Biometrics 63, 714–723
September 2007
DOI: 10.1111/j.1541-0420.2007.00758.x

Gaussian Process Functional Regression Modeling for Batch Data

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Summary. A Gaussian process functional regression model is proposed for the analysis of batch data. Covariance structure and mean structure are considered simultaneously, with the covariance structure modeled by a Gaussian process regression model and the mean structure modeled by a functional regression model. The model allows the inclusion of covariates in both the covariance structure and the mean structure. It models the nonlinear relationship between a functional output variable and a set of functional and nonfunctional covariates. Several applications and simulation studies are reported and show that the method provides very good results for curve fitting and prediction.

Key words: Batch data; B-spline; Functional data analysis; Gaussian process functional regression model; Gaussian process regression model; Multiple-step-ahead forecasting; Nonparametric curve fitting.

1. Introduction

We begin by discussing a motivating example. The application concerns data collected during standing-up maneuvers of paraplegic patients. The *outputs* are the trajectories of the body center of mass (COM), required for a simulator control system; for details see Section 3.3. However, it is very difficult to measure the body position unless some expensive equipment is used and set up in a laboratory environment. Thus, one of the aims of the project is to develop a model for reconstructing the trajectory of the body COM by using some easily measured quantities, such as the forces and torques under the patient's feet, under the arm support, and under the seat while the body is in contact with it. More than 30 such *input* variables are observed in the project. Figure 1 depicts 40 curves of $y(t)$, the vertical trajectories of the body COM, denoted by *comz*. Each curve represents a standing-up maneuver. Eight patients participated in the experiment, and each of them repeated the experiment five times. Our aim is to find a "model" f to model and predict $y(t)$ given covariates $\boldsymbol{x}(t) = (x_1(t), \ldots, x_Q(t))'$:

$$y(t) = f(t, x_1(t), \ldots, x_Q(t)) + \epsilon(t). \tag{1}$$

In each standing-up, both the output variable $y(t)$ and the input variables $\{x_1(t), \ldots, x_Q(t)\}$ are observed at a few hundred time points t_i, for $i = 1, \ldots, N$. If we observe M replications, the mth replication is called the mth batch ($m = 1, \ldots, M$). The data collected are called batch data, terminology that is popular in the engineering community.

We have little information about the physical relationship between the output variable $y(t)$ and the input variables $\{x_1(t), \ldots, x_Q(t)\}$. For such data, it is typically not realistic to use parametric models, or nonparametric linear models such as the functional linear regression models discussed in Ramsay and Silverman (1997) and the varying-coefficient linear models described in Fan, Yao, and Cai (2003). Our idea is to treat the output curve, corresponding to a batch, as a stochastic process and then to estimate the mean and covariance structure simultaneously:

$$y_m(t) = \mu_m(t) + \tau_m(\boldsymbol{x}), \tag{2}$$

where $\mu_m(t) = \mathrm{E}(y_m(t))$ and $\tau_m(\boldsymbol{x})$ is a stochastic process with zero mean and covariance kernel function $C(\boldsymbol{x}, \boldsymbol{x}^*)$ with $\boldsymbol{x} = \boldsymbol{x}(t)$.

To be specific, we will use a Gaussian process regression (GPR) model for $\tau_m(\boldsymbol{x})$ in equation (2). The GPR model has been widely used as a nonparametric approach; see for example O'Hagan (1978), Williams (1998), Neal (1999), and Rasmussen and Williams (2006). In the model, $\tau = f(\boldsymbol{x})$ is an output curve, where $f(\cdot)$ is a function mapping an input $\boldsymbol{x} \in \mathcal{R}^q$ into $\tau \in \mathcal{R}$, and a Gaussian process prior is assumed for $f(\cdot)$: $f(\boldsymbol{x})$ has a normal distribution with zero mean and covariance kernel $C(\boldsymbol{x}, \boldsymbol{x}^*)$. The GPR approach models the nonlinear relationship between $y(t)$ and $\boldsymbol{x}(t)$ through a Gaussian process. Because we assume a zero mean or a given mean for the GPR model, we need first to standardize the data. This is straightforward for a single batch of data, which can be standardized by simply subtracting the sample mean. However, standardization is intractable for batch data, especially when it is used to generate predictions for a completely new batch; see Section 2.2. In Section 3.3, we will show that for the paraplegia example the performance of the GPR model is very good if we use training data collected from a particular patient to predict a new standing-up for the same patient; different standings-up for the same patient have similar mean structures. However, the performance of predictions for a new patient is not so good; mean structures of batches from different patients are quite variable (see Figure 1), because of differences in height, weight, and other factors for the different

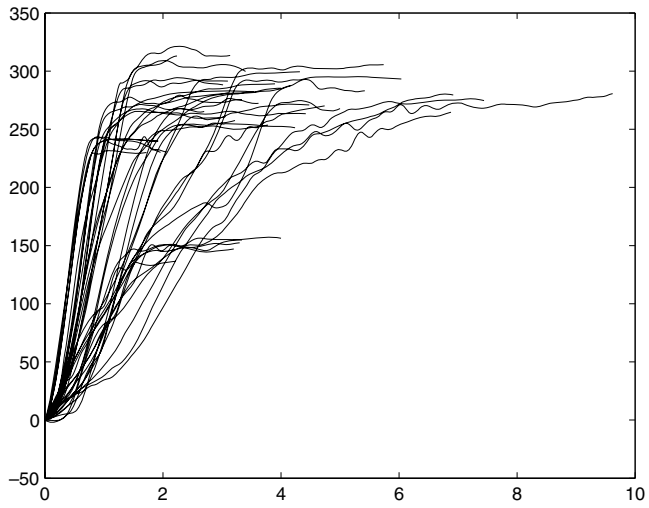


Figure 1. Paraplegia data for eight patients: vertical trajectory of the body COM *comz* coordinate (y-axis, in mm) against time (x-axis, in seconds). Each curve corresponds to one standing-up.

patients. Another limitation of the GPR model is that, although it performs very well in interpolating test data, its extrapolation performance deteriorates very rapidly when the test data are "distant" from the training data. A typical example is that of multiple-step-ahead forecasting. For k-step-ahead forecasting, GPR performs very well when k is small; see, for example, Girard and Murray-Smith (2005). However, when k is large, GPR usually fails in prediction; see Section 3.2. In this article, we try to address these problems and improve the performance of the GPR model by considering the mean structure and covariance structure simultaneously.

To model the mean structure we will use a functional regression model (Ramsay and Silverman, 1997) with functional coefficient parameters and nonfunctional covariates (i.e., we use some batch-based information). We will show that using this type of mean structure within a GPR model can improve the performance substantially.

