

The `bbefkr` Package

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Abstract

Recent advances in computer recording and storing technology have markedly increased the presence of functional data, whose graphical representation can be infinite-dimensional curve, image or shape. When a function-valued predictor and a scalar-valued response is observed, the functional kernel regression provides a flexible way to estimate its possible non-linear relationship. However, as with any type of kernel regression, it requires an optimal selection of smoothing parameter, called bandwidth and an optimal selection of semi-metric. In the literature of nonparametric functional regression, bandwidth parameter is often selected by a functional cross validation. In this article, we present a Bayesian bandwidth estimation method that uses the information about error density to help with the optimal selections of bandwidth and semi-metric in the regression function. We first describe the proposed Bayesian method in a functional nonparametric regression and a semi-functional partial linear regression. Illustrated by two simulation studies and a real data set, the Bayesian method is then implemented using a readily-available R add-on package.

Keywords: bandwidth selection, Bayesian model selection, functional Nadaraya-Watson estimator, kernel error density, marginal likelihood, random-walk Metropolis, simulation inefficiency factor.

1. Introduction

The aim of this article is to describe the R functions that are readily-available in the `bbefkr` package (Shang 2014c), for estimating bandwidth parameters in a functional nonparametric regression and a semi-functional partial linear regression. This article was motivated by the recent developments in nonparametric functional regression estimators for analysing the relationship between a function-valued predictor and a real-valued scalar response. Some commonly used nonparametric functional estimators include: functional Nadayara-Watson (NW) estimator (Ferraty and Vieu 2006), functional local linear estimator (Barrientos-Marin, Ferraty, and Vieu 2010), functional k -nearest neighbour estimator (Burba, Ferraty, and Vieu 2009) and distance-based local linear estimator (Boj, Delicado, and Fortiana 2010). Because of simplicity and mathematical elegance, we consider the functional NW estimator in this paper.

In all of the aforementioned functional estimators, the estimation accuracy of the conditional mean crucially depends on the optimal selections of the bandwidth parameter and semi-metric. Commonly, the optimal bandwidth is selected by the functional cross validation (CV), which is designed to assess the predictive performance of a model by an average of certain measures for the ability of predicting a subset of functions by a model fit, after deleting these functions from the data set only (Rachdi and Vieu 2007). Functional CV aims to minimise L_2 loss function and has the appealing feature that no

estimation of the error variance is required. However, since residuals affect the estimation accuracy of regression function, functional CV may select a sub-optimal bandwidth. This in turn leads to inferior estimation accuracy of regression functions (see for example, [Shang 2013, 2014b](#)). As an alternative, we present a Bayesian bandwidth estimation method that simultaneously estimates the optimal bandwidths in the regression function and kernel-form error density by minimising the generalised loss function (see [Shang 2013](#), for the importance of error density estimation). As a by-product of the Bayesian method, we can also select the optimal semi-metric based on the notion of marginal likelihood.

Before introducing the bandwidth estimation method, we first define the problem more precisely. Let $\mathbf{y} = (y_1, y_2, \dots, y_n)^\top$ be a vector of scalar responses, $\mathbf{T} = (T_1, T_2, \dots, T_n)^\top$ be realisations of a functional predictor and $\mathbf{X} = (X_{i1}, \dots, X_{ip})_{i=1, \dots, n}$ be p -dimensional real-valued predictors, where $^\top$ represents matrix transpose. We consider two regression models, namely a functional nonparametric regression and a semi-functional partial linear regression. The latter is a generalisation of the former, in which the real-valued predictors are also incorporated into the regression function. The semi-functional partial linear regression can be defined as

$$y_i = \mathbf{X}_i \boldsymbol{\beta} + m(T_i) + \varepsilon_i, \quad i = 1, 2, \dots, n, \quad (1)$$

where $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^\top$ is a vector of unknown real-valued regression coefficients in the parametric counterpart, m is an unknown smooth function that performs the mapping from function space to real space and $(\varepsilon_1, \dots, \varepsilon_n)$ are independent and identically distributed (iid) random errors with an unknown error density, denoted as $f(\varepsilon)$. We assume that there is no correlation between the covariates in the regression function and errors, that is

$$\mathbb{E}(\varepsilon_i | \mathbf{X}_i, T_i) = 0.$$

The functional nonparametric regression model has the only nonparametric part of the equation (1). In both regression models, we are interested in accurately estimating the regression function m and $f(\varepsilon)$, which are mainly determined by the optimal selections of bandwidth and semi-metric.

