

# Functional Multicore Gaussian Process Regression Modeling Based on Kalman Filtering

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**Abstract.** Aiming at the regression problem in which the response variable is scalar and the predictor variable is functional-type variable, this paper innovatively proposes a functional-type multicore Gaussian process regression model based on Kalman filtering. Firstly, a functional principal component base expansion method is applied to extract features of functional predictor variables to realize the approximate characterization of functional data; then, the potential function between each principal component score and the response variable is assigned to the Gaussian process a priori and multiple Gaussian process regression submodels are constructed using different kernel functions for fitting; finally, the Kalman filtering algorithm is utilized to dynamically integrate the results of the submodels to obtain the final Prediction results. Compared with the traditional integration learning algorithm, this model integrates the uncertainty estimation into the integration framework, fully considers the adaptability of different regenerative kernel Hilbert space from the probability level, and significantly improves the robustness and generalization ability of the model. Empirical studies on meat and maize near-infrared spectral analysis datasets show that the model in this paper exhibits superior prediction performance in both MSE and MAE metrics compared to benchmark methods such as traditional machine learning models: XGBoost, single-kernel Gaussian process regression (GPR): using RBF kernel function. In addition, the construction of differentiated sub-models by adjusting the number of principal component truncations in functional principal component analysis provides a new path for model performance optimization.

**Keywords:** Functional regression, Gaussian process, functional principal component analysis, Kalman filter algorithm.

## 1. Introduction

With the innovation of modern data acquisition technology, a large amount of observational data with continuous characteristics have emerged in scientific research and engineering practice. The data are not presented in the form of functions defined on a continuous domain, i.e., functional data. This kind of data comes from infinite dimensional space, which gives rise to functional linear regression models, functional nonlinear regression models, partial functional linear models and other functional data regression methods. These methods have shown strong application potential in the fields of biomedicine, industrial inspection, and environmental science. In the industrial field, they help the early warning of equipment vibration signal failure; in climate research, they can effectively model the long-term trend and seasonal fluctuation of temperature and precipitation. This paper focuses on the regression scenario where the independent variable is functional and the dependent variable is scalar, aiming at proposing a functional multicore Gaussian process additivity model based on Kalman filtering to deal with such data more accurately.

Traditional regression analysis methods often treat functional-type data as high-dimensional data and model them using multiple linear regression (MLR), principal component regression (PCR) or partial least squares regression (PLSR), but the results are often unsatisfactory. This is because the number of variables often far exceeds the sample size after the data is discretised into high-dimensional vectors, resulting in some models not being able to be solved stably. Although dimensionality reduction methods can alleviate this problem, it is still difficult to fully exploit the continuity and smoothness characteristics of the data. When functional data are simply treated as high-dimensional vectors, their intrinsic structural features are easily ignored, resulting in information loss. In order to address the limitations of traditional models, James O. Ramsay and Bernard W.

Silverman [1, 2] pioneered the study of functional data and proposed the functional linear model (FLM). In recent years, FLM has been continuously developed, and scholars such as Aue and Dubart Norinho [3] have realized steady-state functional time series prediction based on it. However, FLM assumes a linear relationship between the response and the explanatory variables, which is difficult to adapt to the nonlinear relationship that exists among function data, and is prone to significant distortion and bias. To address this problem, Bosq and Cuevas [4] explored functional kernel regression, while Ferraty and Vieu [5, 6] further introduced the idea of kernel smoothing into the theoretical analysis of functional data and established the framework of functional nonlinear regression models, and Müller and Yao [7] proposed the framework of nonlinear dynamical systems for functional data modeling. Among the nonlinear models, additive models are widely used. However, most of the functional regression models, both linear and nonlinear, can only output a single prediction, which is difficult to satisfy the demand for uncertainty measures of predicted values in engineering and aerospace fields and affects the robustness of the models. Functional Gaussian process regression models provide a new direction to solve the above problems by virtue of the flexible selection of kernel functions and parameters. Bo Wang [8] and other scholars apply Gaussian process methods to nonparametric functional regression with scalar and functional responses, which is suitable for mixed multidimensional functional data; Liu Yingying [9] and others propose an adaptive Gaussian process kernel function selection model; Hau-Po Hsu [10] and others integrate Kalman filtering algorithms into Gaussian process regression models, and the results of these models can be predicted by the Gaussian process. Kalman filter algorithm into Gaussian process model optimization. However, the existing studies still face the challenges of kernel function selection and model integration, and how to construct better function models to realize accurate prediction has become an urgent problem.