The idea of modeling the mean and covariance structure simultaneously has been reported elsewhere. For example, Rice and Silverman (1991) estimated the mean function using a cubic spline and estimated the covariance structure via smooth nonparametric estimates of the relevant eigenfunctions. However, their method is limited to the case of a one-dimensional input variable. Eubank (2003) dealt with a forecasting problem by using a linear functional regression (LFR) model with a special covariance structure.

The article is organized as follows. Section 2 proposes the Gaussian process functional regression (GPFR) model, and shows how to estimate unknown parameters and predict new test data. Several applications are reported in Section 3. Some discussion and further developments are given in Section 4.

2. The Gaussian Process Regression Model with Functional Mean Structure

2.1 *The Gaussian Process Regression Model for Batch Data*

The discrete form of a GPR model for a single batch of N observations is defined as

$$\boldsymbol{y} = (y_1, \ldots, y_N)' \sim N(\boldsymbol{0}, \boldsymbol{C}), \tag{3}$$

where $\boldsymbol{C}$ is an $N \times N$ covariance matrix, of which the ijth element $\boldsymbol{C}_{ij} = C(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is a function of input covariates $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. An example of such a covariance function is

$$\begin{aligned} C(\boldsymbol{x}_i, \boldsymbol{x}_j) &= C(\boldsymbol{x}_i, \boldsymbol{x}_j; \boldsymbol{\theta}) \\ &= v_0 \exp\left\{ -\frac{1}{2} \sum_{q=1}^{Q} w_q (x_{iq} - x_{jq})^2 \right\} \\ &\quad + a_0 + a_1 \sum_{q=1}^{Q} x_{iq} x_{jq} + \sigma_0 \delta_{ij}, \end{aligned} \tag{4}$$

where $\boldsymbol{\theta} = (w_1, \ldots, w_Q, v_0, a_0, a_1, \sigma_0^2)$ denotes the set of unknown parameters, and δ_{ij} is the Kronecker delta. Models (3) and (4) define a nonlinear model for y, given $\boldsymbol{x} = (x_1, \ldots, x_Q)$; some recent developments can be found in Rasmussen and Williams (2006). The GPR is nonparametric, and it is usually not very sensitive to the different choices of kernel covariance functions. In practice, we can use equation (4) for most of problems. Some other types of covariance function and the related problems are discussed in MacKay (1999).

To deal with a data set based on repeated experiments involving similar objects and processes, that is, consisting of several batches, Shi, Murray-Smith, and Titterington (2005) proposed a hierarchical GPR model. Suppose that there are M different batches of data and that, in the mth batch, N_m observations are recorded. The data collected in the mth batch are

$$\begin{aligned} \mathcal{D}_m = \{ &(y_{mi}, t_{mi}, x_{m,1,i}, \ldots, x_{m,Q,i}) \text{ for } i = 1, \ldots, N_m; \\ &\text{and } (u_{m1}, \ldots, u_{mp}) \}, \end{aligned} \tag{5}$$

where t_{mi} is the time point at which we record the data, $y_{mi} = y(t_{mi})$ is the output, for example, the body *comz* position, recorded at t_{mi} and $x_{m,q,i} = x_q(t_{mi})$ is the measurement of the qth input variable for $q = 1, \ldots, Q$. The elements of $\boldsymbol{u}_m = (u_{m1}, \ldots, u_{mp})'$ are not functional data, that is, do not depend on t; they offer information for each curve, such as the patient's height and weight and the technique used in a particular standing-up. In Shi et al.'s hierarchical mixture model we have that

$$\boldsymbol{y}_m \,|\, z_m = k \sim GP_k(\boldsymbol{\theta}), \tag{6}$$

where $\boldsymbol{y}_m = (y_{m1}, \ldots, y_{mN_m})'$, and z_m is an unobservable latent indicator variable corresponding to the mth batch. If $z_m = k$ is given, the model for the N_m correlated observations in batch m is a GPR model $GP_k(\boldsymbol{\theta})$; that is, the process has a normal distribution with zero mean or a given mean μ, and a covariance kernel function $C_k(\boldsymbol{x}_i, \boldsymbol{x}_j; \boldsymbol{\theta})$. The association among the different batches is introduced by the latent variable z_m, for which

$$P(z_m = k) = \pi_k, \quad k = 1, \ldots, K, \tag{7}$$

for specified K. This model is used to address the problem of heterogeneity but without using the batch-based information $\boldsymbol{u}_m$. A special case is the model (6) with $K = 1$:

$$\boldsymbol{y}_m \sim GP(\boldsymbol{\theta}), \tag{8}$$

independently, for $m = 1, \ldots, M$. In this model, the heterogeneity among the different batches is ignored.

2.2 *Gaussian Process Functional Regression Model*

As already mentioned, the Gaussian process defined in equation (6) is usually assumed to have zero mean or a known mean μ. To apply it to batch data, we need to center the data by subtracting its sample batch mean, calculated from the training data for each batch. However, this method has its limitations, as mentioned in Section 1. There are two main problems. First, if the training data are not distributed uniformly over the whole time range, if for example only the data corresponding to the first half of a standing-up were recorded, the batch sample mean calculated from such a data set could be quite different from the real mean. Secondly, it is difficult to use this model to predict a new batch for which there are no training data, in particular for a new patient.

Instead, we model the mean structure as well as the covariance structure. We use a functional regression model to model the mean structure and a Gaussian process to model the covariance structure; that is, we use the model given in equation (2), where $\tau_m(\boldsymbol{x})$ is a zero-mean Gaussian process with covariance function $C(\cdot, \cdot)$, as defined in Section 2.1.

There is a large literature on fitting nonparametric curve $\mu_m(t)$ with a scalar input variable t. To model the dependence of the mean functions on the batch-based covariates, $\boldsymbol{u}_m$, we use a similar idea to that discussed in Ramsay and Silverman (1997) and take

$$\mu_m(t) = \boldsymbol{u}_m' \boldsymbol{\beta}(t), \tag{9}$$

where the coefficient $\boldsymbol{\beta}$ is functional.

If we have observed data in the form of $\mathcal{D}_m$ in equation (5) for the mth batch, it is natural to consider a discrete form of the above model, given by

$$y_{mi} = \mu_{mi} + \tau_{mi}; \quad m = 1, \ldots, M, \quad i = 1, \ldots, N_m, \tag{10}$$

where $\mu_{mi} = \mu_m(t_{mi}) = \boldsymbol{u}_m' \boldsymbol{\beta}(t_{mi})$ and $\boldsymbol{\tau}_m = (\tau_{m1}, \ldots, \tau_{mN_m})'$ is defined in equation (6) or its special case (8). We will refer to this model as the GPFR model.