This article proceeds as follows. The Bayesian bandwidth estimation method is first described and its estimation accuracy is then compared based on the idea of marginal likelihood or Bayes factor. Through a series of simulation studies, the sampling algorithm is demonstrated using the R functions in the **bbefkr** package. Conclusions will then be presented.

2. Bayesian bandwidth estimation

The proposed bandwidth estimation methods aims to accurately estimate the regression function approximated by the functional NW estimator of conditional mean and unknown error density approximated by a kernel density of residuals.

2.1. Estimation of error density

The unknown error density $f(\varepsilon)$ can be approximated by a location-mixture of Gaussian densities (see also [Roeder and Wasserman 1997](#)), given by

$$f(\varepsilon; b) = \frac{1}{n} \sum_{j=1}^n \frac{1}{b} \phi\left(\frac{\varepsilon - \varepsilon_j}{b}\right),$$

where $\phi(\cdot)$ is the probability density function of the standard Gaussian distribution and the component Gaussian densities have means at ε_j , for $j = 1, 2, \dots, n$ and a common standard deviation b . Although error ε_j is unknown, it can be estimated by the functional NW estimator. Thus, the density of y_i is approximated by the estimated error density $\hat{f}(\varepsilon; b)$, expressed as

$$\hat{f}(\varepsilon; b) = \frac{1}{n} \sum_{j=1}^n \frac{1}{b} \phi\left(\frac{\varepsilon - \hat{\varepsilon}_j}{b}\right),$$

where b represents residual bandwidth. In order to avoid the possible selection of $b = 0$, a leave-one-out version of the kernel likelihood is often used, given by

$$\hat{f}(\hat{\varepsilon}_i; b) = \frac{1}{n-1} \sum_{\substack{j=1 \\ j \neq i}}^n \frac{1}{b} \phi\left(\frac{\hat{\varepsilon}_i - \hat{\varepsilon}_j}{b}\right),$$

where $\hat{\varepsilon}_i = y_i - \hat{m}(T_i; h)$ is the i th residual for $i = 1, 2, \dots, n$, in the functional nonparametric regression. In the semi-functional partial linear regression, $\hat{\varepsilon}_i = y_i - \mathbf{X}_i \hat{\boldsymbol{\beta}} - \hat{m}(T_i; h)$, where $\hat{\boldsymbol{\beta}}$ can be obtained by the ordinary least squares (Shang 2014b, Section 2). Given (h, b) and iid assumption of the errors, the leave-one-out version of the kernel likelihood of $\mathbf{y} = (y_1, y_2, \dots, y_n)^\top$ can be approximated by

$$\hat{L}(\mathbf{y}|h, b) = \prod_{i=1}^n \left[\frac{1}{n-1} \sum_{\substack{j=1 \\ j \neq i}}^n \frac{1}{b} \phi\left(\frac{\hat{\varepsilon}_i - \hat{\varepsilon}_j}{b}\right) \right].$$

2.2. Prior density

We now discuss the issue of prior density for the bandwidths. Let $\pi(h^2)$ and $\pi(b^2)$ be the independent prior of squared bandwidths h and b . Since h^2 and b^2 play the role of variance parameters in the Gaussian densities, we assume that the priors of h^2 and b^2 are inverse Gamma density, denoted by $\text{IG}(\alpha_h, \beta_h)$ and $\text{IG}(\alpha_b, \beta_b)$, respectively. Thus, the prior densities of h^2 and b^2 are given by

$$\begin{aligned} \pi(h^2) &= \frac{(\beta_h)^{\alpha_h}}{\Gamma(\alpha_h)} \left(\frac{1}{h^2}\right)^{\alpha_h+1} \exp\left(-\frac{\beta_h}{h^2}\right), \\ \pi(b^2) &= \frac{(\beta_b)^{\alpha_b}}{\Gamma(\alpha_b)} \left(\frac{1}{b^2}\right)^{\alpha_b+1} \exp\left(-\frac{\beta_b}{b^2}\right), \end{aligned}$$

where $\alpha_h = \alpha_b = 1.0$ and $\beta_h = \beta_b = 0.05$ as hyper-parameters. Sensitivity results studied in Shang (2013, 2014b) show that the choices of hyper-parameters and inverse Gamma densities do not influence the estimation of posterior density.