Based on this, this paper proposes a functional-type multicore Gaussian process model based on Kalman filtering. The model applies the functional principal component basis expansion method to extract features from functional predictor variables to realize the approximate characterization of functional data. Multiple functional Gaussian process regression sub-models are established by considering different kernel functions, and the prediction results (a posteriori mean and variance) of the sub-models are inputted into the Kalman filtering algorithm, which realizes the effective fusion of the multiple models under the probabilistic perspective, and improves the model robustness. The proposed method achieved excellent results in the prediction of physical and chemical indexes of meat and corn infrared spectral data, and provided a new effective way for functional data regression analysis.

## 2. Theory and Methods

Consider the observed data  $\{Y_i, X_i(t)\}_{i=1}^N$  as  $N$  independently and identically distributed samples of  $\{Y, X(t)\}$ . Where  $X_i(t)$  is the square-productible random function defined on  $\mathcal{T}$  and  $y_i \in R$  is the scalar response variable. Notate the functional principal component score corresponding to  $X_i(t)$   $\{a_{ik}, k = 1, 2, \dots, n, \dots\}$ , Considering the functional principal component score based on standardization, this paper investigates the following functional model:

$$Y_i = b_0 + \sum_{k=1}^{\infty} f_k(a_{ik}) + \varepsilon_i \quad (1)$$

Functional principal component analysis is used to process the functional predictor variables. Although  $X(t)$  should be a linear combination of infinite eigenfunctions in theory, in the actual data analysis,  $X(t)$  is often expressed as a linear combination of finite eigenfunctions, and the original discrete observation  $\{X_i(t_j)\}$  is functionally reconstructed using the form of basis function expansion for approximation and reconstruction, to eliminate the measurement noise and to ensure the continuity of the function in the form of the following:

$$\hat{X}_i(t) = \sum_{k=1}^K c_{ik} \phi_k(t) \quad (2)$$

Where  $\phi_k(t)$  is the pre-selected basis function,  $c_{ik} \in R$ . Calculate the function mean  $\mu(t) = \frac{1}{n} \sum_{i=1}^n \tilde{X}_i(t)$ , and define the centering function as  $X'_i(t) = \tilde{X}_i(t) - \mu(t)$ . Based on the covariance operator  $C(s, t) = Cov(X^c(s), X^c(t))$ , solve the Fredholm integral equation to extract the principal components:  $\int_T C(s, t) \psi_k(s) ds = \lambda_k \psi_k(t), k = 1, 2, \dots$ , where  $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$  is the eigenvalue and  $\{\psi_k(t)\}$  is the corresponding orthogonal eigenfunction (principal component function). Project the centrality function  $X'_i(t)$  to the first  $K$  principal component directions:  $a_{ik} = \int_T X'_i(t) \psi_k(t) dt, k = 1, \dots, K$ . At this point, the functional data can be approximated as:  $X_i(t) \approx \mu(t) + \sum_{k=1}^K \xi_{ik} \psi_k(t)$ . Using the principal component scores  $\{a_{ik}\}$  as the input variables of the additive model, the following functional model is constructed:

$$Y_i = \alpha + \sum_{k=1}^K f_k(\xi_{ik}) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2) \quad (3)$$

For the above model, in order to make it have an uncertainty measure, each function  $f_j(\cdot)$  obeys an independent Gaussian process with zero mean, i.e:

$$f_j(\cdot) \sim GP(0, k_j) \quad (4)$$

Where  $k_j$  is the covariance function of the first  $j$  component, and the prior distributions of each  $f_j(\cdot)$  are independent of each other and of the noise term  $\epsilon_i$ .  $f_j(\cdot) \sim GP(0, k_j)$ , Then the model  $\sum_{j=1}^p f_j(\cdot)$  obeys the Gaussian process  $GP(0, \sum_{j=1}^p k_j)$ . In the task of Gaussian process regression prediction, it is extremely important to train the hyperparameters, and in the general task, the most common kernel function in machine learning, i.e., the squared exponent, is often used. For different tasks, the selection of the kernel function will affect the final prediction results of the model. Table 1 shows the common Gaussian process kernel functions.