This model is quite distinct from the LFR model discussed in Ramsay and Silverman (1997), which models the mean structure only. This is illustrated by the example given in Figure 2a, in which the solid line represents the true mean curve whereas the dotted line represents the curve with a random error, fluctuating around the true mean curve. The dashed line represents a curve with dependent errors, which is a Gaussian process depending on a functional input variable x; for details see Section 3.1. This curve is systematically different from the true mean curve; 30 such sample curves are presented in Figure 2b.

2.3 *Estimation*

It is not difficult to write down a penalized likelihood for model (10), and then estimate the unknown parameters involved in both the mean structure and the covariance structure. However, the implementation is tedious and there may be computational problems. We use a two-stage approach in this article. In the first stage we estimate the mean structure by using B-spline smoothing; see for example Rice and Silverman (1991), Faraway (1997, 2001) and Ramsay and Silverman (1997). We approximate each curve $y_m(t)$ ($m = 1, \ldots, M$) by

$$y_m(t) = \boldsymbol{A}_m' \boldsymbol{\Phi}(t),$$

where $\boldsymbol{\Phi}(t) = (\Phi_1(t), \ldots, \Phi_K(t))'$ are the B-spline basis functions and $\boldsymbol{A}_m = (\boldsymbol{A}_{m1}, \ldots, \boldsymbol{A}_{mK})'$. The coefficients $\boldsymbol{A} = (\boldsymbol{A}_{mk})$ form an $M \times K$ matrix, whose elements are chosen to minimize

$$\int \left(y_m(t) - \sum_{k=1}^{K} \boldsymbol{A}_{mk} \boldsymbol{\Phi}_k(t) \right)^2 dt.$$

The functional parameters can be expanded as $\boldsymbol{\beta}(t) = \boldsymbol{B}\boldsymbol{\Phi}(t)$, where $\boldsymbol{B}$ is a $p \times K$ matrix, which can be estimated by $\hat{\boldsymbol{B}} = (\boldsymbol{U}'\boldsymbol{U})^{-1}\boldsymbol{U}'\boldsymbol{A}$, where $\boldsymbol{U} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_M)'$ is an $M \times p$ matrix. An estimate of the mean function is given by

$$\hat{\mu}_m(t) = \boldsymbol{u}_m' \hat{\boldsymbol{B}} \boldsymbol{\Phi}(t). \tag{11}$$

Selection of the form and number of the basis functions is discussed by Faraway (1997, 2001). From our empirical experience, the accuracy of the model depends mainly on successful modeling of the covariance structure when the output curves depend on many input functional covariates. Thus, we do not need to use many basis functions in this first stage. For the examples discussed in the next section, we found that 20 basis functions were enough.

In the second stage, we replace μ_{mi} in equation (10) by its estimate $\hat{\mu}_{mi} = \hat{\mu}_m(t_{mi})$ from equation (11). Thus,

$$\hat{\tau}_{mi} = y_{mi} - \hat{\mu}_{mi}$$

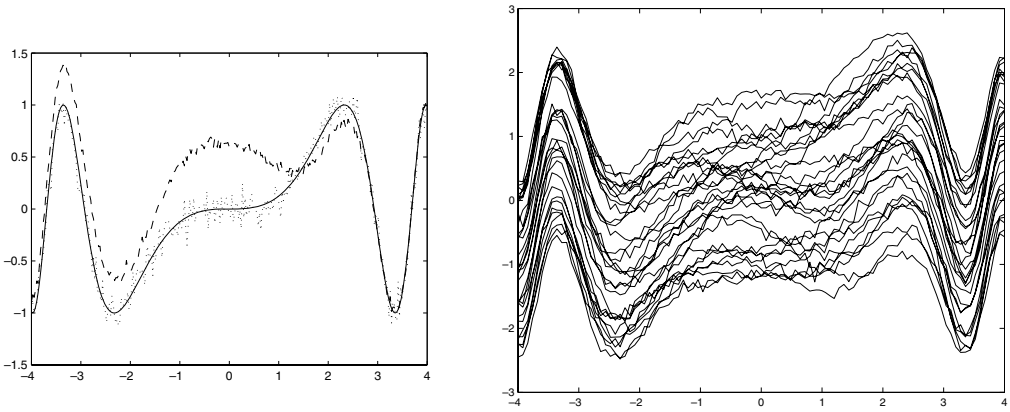
is modeled by a Gaussian process as defined in equations (6) or (8) with covariance function $C(\cdot, \cdot; \boldsymbol{\theta})$. A standard method such as a maximum likelihood or a Markov chain Monte Carlo approach can be used to estimate the unknown parameters $\boldsymbol{\theta}$, leading to $\hat{\boldsymbol{\theta}}$ say; see, for example, Rasmussen (1996) and Williams (1998). Implementation in the case of batch data is described by Shi et al. (2005).

2.4 *Prediction*

We now consider the generation of a prediction y^* at a new test point $(t^*, \boldsymbol{x}^*)$ with $\boldsymbol{x}^* = \boldsymbol{x}(t^*)$. From equation (2), $\hat{y}^* = \hat{\mu}(t^*) + \hat{\tau}(\boldsymbol{x}^*)$, where $\tau^* = \tau(\boldsymbol{x}^*)$ is predicted by its conditional mean $\mathrm{E}(\tau^* \,|\, \mathcal{D})$ through the Gaussian process with estimated covariance function $C(\cdot, \cdot; \hat{\boldsymbol{\theta}})$. We will discuss two types of prediction in this subsection. First we suppose that we have already observed some training data in a batch, the $(M + 1)$th batch say, and want to predict the output for a new set of inputs. In addition to the training data observed in the first M batches, we assume that N observations are obtained in the new batch, providing data

$$\mathcal{D}_{M+1} = \big\{ \big(y_{M+1,i}, t_{M+1,i}, x_{M+1,1,i}, \ldots, x_{M+1,Q,i} \big) \text{ for } i = 1, \ldots, N; \text{ and } \boldsymbol{u}_{M+1} \big\}.$$

We therefore have training data $\mathcal{D} = \{\mathcal{D}_1, \ldots, \mathcal{D}_M, \mathcal{D}_{M+1}\}$. It is of interest to predict y^* at a new test data point t^* in the $(M + 1)$th batch. Let $\boldsymbol{x}^* = \boldsymbol{x}(t^*)$ be the observed test inputs.