2.3. Posterior density

Let $\boldsymbol{\theta} = (h^2, b^2)$ be the parameter vector and $\mathbf{y} = (y_1, \dots, y_n)^\top$ be the data. According to the Bayes theorem, the posterior of $\boldsymbol{\theta}$ is written by

$$\pi(\boldsymbol{\theta}|\mathbf{y}) = \frac{\hat{L}(\mathbf{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})}{L(\mathbf{y})}, \quad (2)$$

where $\widehat{L}(\mathbf{y}|\boldsymbol{\theta})$ is the approximated likelihood function with squared bandwidths and $L(\mathbf{y})$ is the marginal likelihood, which can be expressed as

$$\int \widehat{L}(\mathbf{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta}.$$

In practice, the posterior in (2) can be approximated by (up to a normalising constant):

$$\pi(\boldsymbol{\theta}|\mathbf{y}) \propto \widehat{L}(\mathbf{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta}).$$

We use the adaptive random-walk Metropolis algorithm to sample $\boldsymbol{\theta}$ (see [Shang 2013, 2014b](#), for details). In order to assess the convergence of the Markov chain Monte Carlo (MCMC) algorithm, we use the notion of simulation inefficiency factor ([Meyer and Yu 2000](#)). This is a measure of autocorrelation among iterations and provides an indication of how many iterations are required to have the iid draws from the posterior distributions. It is noteworthy that a full range of diagnostic tools in the `cod` package ([Plummer, Best, Cowles, and Vines 2006](#)) can also be applied to check the convergence of MCMC.

2.4. Adaptive estimation of error density

In kernel density estimation, it has been noted that the leave-one-out estimator may be heavily affected by extreme observations in the data sample (see for example, [Bowman 1984](#)). Because of the use of a global bandwidth, the leave-one-out kernel error density estimator is likely to overestimate the tails of the density. To overcome this deficiency, it is possible to use localised bandwidths by assigning small bandwidths to the residuals in the high density region and large bandwidths to the residuals in the low density region. The localised error density estimator can be given by

$$\widehat{f}(\widehat{\varepsilon}_i; b, \tau_\varepsilon) = \frac{1}{n-1} \sum_{\substack{j=1 \\ j \neq i}}^n \frac{1}{b(1+\tau_\varepsilon|\widehat{\varepsilon}_j|)} \phi\left(\frac{\widehat{\varepsilon}_i - \widehat{\varepsilon}_j}{b(1+\tau_\varepsilon|\widehat{\varepsilon}_j|)}\right), \quad (3)$$

where $b(1+\tau_\varepsilon|\widehat{\varepsilon}_j|)$ is the bandwidth assigned to residual $\widehat{\varepsilon}_j$ and the vector of parameters is now (h, b, τ_ε) . Again, the random-walk Metropolis algorithm can be used to sample these parameters, where the prior density of $\tau_\varepsilon \sim U(0, 1)$.

3. Bayesian model selection

How could the Bayesian model selection be useful in functional kernel regression? The answer lies in the choice of semi-metric, which is important to obtain good statistical properties of the nonparametric method in the function space. As pointed out by [Ferraty and Vieu \(2009\)](#), the choice of semi-metric has effects on the size and the form of neighborhoods and can thus control the concentration properties of functional data. From a practical viewpoint, a semi-metric based on derivative should be used for a set of smooth functional data; a semi-metric based on dimension reduction technique, such as functional principal component analysis, should be used for a set of rough functional data ([Ferraty and Vieu 2006](#), Chapters 3 and 13). Although [Ferraty and Vieu \(2006, p.193\)](#) remarked that the optimal selection of semi-metric remains an open question, there is

no method to quantify which semi-metric is more adequate, or how to select the optimal one. Here, we propose to use the marginal likelihood to select the optimal semi-metric.

In Bayesian inference, model selection or averaging is often conducted through the Bayes factor of the model of interest against a competing model. The Bayes factor reflects a summary of evidence provided by the data supporting the model as opposed to its competing model. The Bayes factor can be defined as the ratio of the marginal likelihoods under different models. The marginal likelihood is defined as the expectation of likelihood with respect to the prior of parameters. It is seldom computed as the integral of the product of the likelihood and prior of parameters, but instead, is often computed numerically (Gelfand and Dey 1994; Newton and Raftery 1994; Chib 1995; Kass and Raftery 1995; Geweke 1999, among others). We utilised the method proposed by Chib (1995) to compute the marginal likelihood.

