3D protein structural data set was converted into discrete data sets using the XYZ-coordinates values of the $\alpha$-carbon atoms which were typical atoms of amino-acids. Each $\alpha$-carbon atom corresponds to an amino-acid. We then had a discrete data set for each coordinate, and the smoothing method using Gaussian basis functions was performed for each discrete data set. We considered values for $M$ of $3, 4, \cdots, 20$, values for $\nu$ of $1, 2, \cdots, 50$ and values for $\beta_{il}$ of $10^{-10}, 10^{-9}, \cdots, 10^{-1}$ and found optimal values of $M = 15$, $\nu = 11.6$ and $\beta_{il} = 10^{-8} \sim 10^{-5}$. The selected values of $M$ and $\nu$ were the mode and mean of that for all individuals and coordinates, respectively.

To unify the coordinates, we rotated the estimated functional data sets obtained by smoothing, since the coordinate systems differ for each protein. Optimization was performed in rotating each protein to an another base protein. A root mean square deviation (RMSD) for two functional data $\{x(t), y(t), z(t) \ ; \ t \in \mathcal{T}\}$ and $\{x'(t), y'(t), z'(t) \ ; \ t \in \mathcal{T}\}$ was utilized as a criterion for the optimization, and it was here defined by

$$\mathrm{RMSD}_F = \left\{ \frac{1}{|\mathcal{T}|} \left[ \ \int_{\mathcal{T}} \left\{ (x(t) - x'(t) \right\}^2 dt \right. \right.$$

$$\left. \left. + \int_{\mathcal{T}} \left\{ y(t) - y'(t) \right\}^2 dt + \int_{\mathcal{T}} \left\{ z(t) - z'(t) \right\}^2 dt \ \right] \right\}^{1/2} .$$

We employed Euler's angle $\theta_1, \theta_2, \theta_3$ as a rotation method with step size 10 degree, and the

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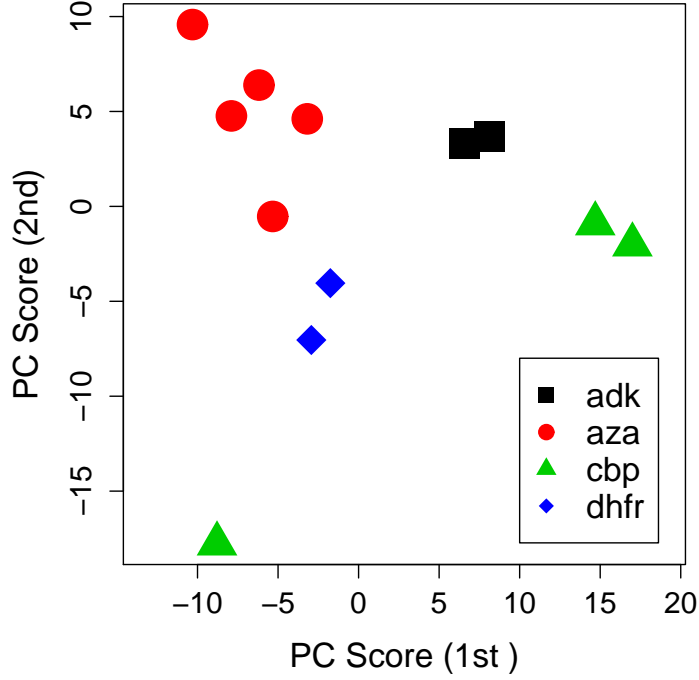
Fig. 5: The principal component (PC) scores for each family. The proteins in the adk, aza and dhfr families are clustered in their respective groups, while the cbp family has an un-clustered protein.

selected angles $\theta_1^*, \theta_2^*, \theta_3^*$ were then varied with step size 1 degree. Fig4 shows an example of the 3-dimensional functional data sets (upper) and the rotated ones (lower). In this figure, we show a rotation of two proteins. The regularized functional PCA was applied to the rotated 3-dimensional functional data sets.

Using cross validation resulted in $\lambda_1 = 6.31 \times 10^{-6}$, $\lambda_2 = 2.51 \times 10^{-6}$ and $\lambda_3 = 3.98 \times 10^{-6}$ as optimal smoothing parameters, where we set the candidate values of $\lambda_l (l = 1, 2, 3)$ to $\lambda_{li} = 10^{11-i}$ $(i = 1, \cdots, 10)$ and $\lambda_{li} = 10^{(i-71)/10}$ $(i = 1, \cdots, 21)$. With the selected smoothing parameters, we estimated PC curves and PC scores and plotted the PC scores for each family (Fig5). The proteins belonging to the adk, aza and dhfr families were clustered in respective family groups; however, the cbp family contained an unclustered protein. This problem may be caused by the "slim" structure of proteins in the cbp family, while we successfully captured the "ball" structure characteristic of proteins in the adk, aza and dhfr families. Thus, using our functionalization method, 3D protein structures can be captured without relying on their sequence information, physicochemical properties and a visual census of an enormous number of proteins. However, we may have to use a robust representation of a 3D protein structure for rotation.

# 6. Concluding remarks

We introduced regularized functional PCA for multidimensional functional data sets, using Gaussian basis functions. The results of the Monte Carlo experiments showed that our regularized functional PCA based on Gaussian basis functions performed well, and was superior to that based on cubic $B$-splines in the sense of minimizing the mean square error and its standard deviation for unbalanced data. The proposed procedure extracted useful information from unbalanced data like the protein structural data. The analysis of the real data set showed that the 3D protein structures could be characterized by our method without relying on their sequence information and physicochemical properties. Future works that remains to be done include derivation of model selection criteria from an information-theoretic perspective and also the application of Bayesian approaches instead of cross validation.