(a) (b)

Figure 2. The sample curves. (a) Solid line—the true mean curve; dotted line—the curve with random errors; dashed line—the curve with errors having GP covariance structure depending on x. (b) Thirty sample curves with GP errors.

We use the Gaussian process assumption for the $(M + 1)$th batch,

$$\left(\tau_{M+1,1}, \ldots, \tau_{M+1,N}, \tau^*\right)' \sim N(0, \boldsymbol{\Omega}) \tag{12}$$

where $\tau = y - \mu$ and $\boldsymbol{\Omega}$ is an $(N + 1) \times (N + 1)$ covariance matrix

$$\boldsymbol{\Omega} = \begin{bmatrix} \boldsymbol{C} & \boldsymbol{C}\left(\boldsymbol{x}^*, \boldsymbol{x}_{M+1}\right) \\ \boldsymbol{C}'\left(\boldsymbol{x}^*, \boldsymbol{x}_{M+1}\right) & C(\boldsymbol{x}^*, \boldsymbol{x}^*) \end{bmatrix} \tag{13}$$

where $\boldsymbol{C}(\boldsymbol{x}^*, \boldsymbol{x}_{M+1}) = (C(\boldsymbol{x}^*, \boldsymbol{x}_{M+1,1}), \ldots, C(\boldsymbol{x}^*, \boldsymbol{x}_{M+1,N}))'$, is the covariance matrix between y^* and $\boldsymbol{y}_{M+1} = (y_{M+1,1}, \ldots, y_{M+1,N})'$, and $\boldsymbol{C}$ is the $N \times N$ covariance matrix of $\boldsymbol{y}_{M+1}$ or $\boldsymbol{\tau}_{M+1}$, which depends on $\boldsymbol{x}_{M+1}$. The covariance can be calculated by, for example, equation (4) with the parameters estimated as in the previous subsection. Thus, the predictive distribution of y^*, given training data $\mathcal{D}$ and the mean $\boldsymbol{\mu}(t)$, is also a Gaussian distribution. Its mean and variance are given by

$$\mathrm{E}(y^* \mid \mathcal{D}, \boldsymbol{\mu}) = \mu_{M+1}(t^*) + \boldsymbol{H}'(\boldsymbol{y}_{M+1} - \boldsymbol{\mu}_{M+1}(\boldsymbol{t})), \tag{14}$$

$$\sigma^{*2}_{GP} = \mathrm{Var}(y^* \mid \mathcal{D}, \boldsymbol{\mu}) = C(\boldsymbol{x}^*, \boldsymbol{x}^*) - \boldsymbol{H}'\boldsymbol{C}\boldsymbol{H}, \tag{15}$$

where $\boldsymbol{\mu}_{M+1}(\boldsymbol{t}) = (\mu_{M+1}(t_1), \ldots, \mu_{M+1}(t_N))'$ is the vector of means at data points $\boldsymbol{t} = (t_1, \ldots, t_N)$, and $\boldsymbol{H}' = [\boldsymbol{C}(\boldsymbol{x}^*, \boldsymbol{x}_{M+1})]'\boldsymbol{C}^{-1}$. Thus the prediction for y^* is given by

$$\hat{y}^*_{M+1} = \hat{\mu}_{M+1}(t^*) + \boldsymbol{H}'(\boldsymbol{y}_{M+1} - \hat{\boldsymbol{\mu}}_{M+1}(\boldsymbol{t})), \tag{16}$$

where $\hat{\mu}_{M+1}(t^*)$ and $\hat{\boldsymbol{\mu}}_{M+1}(\boldsymbol{t})$ are given by equation (11), that is, $\hat{\mu}_{M+1}(\cdot) = \boldsymbol{u}'_{M+1}\hat{\boldsymbol{B}}\boldsymbol{\Phi}(\cdot)$. The prediction variance can be calculated from the conditional variances in equations (14) and (15):

$$\begin{aligned} \hat{\sigma}^{*2}_{M+1} = \mathrm{Var}(y^* \mid \mathcal{D}) &= \mathrm{E}\{\mathrm{Var}(y^* \mid \mathcal{D}, \boldsymbol{\mu})\} + \mathrm{Var}\{\mathrm{E}(y^* \mid \mathcal{D}, \boldsymbol{\mu})\} \\ &= \hat{\sigma}^{*2}_{GP}\left(1 + \boldsymbol{u}'_{M+1}(\boldsymbol{U}'\boldsymbol{U})^{-1}\boldsymbol{u}_{M+1}\right), \end{aligned} \tag{17}$$

where $\hat{\sigma}^{*2}_{GP}$ is given by equation (15), in which all the parameters are replaced by their estimators. The derivation of equation (17) is given in Appendix A.

The second type of prediction is to predict for a completely new batch. We shall still refer to the new batch as the $(M + 1)$th batch, with batch-based covariate $\boldsymbol{u}_{M+1}$. We want to predict y^* at $(t^*, \boldsymbol{x}^*)$. In this case, the training data are $\mathcal{D} = \{\mathcal{D}_1, \ldots, \mathcal{D}_M\}$. Because we have not observed any data in the $(M + 1)$th batch, we cannot use the predictive mean and covariance matrix discussed above, which is based on the Gaussian process assumption (12). The argument in Shi et al. (2005) is that batches $1, \ldots, M$ provide an empirical distribution of the set of all possible batches. We will use a similar idea here but only for the Gaussian process component $\tau_{M+1}(\cdot) = y_{M+1}(\cdot) - \hat{\mu}_{M+1}(\cdot)$. We assume that, for $m = 1, \ldots, M$, $P(\tau^* \text{ belongs to } m\text{th batch}) = 1/M$. To say that τ^* belongs to the mth batch means that $(\tau_{m,1}, \ldots, \tau_{m,N_m}, \tau^*) \sim N(0, \boldsymbol{\Omega}_m)$, where $\boldsymbol{\Omega}_m$ is an $(N_m + 1) \times (N_m + 1)$ covariance matrix which is defined similar to equation (13). We can, therefore, calculate $\hat{y}^*_m$ and $\hat{\sigma}^{*2}_m$ from equations (16) and (17), respectively, as if the test data belongs to the mth batch. Because the empirical distribution is relevant to the Gaussian process component only, $\hat{y}^*_m$ is given by

$$\hat{y}^*_m = \hat{\mu}_{M+1}(t^*) + \boldsymbol{H}'(\boldsymbol{y}_m - \hat{\boldsymbol{\mu}}_m(\boldsymbol{t})). \tag{18}$$

The value of $\hat{\sigma}^{*2}_m$ is given by equations (17) and (15), but the related covariance matrices are calculated at $\boldsymbol{x}^*$ and $(\boldsymbol{x}_{m,1}, \ldots, \boldsymbol{x}_{m,N_m})$.