Chib (1995) showed that the marginal likelihood under semi-metric A is expressed as

$$L_A(\mathbf{y}) = \frac{\widehat{L}_A(\mathbf{y}|\boldsymbol{\theta})\pi_A(\boldsymbol{\theta})}{\pi_A(\boldsymbol{\theta}|\mathbf{y})},$$

where $\widehat{L}_A(\mathbf{y}|\boldsymbol{\theta})$, $\pi_A(\boldsymbol{\theta})$ and $\pi_A(\boldsymbol{\theta}|\mathbf{y})$ denote the kernel likelihood, prior and posterior under semi-metric A, respectively. $L_A(\mathbf{Y})$ is often computed at the posterior estimate of $\boldsymbol{\theta}$. The numerator has a closed form and can be computed analytically, but the denominator can be approximated by the MCMC posterior draws. However, for relatively small number of parameters, the denominator can be estimated by its kernel density estimator based on the simulated chain of $\boldsymbol{\theta}$ through a posterior sampler.

The Bayes factor of semi-metric A against semi-metric B is defined as

$$\frac{L_A(\mathbf{y})}{L_B(\mathbf{y})}.$$

Based on the Bayes factor, we can determine which model is more superior than a competing model with different levels of evidence (see Kass and Raftery 1995, for more details); it is also possible to combine different semi-metrics using the idea of Bayesian model averaging.

4. Simulation studies

We describe the construction of the simulated data. First of all, a set of discretised data points of a functional curve is simulated:

$$T_i(t_j) = a_i \cos(2t_j) + b_i \sin(4t_j) + c_i(t_j^2 - \pi t_j + \frac{2}{9}\pi^2), \quad i = 1, 2, \dots, n, \quad (4)$$

where $0 \leq t_1 \leq t_2 \leq \dots \leq t_{100} \leq \pi$ are equispaced points, a_i, b_i and c_i are independently drawn from a uniform distribution on $[0, 1]$ and n represents the sample size. The functional form in (4) was taken from Ferraty, Van Keilegom, and Vieu (2010) and has also been studied by Shang (2013, 2014b). Figure 1 presents 20 simulated smooth curves as an example.

Once the curves are defined, one simulates a functional regression model to compute the scalar responses, given below:

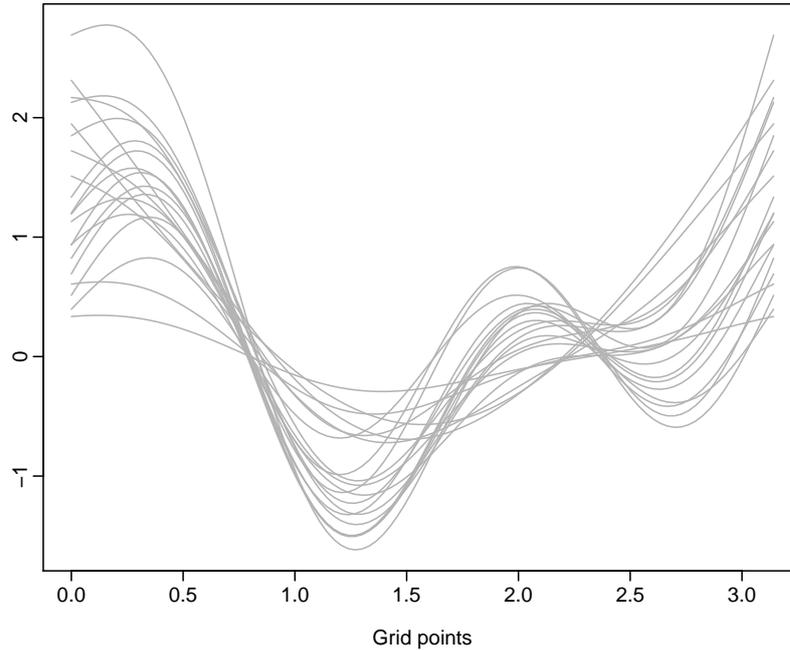


Figure 1: 20 simulated smooth curves.