**Table 1.** Common Gaussian process kernel functions

Kernel function name	math expression
Square Exponent (SE) Kernel	$k(x, x') = \sigma^2 \exp\left(-\frac{\ x - x'\ ^2}{2l^2}\right)$
Matérn 3/2 nuclear	$k(x, x') = \sigma^2 \left(1 + \frac{\sqrt{3} \ x - x'\ }{l}\right) \exp\left(-\frac{\sqrt{3} \ x - x'\ }{l}\right)$
index nucleus	$k(x, x') = \sigma^2 \exp\left(-\frac{\ x - x'\ }{l}\right)$
periodic nucleus	$k(x, x') = \sigma^2 \exp\left(-\frac{2 \sin^2\left(\pi \frac{\ x - x'\ }{p}\right)}{l^2}\right)$
Rational quadratic kernel	$k(x, x') = \sigma^2 \left(1 + \frac{\ x - x'\ ^2}{2\alpha l^2}\right)^{-\alpha}$
linear kernel (math.)	$k(x, x') = \sigma_b^2 + \sigma_v^2(x \cdot x')$

Using different kernel functions, different sub-models can be obtained, for which the Kalman filtering algorithm is used for fusion. Kalman filtering is a recursive estimation algorithm based on the minimum mean square error criterion, and its core idea is to realize the optimal state estimation under the noise interference through the state space model of the dynamic system. The algorithm gradually optimizes the estimation results through a "prediction-correction" cycle, which mainly consists of two recursive phases: based on the state equations of the system and the a posteriori estimation of the previous moment, the a priori estimation of the state at the current moment is deduced, and at the same time, the state covariance matrix is updated to quantify the prediction uncertainty. This phase relies on the dynamic model of the system for state evolution prediction. By introducing real-time observations and calculating the Kalman gain matrix to dynamically balance

the weights of model predictions and measurements, the a priori estimates are fused with the observations to obtain a modified a posteriori estimate. The process simultaneously updates the covariance matrix to provide an optimized basis for the prediction at the next moment. The algorithm effectively suppresses the interference of system noise and observation noise through the continuous iterative prediction and correction process, and realizes highly accurate real-time estimation of the dynamic system state. Its recursive nature avoids the data storage burden of traditional batch processing methods and is particularly suitable for online estimation scenarios. The core objective of the Kalman filter algorithm is to minimize the mean square value of the a posteriori state error through recursive estimation, i.e., the optimization objective can be transformed into minimizing the trace of the a posteriori estimation covariance matrix  $P_{k|k}$ . Based on this, the optimal Kalman gain at step  $k$  can be derived as

$$K_k = \frac{P_{k|k-1}H_k^T}{H_k P_{k|k-1}H_k^T + R_k} \quad (5)$$

Where  $P_{k|k-1}$  is the a priori covariance matrix,  $H_k$  is the observation matrix and  $R_k$  is the observation noise covariance matrix. The algorithm is divided into two phases: a priori estimation and updating. In the a priori estimation phase, the state estimates and covariance matrices are predicted by the following equations:

$$\hat{X}_{k|k-1} = F_k \hat{X}_{k-1|k-1} + B_k u_k + w_k \quad (6)$$

$$P_{k|k-1} = F_k P_{k-1|k-1} F_k^T + Q_k \quad (7)$$

Where  $\hat{X}_{k-1|k-1}$  is the optimal state estimation at step  $k-1$ ,  $F_k$  is the state transfer matrix,  $B_k$  is the control matrix,  $u_k$  is the control quantity,  $w_k \sim N(0, Q_k)$  is the process noise, and  $Q_k$  is its covariance matrix. In the update stage, the actual observations  $z_k$  are used to correct the predictions:

$$\hat{X}_{k|k} = \hat{X}_{k|k-1} + K_k (z_k - H_k \hat{X}_{k|k-1}) \quad (8)$$

$$P_{k|k} = (I - K_k H_k) P_{k|k-1} \quad (9)$$

Where  $\hat{X}_{k|k}$  is the optimal state estimate at step  $k$  and  $P_{k|k}$  is the updated covariance matrix. Figure 1 shows the flowchart of the Kalman filtering algorithm.