Based on the above empirical assumption, the prediction for the response associated with a test input $\boldsymbol{x}^*$ at t^* in a completely new batch is

$$\hat{y}^* = \sum_{m=1}^{M} \hat{y}^*_m / M, \tag{19}$$

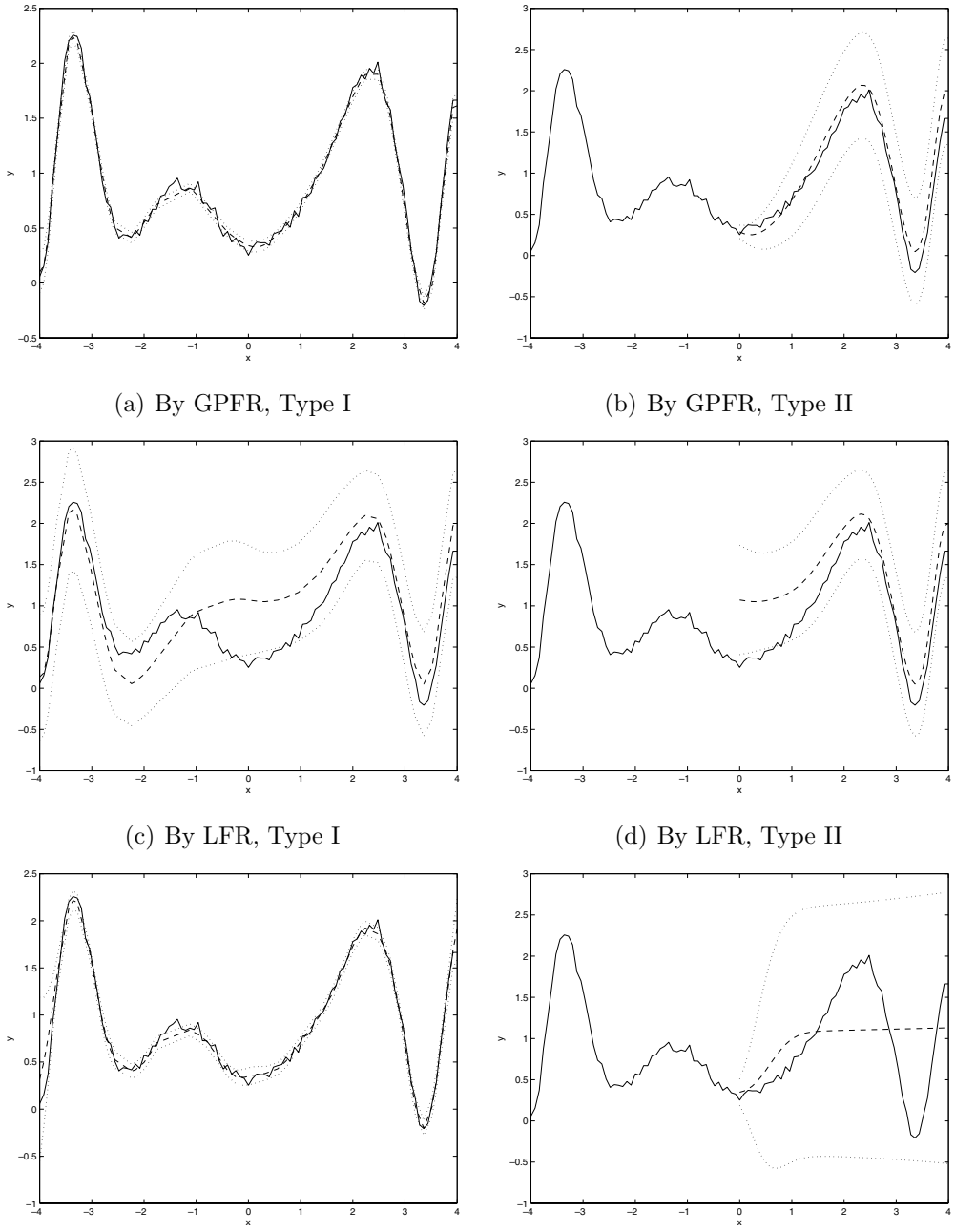
and the predictive variance is

$$\hat{\sigma}^{*2} = \sum_{m=1}^{M} \hat{\sigma}^{*2}_m / M + \left(\sum_{m=1}^{M} \hat{y}^{*2}_m / M - \hat{y}^{*2}\right). \tag{20}$$

3. Applications

3.1 *Learning and Prediction for Large Batch Data Sets*

We first consider an example with simulated data. The true model used to generate the data is $y_{mi}(x_{mi}) = u_m + \sin(0.5x_{mi})^3 + \tau_{mi}$, where, for each m, $x_{mi} \in (-4, 4)$ and $\{\tau_{mi}\}$



(a) By GPFR, Type I

(b) By GPFR, Type II

(c) By LFR, Type I

(d) By LFR, Type II

(e) By GPR, Type I

(f) By GPR, Type II

Figure 3. The predictions obtained by the different methods, where the solid line represents the true curve, the dashed line represents the predictions, and the dotted lines represent 95% prediction intervals.