- 1) construct a nonparametric component $m(T_i) = 10 \times (a_i^2 - b_i^2)$, which performs the mapping from function-valued space to real-valued space.
- 2) in the functional nonparametric regression, the regression function consists of only a nonparametric component. Thus, we have $\tau_i = m(T_i)$. In the semi-functional partial linear regression, we also have a parametric component. In this case, let X_{i1} and X_{i2} be independently drawn from a uniform distribution $U(0, 1)$ for $i = 1, 2, \dots, n$. The true values of regression coefficients are set to be $\beta = (-1, 2)$. The regression function is constructed as

$$\tau_i = m(T_i) + \mathbf{X}_i\beta, \quad \text{for } i = 1, 2, \dots, n.$$

- 3) generate $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$ from a standard normal distribution.
- 4) compute the corresponding response:

$$y_i = \tau_i + \varepsilon_i.$$

4.1. Smooth curves

First, we consider a set of smoothed curves as realisations of a functional predictor and choose a semi-metric based on the second derivative to measure the distances among curves. The relationship between a functional predictor and a scalar response can be modelled by either a functional nonparametric regression or a semi-functional partial linear regression. In the case of a functional nonparametric regression, the optimal selection of semi-metric and the estimated bandwidths, regression function and error density can be obtained as follows:

```

R> ## install and load the R package
R> install.packages("bbefkr")
R> require(bbefkr)
R> ## set random seed
R> set.seed(123456)
R> ## error density is approximated by a kernel density of residuals with a global
R> ## bandwidth, q=2 represents the semi-metric based on the second derivative,
R> ## since functions can be estimated by a basis representation, a B-spline
R> ## basis representation is used with 20 knots
R> np_global <- bayMCMC_np_global(data_x=simcurve_smooth_normerr,
+   data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr,
+   warm=1000, M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## estimated bandwidth parameters (h,b)
R> np_global$xpfinalres
R> ## estimated values for the regression function
R> np_global$mhat
R> ## simulation inefficiency factor to evaluate the convergence of MCMC
R> ## it measures how many iterations are required to have the iid draws
R> ## from the posterior
R> np_global$sif_value
R> ## log marginal likelihood computed by Chib (1995)'s method
R> np_global$mlikeres
R> ## acceptance rates of the random-walk Metropolis sampling algorithm with target of
R> ## 0.44 for the bandwidths in the regression function and kernel-form error density
R> c(np_global$acceptnwMCMC, np_global$accepterroMCMC)
R> ## estimated error density (probability density function)
R> np_global$fore.den.mkr
R> ## estimated error density (cumulative probability density function)
R> np_global$fore.cdf.mkr

```

By using localised bandwidths, the estimation of error density can generally be more accurate than a global bandwidth because residuals with large magnitude are assigned relatively large bandwidths, while residuals with small magnitude are assigned relatively small bandwidths. An example is provided below:

```

R> ## error density is approximated by a kernel density of residuals with localised
R> ## bandwidths
R> np_local <- bayMCMC_np_local(data_x=simcurve_smooth_normerr,
+   data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr, warm=1000,
+   M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## estimated bandwidth parameters (h, b, badj)
R> np_local$xpfinalres
R> ## estimated values for the regression function
R> np_local$mhat
R> ## simulation inefficiency factor to evaluate the convergence of MCMC

```

```
R> np_local$sif_value
R> ## log marginal likelihood computed by Chib (1995)'s method
R> np_local$mlikeres
R> ## acceptance rates of the random-walk Metropolis algorithm for the bandwidths
R> c(np_local$acceptnwMCMC, np_local$accepterroMCMC, np_local$acceptepsilonMCMC)
R> ## estimated error density (probability density function)
R> np_local$fore.den.mkr
R> ## estimated error density (cumulative probability density function)
R> np_local$fore.cdf.mkr
```

Based on the log marginal likelihood (LML), the kernel-form error density with localised bandwidths is preferred to a global bandwidth. The Bayes factor can be derived from the difference in LML:

$$\exp(\text{LML}_G - \text{LML}_L),$$

where G and L represent the kernel density estimators of error density, with a global bandwidth or localised bandwidths as described in (3).

In a semi-functional partial linear regression, the algorithm is similar to a functional nonparametric regression. Thus, we only highlight the additional output produced, such as the estimation of regression coefficients in the parametric part of the regression function. This is described as follows:

```
R> ## error density is approximated by a kernel density of residuals with a global
R> ## bandwidth, Xvar is a n by 2 matrix, where each column variable is simulated
R> ## from U(0,1)
R> semi_global <- bayMCMC_semi_global(data_x=simcurve_smooth_normerr,
+ data_y=simresp_semi_normerr, data_xnew=simcurve_smooth_normerr,
+ Xvar=Xvar, warm=1000, M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## estimated regression coefficients
R> semi_global$betahat
R> ## log marginal likelihood computed by Chib (1995)'s method
R> semi_global$mlikeres
R> ## error density is approximated by a kernel density of residuals with localised
R> ## bandwidths
R> semi_local <- bayMCMC_semi_local(data_x=simcurve_smooth_normerr,
+ data_y=simresp_semi_normerr, data_xnew=simcurve_smooth_normerr,
+ Xvar=Xvar, warm=1000, M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## estimated regression coefficients
R> semi_local$betahat
R> ## log marginal likelihood computed by Chib (1995)'s method
R> semi_local$mlikeres
```