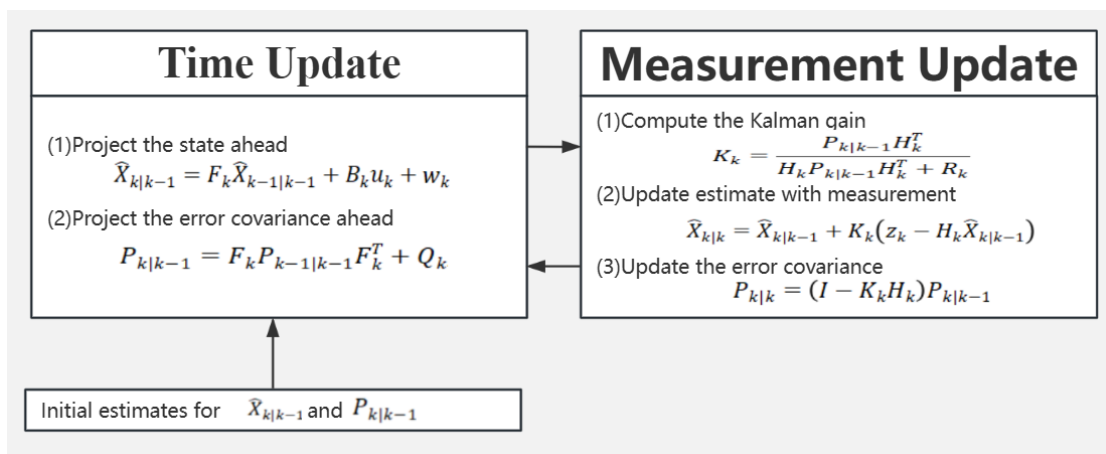


Figure 1. Kalman filter algorithm flow

### 3. Data analysis

#### 3.1. Data sources and experimental setups

The dataset used for this experiment was obtained from <http://lib.stat.cmu.edu/datasets/tecator>. It was obtained from the Tecator Infratec food and feed analyzer, collected by near infrared transmission

(NIT) technology in the wavelength range of 850-1050 nm. The data contained 240 meat samples, where the functional data consisted of 100-channel NIR absorbance spectra (i.e., predictor variables), with absorbance defined as the negative logarithm of the transmittance (. Scalar-type data moisture, fat and protein content (response variables) determined by chemical analysis. In this paper, only protein content was studied. The second dataset was obtained from the website <http://www.eigenvector.com/data/Corn/index.html>. This dataset included a total of 80 corn samples with three sensors, each sensor measurement covering the band range of 1100-2498 nm respectively, at 2 nm intervals collection, and 700 absorbance data points. A total of 700 function-type data (i.e., predictor variables) from one sensor in the near-infrared spectral data based on maize samples, as well as scalar-type data (response variables) of four physicochemical indices, namely, oil, moisture, protein, and starch, were investigated. To capture the continuous nature of the spectral data, functional data analysis was used to smooth and base-expand the discrete spectra, map the spectral band ranges to the standardized intervals  $t \in [0,1]$ , Fourier bases were selected to generate basis functions to convert the raw spectral data into continuous functional objects to eliminate measurement noise and retain the overall morphological characteristics of the spectral curves. Principal component analysis was performed on the functional data to reduce the dimensionality of the data and extract the key spectral modes, and a low-dimensional feature matrix was generated based on the first 10 principal components according to the cumulative variance contribution. In order to realize the nonlinear modeling of spectral data, a multikernel Gaussian process regression additive model is used, and eight kinds of kernel functions are selected to form a collection, including the radial basis kernel (RBF), the Matern kernel (with different smoothing parameters), the periodic kernel (ExpSineSquared), the linear kernel (DotProduct) and its composite form, forming multiple submodels to be trained in parallel. Each model outputs the predicted mean and standard deviation for the test samples, and constructs an ensemble of prediction distributions to quantify the uncertainty of single-model prediction. To address the heterogeneity and uncertainty of the multi-model prediction results, a dynamic fusion strategy based on Kalman filtering is used, in which the predicted mean and variance of each model are regarded as a sequence of time-ordered observations, which are sequentially input into the Kalman filtering framework. Based on the fusion result of the previous model, the a priori estimate of the current state is computed combining the observations and confidence level of the current model, and the Kalman gain is adaptively adjusted to update the a posteriori mean and covariance. Iteratively fusing all model predictions, the final output a posteriori mean is used as the optimized prediction. In order to validate the effectiveness of Kalman filter-based multikernel Gaussian process fusion model (Kalman-FMGPR), this study designs multiple sets of comparative experiments covering the following: Kalman-FMGPR (the method of this study); traditional machine learning models: XGBoost, Random Forest, Support Vector Regression (SVR), ElasticNet Network (ElasticNet); single-kernel Gaussian Process Regression (GPR): the RBF kernel function is used; the dataset is randomly divided into the training set and the test set in the ratio of 4:6 (test\_size=0.4); the experiments are repeated for 10 times independently to eliminate the effect of randomness, and the results are taken as the mean and standard deviation. Besides, this experiment also reduces the function type data to high dimensional data for direct modeling. Before performing the experiment, the data need to be smoothed.