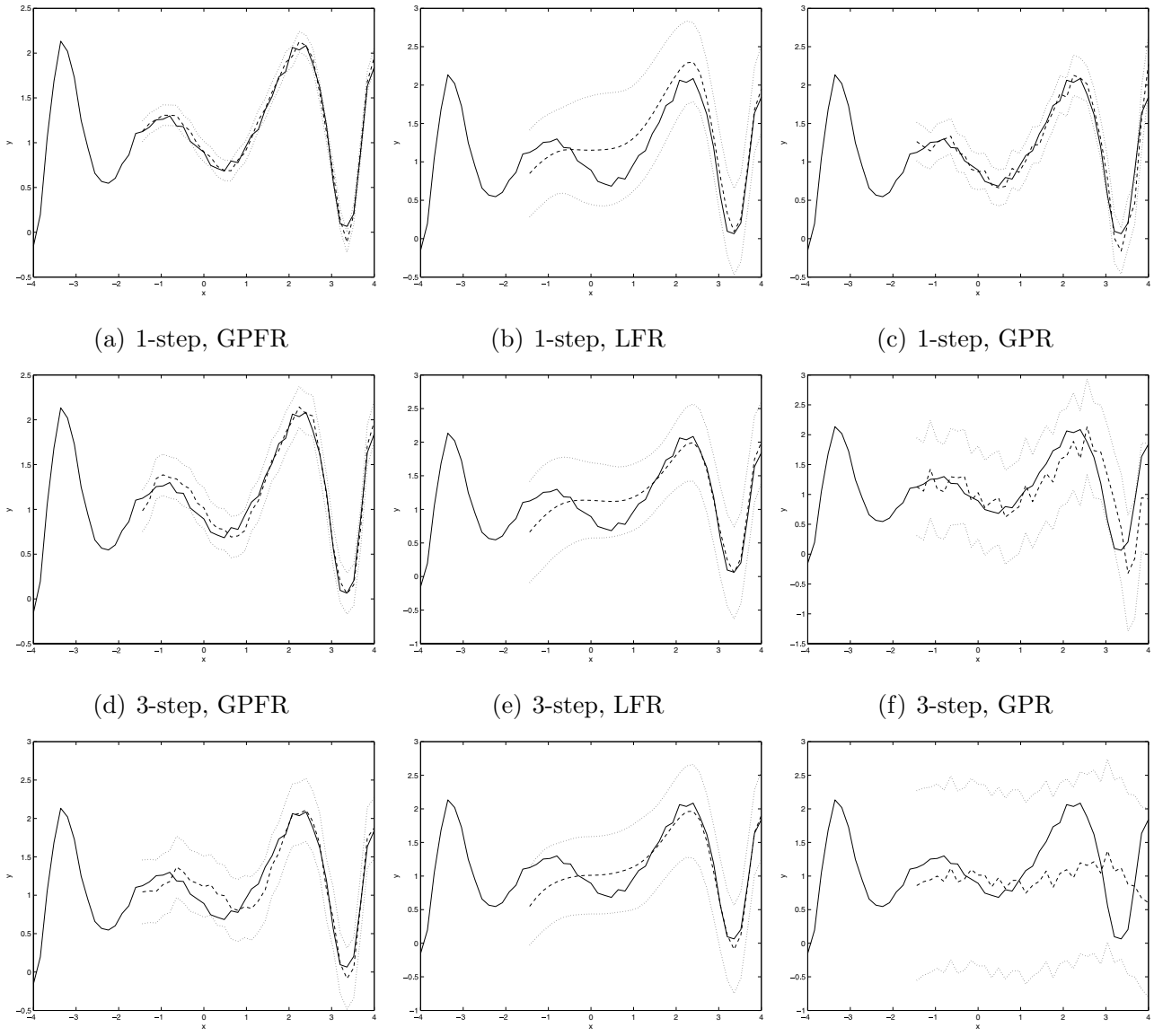
is a Gaussian process with zero mean and covariance function $C(x_{mi}, x_{mj}) = v_0 \exp\{-\frac{1}{2} w_0 (x_{mi} - x_{mj})^2\} + \sigma_0 \delta_{ij}$, with $v_0 = 0.1$, $w_0 = 1.0$ and $\sigma_0^2 = 0.0025$. In this example, x_{mi} is the same as t_{mi}. Thirty independent curves are generated and are presented in Figure 2b, where $u_m = 0$ for batches 1 to 10, $u_m = -1$ for batches 11 to 20, and $u_m = 1$ for the remaining 10 batches. In each batch, 100 data points are generated. We randomly select half of the data points as training data.

In this example, only one discrete covariate u_m is used in the mean structure model (9). The model is such that $\mu_m(t) = \beta_1(t)$ when $u_m = -1$, $\mu_m(t) = \beta_2(t)$ when $u_m = 0$, and $\mu_m(t) = \beta_3(t)$ when $u_m = 1$. We use cubic B-spline smoothing with 18 knots equally spaced in $(-4, 4)$ and the method discussed in Section 2.3 to estimate $\beta_i(t)$, for $i = 1$, 2, 3. We then apply a GPR model to $\hat{\tau}_m(t) = y_m(t) - \hat{\mu}_m(t)$ with covariance function (4), depending on the scalar input

Table 1
The values of rmse and r between true and predicted responses

		Type I		Type II			
Results for	Model	*rmse*	*r*	*rmse*			*r*
Figure 3	GPFR	0.0485	0.9976	0.1634			0.9814
	LFR	0.3616	0.8718	0.4054			0.9510
	GPR	0.1066	0.9865	0.5693			0.4455
		rmse	*r*	*rmse*[a]	*r*	*rmse*[b]	*rmse*[c]
Simu. Study	GPFR	0.0588	0.9954	0.2802	0.9270	0.1321	0.3116
	LFR	0.3244	0.9068	0.3318	0.9143	0.2874	0.3352
	GPR	0.0830	0.9911	0.6044	0.1246	0.2271	0.6843

[a]The overall *rmse* comparing true and predicted responses in range [0, 4].
[b]The *rmse* comparing true and predicted responses in range [0, 1].
[c]The *rmse* comparing true and predicted responses in range [1, 4].



(a) 1-step, GPFR (b) 1-step, LFR (c) 1-step, GPR

(d) 3-step, GPFR (e) 3-step, LFR (f) 3-step, GPR

(g) 6-step, GPFR (h) 6-step, LFR (i) 6-step, GPR

Figure 4. The k-step-ahead forecasts and the associated 95% prediction intervals.

Table 2
Numerical results of rmse and r for k-step-ahead forecasting

		1 step		3 step		6 step	
Results for	Model	*rmse*	*r*	*rmse*	*r*	*rmse*	*r*
Figure 4	GPFR	0.0697	0.9925	0.1001	0.9838	0.1658	0.9502
	LFR	0.2564	0.9291	0.2241	0.9054	0.2314	0.9044
	GPR	0.1452	0.9683	0.3972	0.7010	0.5842	−0.0439
Simu. Study	GPFR	0.0785	0.9896	0.1229	0.9769	0.2169	0.9360
	LFR	0.3013	0.8989	0.3097	0.8820	0.3242	0.8172
	GPR	0.1487	0.9670	0.4375	0.6640	0.5994	0.0021

variable x as discussed in Section 2.3. Prediction can then be carried out by the method discussed in Section 2.4.