# Acknowledgements

# Appendix. Evaluation of the cross product matrix for cubic $B$-splines

This section shows an outline of the evaluation for the cross product matrix $W^* = \{W_{mn}^* = \int_{\mathcal{T}} \phi_m(t)\phi_n(t)\,dt\}_{m,n=1}^M$ via cubic $B$-splines $\{\phi_m(t)\}$ with the equispaced knots $k_1 < k_2 < \cdots < k_{M+4}$, where $\mathcal{T} = [k_4, k_{M+1}]$. We refer to De Boor (2001) and Imoto and Konishi (2003) for $B$-splines.

It is known that $B$-splines $\phi_1(t;r), \cdots, \phi_M(t;r)$ with degree $r \in \{1, 2, \cdots\}$ and knots $k_1 < k_2 < \cdots < k_{M+r+1}$ are given by the sequential equation (de Boor 2001);

$$\phi_m(t;r) = \frac{t - k_m}{k_{m+r} - k_m}\phi_m(t;r-1) - \frac{t - k_{m+r+1}}{k_{m+r+1} - k_{m+1}}\phi_{m+1}(t;r-1),$$

where $\phi_m(t;0) = 1$ ($k_m \le t < k_{m+1}$), $= 0$ (otherwise). The cubic $B$-splines $\{\phi_m(t;3)\}$ are here denoted by $\{\phi_m(t)\}$. Fig6 shows an example of the cubic $B$-splines with $\mathcal{T} = [0, 1]$ and $M = 9$.

The diagonal components $W_{mm}^*$ of $W^*$ can be evaluated through the integrations $I_1^d = \int_{k_1}^{k_2} \phi_1(t)^2 dt = h/252$ and $I_2^d = \int_{k_2}^{k_3} \phi_1(t)^2 dt = 33h/140$ with the width $h$ of the

15
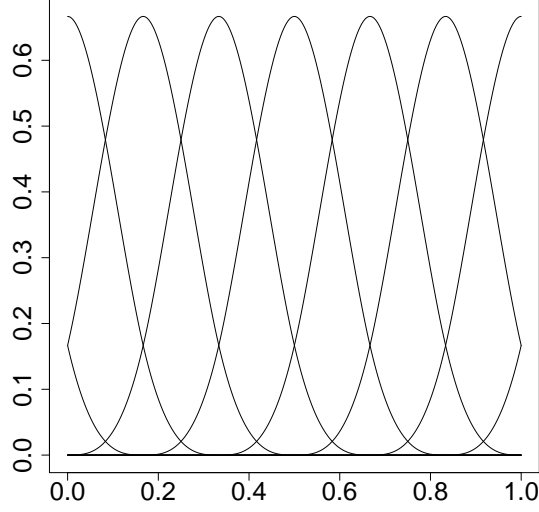
Fig.6: Cubic $B$-splines ($\mathcal{T} = [0,1]$, $M = 9$).

equidistant knots sequence;

$$W_{11}^* = I_1^d \ (= W_{MM}^*) \,, \qquad\qquad W_{22}^* = I_1^d + I_2^d \ (= W_{M-1,M-1}^*) \,,$$
$$W_{33}^* = I_1^d + 2I_2^d \ (= W_{M-2,M-2}^*) \,, \quad W_{mm}^* = 2I_1^d + 2I_2^d \quad (m = 4, 5, \cdots, M-3) \,.$$

It may be noted that the $B$-splines are symmetric and $\phi_m(t) = 0$ ($t < k_m$, $k_{m+4} \le t$). Furthermore, each $B$-spline function $\phi_m(t)$ is given by the parallel translation of the other $B$-splines $\phi_n(t)$ ($n \ne m$).

The calculation of the non-diagonal components $W_{mn}^*$ ($m < n$) requires the 4 integrations $I_1^{nd} = \int_{k_4}^{k_5} \phi_1(t)\phi_2(t) \ dt = h/210$, $I_2^{nd} = \int_{k_4}^{k_5} \phi_1(t)\phi_3(t) \ dt = h/84$, $I_3^{nd} = \int_{k_4}^{k_5} \phi_1(t)\phi_4(t) \ dt = h/5040$ and $I_4^{nd} = \int_{k_3}^{k_4} \phi_1(t)\phi_2(t) \ dt = 311h/1680$. We then have the components in the 1st to 3rd rows;

$$W_{12}^* = \qquad\qquad I_1^{nd} \,, \quad W_{13}^* = \ I_2^{nd} \,, \quad W_{14}^* = I_3^{nd} \,, \quad W_{15}^* = \cdots = W_{1M}^* = 0 \,,$$
$$W_{23}^* = \qquad I_1^{nd} + I_4^{nd} \,, \quad W_{24}^* = 2I_2^{nd} \,, \quad W_{25}^* = I_3^{nd} \,, \quad W_{26}^* = \cdots = W_{2M}^* = 0 \,,$$
$$W_{34}^* = \qquad 2I_1^{nd} + I_4^{nd} \,, \quad W_{35}^* = 2I_2^{nd} \,, \quad W_{36}^* = I_3^{nd} \,, \quad W_{37}^* = \cdots = W_{3M}^* = 0 \,.$$

In a similar way, the components in the 4th,5th,$\cdots$ rows can be obtained. Especially, the components in the $(M-2)$-th and $(M-1)$-th rows are given by $W_{M-2,M-1}^* = I_1^{nd} + I_4^{nd} (= W_{23}^*)$, $W_{M-2,M}^* = I_2^{nd} (= W_{13})$ and $W_{M-1,M}^* = I_1^{nd} (= W_{12})$.

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