Rough curves

We also consider a set of rough curves as realisations of a functional predictor. The same functional form is given in (4), but one extra variable $d_j \stackrel{\text{iid}}{\sim} U(-0.1, 0.1)$ is included. Figure 2 presents 20 simulated rough curves as an example.

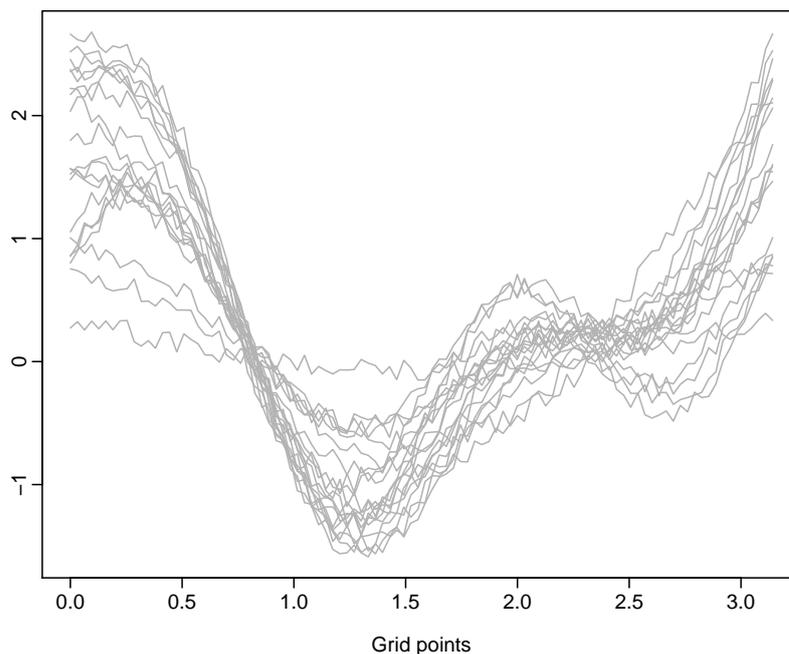


Figure 2: 20 simulated rough curves.

For modelling a set of rough curves, the semi-metric based on functional principal components should be used (Ferraty and Vieu 2006). From one to five functional principal components, Shang (2014b) found that retaining three functional principal components produces the smallest estimation error in this data set and should be sufficient to explain main mode of variation. Therefore, we compare the LMLs between the semi-metric based on the second derivative and the semi-metric based on three retained functional principal components. This can be implemented as follows:

```
R> ## error density is approximated by a kernel density of residuals with a global
R> ## bandwidth using the semi-metric based on the second derivative
R> rough_np_global_deriv <- bayMCMC_np_global(data_x=simcurve_rough_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_rough_normerr, warm=1000,
+ M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## a global bandwidth using the semi-metric based on three retained
R> ## principal components
R> rough_np_global_pca <- bayMCMC_np_global(data_x=simcurve_rough_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_rough_normerr, warm=1000,
+ M=1000, semimetric="pca", q=3)
R> ## comparing two semi-metrics based on their log marginal likelihoods
R> c(rough_np_global_deriv$mlikeres, rough_np_global_pca$mlikeres)
```

Similar findings also held for the functional nonparametric regression model with localised bandwidths. These can be implemented as follows:

```

R> ## error density is approximated by a kernel density of residuals with
R> ## localised bandwidths using the semi-metric based on the second derivative
R> rough_np_local_deriv <- bayMCMC_np_local(data_x=simcurve_rough_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_rough_normerr, warm=1000, M=1000,
+ range.grid=c(0,pi), q=2, nknot=20)
R> ## localised bandwidths using the semi-metric based on three retained
R> ## principal components
R> rough_np_local_pca <- bayMCMC_np_local(data_x=simcurve_rough_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_rough_normerr, warm=1000,
+ M=1000, semimetric="pca", q=3)
R> ## comparing two semi-metrics based on their log marginal likelihoods
R> c(rough_np_local_deriv$mlikeres, rough_np_local_pca$mlikeres)