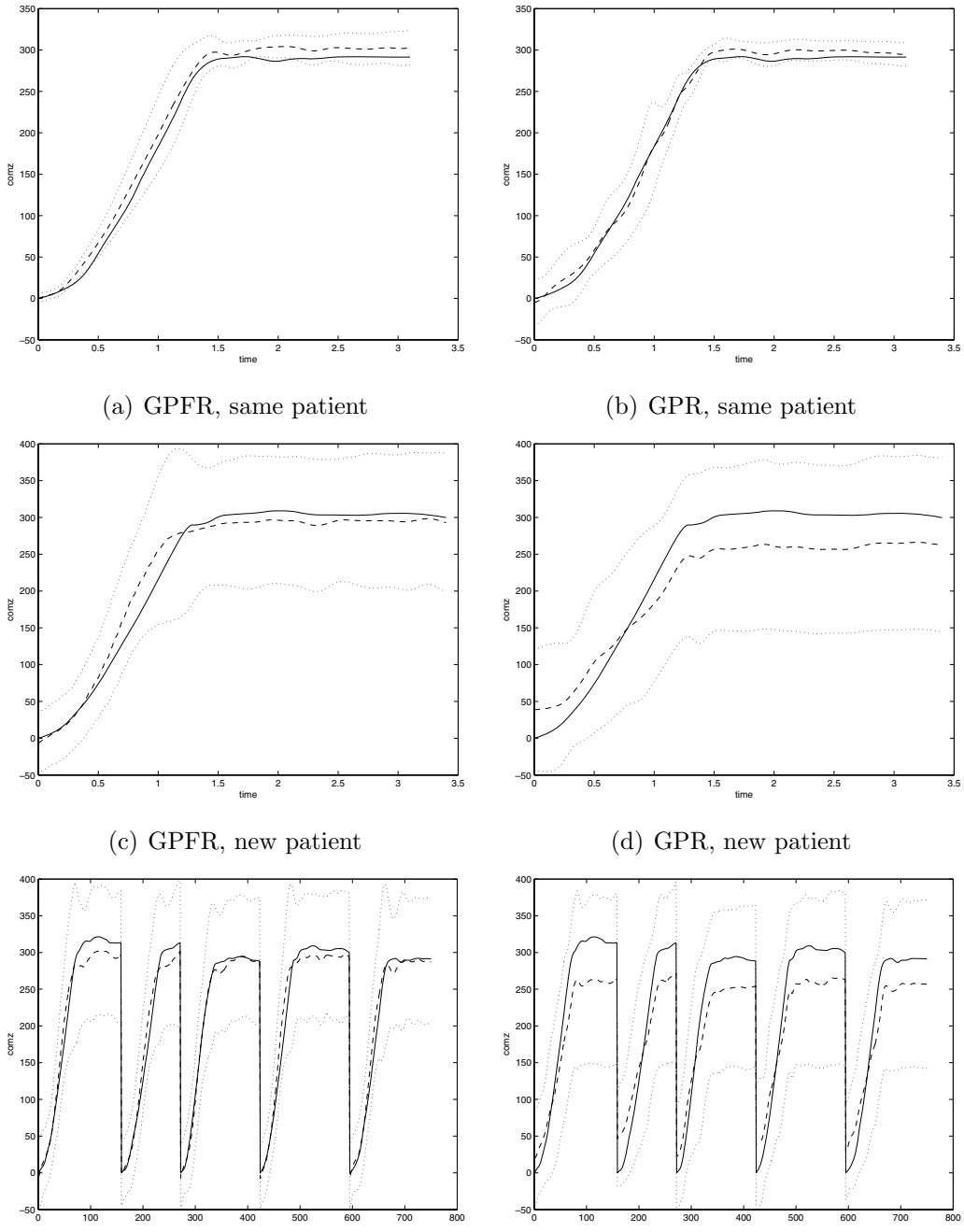
To assess the performance of the method, we calculate predictions for a new batch and compare them with the actual output values of the test data. One hundred data points are generated in a new batch with $u_m = 1$. Half of the data are selected as part of the training data and are used to predict the rest. Two types of training data are considered. Type I data are selected randomly from the whole set of 100 points. In type II data, data points corresponding to $x \in (-4, 0)$ are used as training data and the rest are used as test data. Thus, type I prediction is essentially interpolation, while type II prediction involves extrapolation, which is obviously harder. For comparison, GPR and LFR are also applied to the same data set.

The predictions obtained by the different methods, along with the actual values of the test data, are plotted in Figure 3 and presented in Table 1, in which *rmse* is the root mean squared error between the predictions and the true test values, and r is the related correlation coefficient. The left-hand side panels in Figure 3 report the results for type I prediction, that is, interpolation. Both GPFR and GPR predict the output very precisely. It is not surprising that the result using LFR is less good, because LFR models the common mean structure only. The results for type II prediction are given in the right-hand side panels in Figure 3. GPFR still gives very precise predictions. LFR predicts the common mean structure, so that its performance is quite similar for both types of test data. GPR fails to predict this type of test data well except for a few points close to 0. GPR models the covariance structure only, and does not reliably predict the test data if they are "far away" from the training data. When test data are "close" to training data, the GPFR model uses both the mean structure and the covariance structure to calculate predictions, and gives a very precise result; when test data are distant from the training data, GPFR would rely mainly on the mean structure to predict test data and could still give a reasonably good result. This is confirmed by the simulation study, based on 50 replications, reported in Table 1. The overall performance of GPFR for type II prediction is better than LFR and GPR. In the range [0, 1], which is close to the training data, GPFR($rmse = 0.1321$) is much better than LFR($rmse = 0.2874$) and GPR($rmse = 0.2271$). In the range [1, 4], which is further away from the training data, GPFR($rmse = 0.3116$) is slightly better than LFR($rmse = 0.3352$), as expected, and GPR fails in the prediction of output in this range ($rmse = 0.6843$, see also Figure 3f).

3.2 *Multiple-Step-Ahead Forecasting*

If, in a discrete-time dynamic system, we have available data up to time t_i, we may wish to predict the output at time t_{i+k}. This is called k-step-ahead forecasting. Many dynamic systems are periodic in real-life problems, and data collected in each period form a batch. We may refer to the data collected in previous periods as historical data. In the current period, we use the data up to time t_i as well as the historical data to train the model and forecast the output at time t_{i+k}.

We use the artificial model used in Section 3.1 to generate a set of batch data. Values for 30 curves are generated, each at 50 equally spaced points. For the k-step-ahead forecasting problem, we assume that there are two functional input variables associated with each output y_i, namely x_i and y_{i-k}. We first use the data for those 30 curves and the related input variables to train the model, and then do k-step-ahead forecasting after one-third of the data in a new batch has been observed. For comparison, the GPFR, LFR and GPR methods are applied to the same data set. A simulation study with 50 replications was conducted. The results from the simulation study and the result from one typical replication, for 1−, 3−, and 6-step-ahead forecasts, are reported in Table 2. The results for the single replication are also presented in Figure 4. The values of *rmse* and r are calculated by comparing the forecast values with the actual simulated values. The GPFR model performs very well in all the cases and becomes more and more accurate as the end of the period is approached, by which time more observations have been obtained. The LFR model gives reasonably good predictions in all the cases. The precision achieved does not vary much with k. As expected, LFR does not give very accurate predictions because only the common mean structure is modeled. When k is small, GPR gives good predictions; see for example the 1-step-ahead results reported in Table 2. However, the precision decreases very rapidly as k increases. It fails when k is larger than six in this example. Of course, the precision of the forecasting obtained by GPFR also decreases as k increases, but the rate of decrease is much slower than for the GPR model. When k is very large, the forecast obtained by GPFR will be close to that given by LFR, that is, it will give a forecast based on a common mean structure. This is still a useful forecast.



(a) GPFR, same patient

(b) GPR, same patient

(c) GPFR, new patient

(d) GPR, new patient

(e) GPFR, new patient

(f) GPR, new patient

Figure 5. Paraplegia data: the true test data (solid line), the prediction (dashed line), and the 95% prediction intervals (dotted line). (a)–(b) Prediction of a new standing-up as for the same patient. (c)–(d) Prediction of a new standing-up as for a new patient. (e)–(f) Prediction of five new standings-up for a new patient.

3.3 *Modeling of Standing-Up Maneuvers by Paraplegic Patients*

Our application, as introduced in Section 1, involves the analysis of the standing-up maneuver in the context of paraplegia; for operational details see Kamnik, Bajd, and Kralj (1999) and Kamnik et al. (2005). Here we model the vertical trajectory of the body COM as output, and select 14 input variables. In one standing-up, output and inputs are recorded for a few hundred time points. The experiment was repeated several times for each patient. The vertical trajectories of the body COM are presented in Figure 1 for 40 standings-up, 5 for each of 8 patients.

For modeling the mean structure in the GPFR model, we use three covariates for $\boldsymbol{u}_m$, namely the patient's height,

weight and sex. These are natural covariates for the mean structure model. Figure 1 indicates that the time scale may be different for different standings-up. Some registration methods are used before estimating the mean structure; see Ramsay and Silverman (1997) and Ramsay and Li (1998). We then estimate the mean structure and covariance structure by the method discussed in Section 2 with the covariance function (4), and use this model to predict a new standing-up. For comparison, results from GPR models are also obtained.

We consider two important types of prediction here. Type A uses the data that have already been observed for one patient to predict a new standing-up for the same patient, whereas type B predicts a standing-up for a new patient. For type A prediction, we use the training data from the same patient, which should have similar mean structure, so that GPR should predict well. However, it may be less satisfactory for type B prediction. This is confirmed by the numerical results. Figure 5a and 5b presents the type A prediction by GPFR and GPR, respectively, both giving very good results. Figure 5c–5f shows type B predictions. Figure 5c and 5d presents the prediction for a single standing-up for a new patient by using the GPFR and GPR models, respectively. The values of *rmse* are 18.6180 and 47.8120, respectively, which shows that GPFR performs much better than GPR. Figure 5e and 5f shows the predictions for all five standings-up for this new patient. The average value of *rmse* is 14.6661 for GPFR and 40.95550 for GPR, showing that GPFR performs consistently better than GPR.

We selected one of the eight patients as the new patient in turn, and used the data obtained from the rest as the training data. The results are very similar to those reported in Figure 5 except for one patient. However, that patient is atypical, being a thin (59 kg) and very tall (178 cm) woman. She is an outlier in terms of the mean structure model, and thus the GPFR model fails to improve much on the result obtaining by GPR. For this patient, the average value of *rmse* for five standings-up is 62.8 for the GPFR and 51.74 for the GPR model.

4. Discussion

Nonparametric and nonlinear regression analysis for batch data (functional data or longitudinal data) is a difficult problem with a large literature. However, most methods are limited to scenarios with one- or two-dimensional covariates (Lin and Carroll, 2000; Yao, Müller, and Wang, 2005), or the nonparametric linear regression model (Ramsay and Silverman, 1997; Fan et al., 2003). However, for our motivating example discussed in Section 1 and Section 3.3 and many other applications, one needs a nonparametric nonlinear model that copes with high-dimensional input functional covariates.

Rice and Silverman (1991) treat the output curve (batch) as a stochastic process and then estimate both the mean and covariance structure: $y_m(t) = \mu_m(t) + \tau_m(t)$, where $\mu_m(t) = \mathrm{E}(y_m(t))$ and $\tau_m(t)$ is a stochastic process with zero mean and kernel covariance function $C(t, t^*) = \mathrm{Cov}(y(t), y(t^*))$. In our method the stochastic process $\tau_m(\boldsymbol{x})$ and the related covariance kernel C depend on input variables $\boldsymbol{x}$, that is, $\mathrm{Cov}(y(t), y(t^*)) = C(\boldsymbol{x}, \boldsymbol{x}^*)$, as in model (2). Yao et al. (2005) approximated the covariance matrix $C(t, t^*)$ by a smooth surface estimate and then estimated the related eigenvalues and eigenfunctions. The stochastic process $\tau_m(t)$ can be expanded in terms of those eigenfunctions. However, it is very difficult to extend their method to the model involving $C(\boldsymbol{x}, \boldsymbol{x}^*)$ when the dimension of $\boldsymbol{x}$ is larger than one. In this article, we assume a Gaussian process for $\tau_m(\boldsymbol{x})$ and estimate it by a predictive mean as discussed in Section 2.4.

For the problem of curve fitting and prediction with high-dimensional input variables, neural network models are another popular approach; see Cheng and Titterington (1994) for a review. Shi et al. (2005) and Kamnik et al. (2005) showed that the GPR model gives a better fit for the paraplegia data than did the neural network models. However, the GPR model models the covariance structure only.

In future work it would be worthwhile to explore a unified Bayesian approach to the GPFR model; see, for example, DiMatteo, Genovese, and Kass (2001) and Shi et al. (2005).

5. Supplementary Materials

Appendix A. Derivation of equation (17) is accessed at the *Biometrics* website `http://www.tibs.org/biometrics`. The related Matlab Codes are available at the website `http://www.staff.ncl.ac.uk/j.q.shi`.

Acknowledgements

Dr Wang is grateful for support of the UK Engineering and Physical Sciences Research Council for grant EPSRC GR/T29253/01. We would also like to thank Dr R. Kamnik and Prof T. Bajd of the Laboratory of Biomedical Engineering of the University of Ljubljana for allowing us to use their experimental data. We are grateful to the associate editor and the reviewers for very helpful comments.

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Received September 2005. *Revised October* 2006.
Accepted October 2006.