```

Thus, for a set of rough curves, the semi-metric based on functional principal components is more suitable than the semi-metric based on the second derivative. However, for a set of smooth curves, it is advantageous to use the semi-metric based on the second derivative, as shown below:

```

R> ## error density is approximated by a kernel density of residuals with a global
R> ## bandwidth using the semi-metric based on the second derivative
R> smooth_np_global_deriv <- bayMCMC_np_global(data_x=simcurve_smooth_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr, warm=1000,
+ M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## a global bandwidth using the semi-metric based on functional
R> ## principal components
R> smooth_np_global_pca <- bayMCMC_np_global(data_x=simcurve_smooth_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr, warm=1000,
+ M=1000, semimetric="pca", q=3)
R> ## comparing two semi-metrics based on their log marginal likelihoods
R> c(smooth_np_global_deriv$mlikeres, smooth_np_global_pca$mlikeres)
R> ## localised bandwidths using the semi-metric based on the second derivative
R> smooth_np_local_deriv <- bayMCMC_np_local(data_x=simcurve_smooth_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr, warm=1000,
+ M=1000, range.grid=c(0,pi), q=2, nknot=20)
R> ## localised bandwidths using the semi-metric based on functional
R> ## principal components
R> smooth_np_local_pca <- bayMCMC_np_local(data_x=simcurve_smooth_normerr,
+ data_y=simresp_np_normerr, data_xnew=simcurve_smooth_normerr, warm=1000,
+ M=1000, semimetric="pca", q=3)
R> ## comparing two semi-metrics based on their log marginal likelihoods
R> c(smooth_np_local_deriv$mlikeres, smooth_np_local_pca$mlikeres)

```

Among a set of possible semi-metrics, the computation of marginal likelihood allows us to determine the optimal semi-metric and possibly combine different semi-metrics. The latter one remains an open question.

5. Spectroscopy application

Let us consider a food quality control application, where the focus is on the prediction of the fat content of meat products based on near-infrared absorbance spectroscopy. This data set was first studied by Borggaard and Thodberg (1992) and has since been studied by Ferraty and Vieu (2006), Aneiros-Pérez and Vieu (2006), Shang (2013, 2014b,a), Goldsmith and Scheipl (2014), among many others. The data set was obtained from <http://lib.stat.cmu.edu/datasets/tecator>. Each food sample contains finely chopped pure meat with different percentages of the fat, protein and moisture contents. For each unit i (among 215 pieces of finely chopped meat), we observe one spectrometric curve, denoted by T_i , which corresponds to the absorbance measured at a grid of 100 wavelengths, from 852nm to 1050nm in the step of 2nm. Given a new spectrometric curve T_{new} , we aim to predict its corresponding fat content. As pointed out by Ferraty and Vieu (2006), the motivation is that obtaining a spectrometric curve is less time and cost consuming than the analytic chemistry needed for determining the fat content. A graphical display of spectrometric curves is shown in Figure 3.

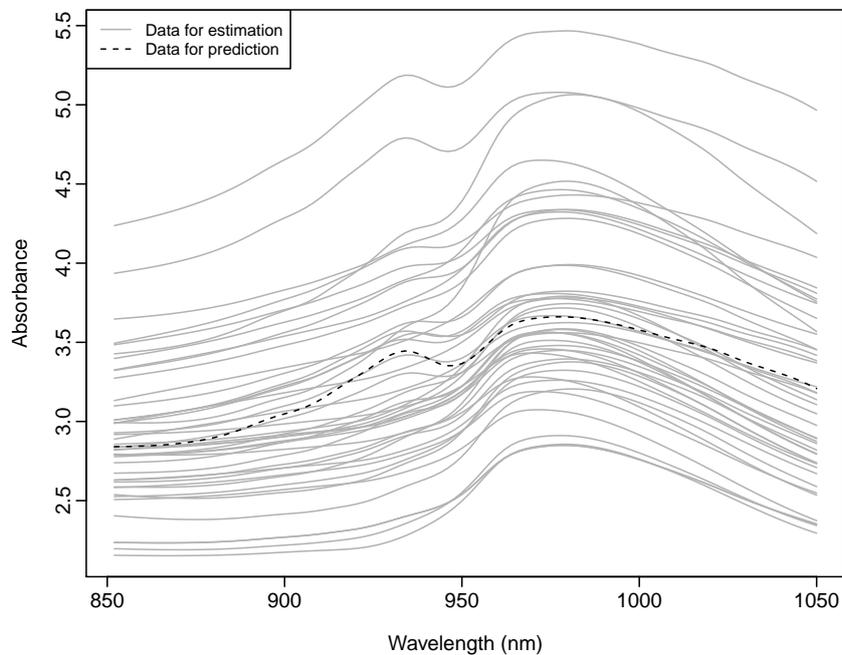


Figure 3: The first 45 spectrometric curves. Among these curves, the first 44 curves are used for the estimation of bandwidths, while the 45th curve is used for the prediction of fat content.

To predict the fat content, we consider a functional nonparametric regression and a semi-functional partial linear regression. As shown in Shang (2014b), the semi-functional partial linear regression gives more accurate forecasts than the functional nonparametric regression, since it uses additional information about protein and moisture contents. The point and interval forecasts can be obtained as follows:

```
R> ## We use the first 44 pairs of data to estimate the relationship. Based on a
R> ## new curve, we can then predict its response using a functional
```

```

R> ## nonparametric regression
R> fat_np_global <- bayMCMC_np_global(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], range.grid=c(0,pi), q=2, nknot=20)
R> ## Point forecast
R> fat_np_global$pointforecast
R> ## 95% prediction interval
R> fat_np_global$PI
R> ## Using a functional nonparametric regression with localised bandwidths
R> fat_np_local <- bayMCMC_np_local(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], range.grid=c(0,pi), q=2, nknot=20)
R> ## Point forecast
R> fat_np_local$pointforecast
R> ## 95% prediction interval
R> fat_np_local$PI
R> ## Using a semi-functional partial linear regression with a global bandwidth
R> fat_semi_global <- bayMCMC_semi_global(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], Xvar = cbind(protein[1:44], moisture[1:44]),
+   Xvarpred = matrix(c(protein[45], moisture[45]), nrow=1),
+   range.grid=c(0,pi), q=2, nknot=20)
R> ## Point forecast
R> fat_semi_global$pointforecast
R> ## 95% prediction interval
R> fat_semi_global$PI
R> ## Using a semi-functional partial linear regression with localised bandwidths
R> fat_semi_local <- bayMCMC_semi_local(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], Xvar = cbind(protein[1:44], moisture[1:44]),
+   Xvarpred = matrix(c(protein[45], moisture[45]), nrow=1),
+   range.grid=c(0,pi), q=2, nknot=20)
R> ## Point forecast
R> fat_semi_local$pointforecast
R> ## 95% prediction interval
R> fat_semi_local$PI

```

Among the semi-metrics based on first derivative, second derivative, functional principal component analysis with three retained principal components, we found that the semi-metric based on the second derivative has the largest marginal likelihood and smallest prediction error in this example. As a demonstration with a global bandwidth in the functional nonparametric regression, the LMLs of the three semi-metrics are computed as follows:

```

R> fat_np_global_d1 <- bayMCMC_np_global(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], range.grid=c(0,pi), q=1, nknot=20)
R> fat_np_global_d2 <- bayMCMC_np_global(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], range.grid=c(0,pi), q=2, nknot=20)
R> fat_np_global_pca <- bayMCMC_np_global(data_x = specurves[1:44,], data_y = fat[1:44],
+   data_xnew = specurves[45,], semimetric="pca", q=3)
R> c(fat_np_global_d1$mlikeres, fat_np_global_d2$mlikeres, fat_np_global_pca$mlikeres)

```

6. Conclusion

This article describes the Bayesian bandwidth estimation method and its implementations in a functional nonparametric regression and a semi-functional partial linear regression, using the R functions that are readily-available in the **bbefkr** package. The method is proposed to simultaneously estimate optimal bandwidths in the regression function approximated by the functional NW estimator and kernel-form error density. Illustrated by a series of simulation studies, we found that the use of localised bandwidths is preferable to a global bandwidth based on marginal likelihood or Bayes factor. For modelling a set of smooth curves, it is advantageous to use a semi-metric based on second derivative, whereas a semi-metric based on functional principal components should be used for a set of rough curves. From the spectroscopy data set, we demonstrated that the proposed Bayesian method is able to simultaneously produce point and interval forecasts and the semi-metric based on the second derivative is advantageous to the semi-metric based on principal components for this data set.

In future, the Bayesian method described may be extended to other nonparametric functional estimators for estimating regression function, such as functional local linear estimator (Baíllo and Grané 2009). Furthermore, it may also be extended to other scalar-on-function regression models, such as functional partial linear regression (Lian 2011).

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