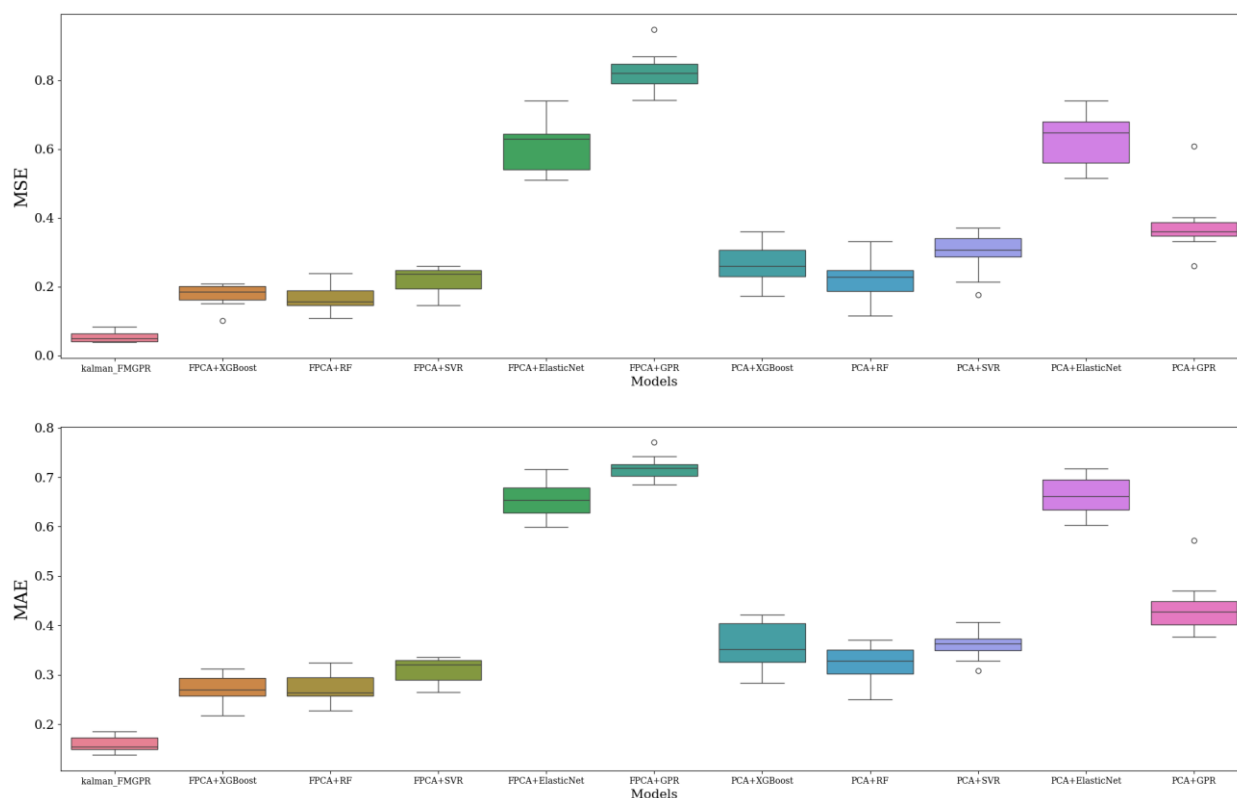
### 3.2. Analysis of experimental results

After On the meat dataset, using protein as the response variable, this paper compares a number of models based on different combinations of feature extraction and modeling methods based on two metrics, Mean Squared Error (MSE) and Mean Absolute Error (MAE). The data results are shown in Table 2.

**Table 2.** Comparison of model prediction errors based on the meat dataset

Model name	mean square error	absolute error
Kalman-FMGPR	0.0545	0.1585
FPCA+XGBoost	0.1769	0.2706
FPCA+RF	0.1657	0.2727
FPCA+SVR	0.2206	0.3100
FPCA+ElasticNet	0.6089	0.6527
FPCA+GPR	0.8256	0.7187
PCA+XGBoost	0.2638	0.3582
PCA+RF	0.2207	0.3229
PCA+SVR	0.2963	0.3603
PCA+ElasticNet	0.6283	0.6643
PCA+GPR	0.3780	0.4355

Figure 2 presents the distribution of box-and-line plots for each model on the two indicator dimensions.



**Figure 2.** Model prediction error boxplot based on meat dataset

In terms of overall performance, the model constructed based on the FPCA feature extraction method is overall better than the model based on the traditional PCA. The Kalman-FMGPR model significantly outperforms the rest of the models in both evaluation metrics, showing the smallest error value and the most stable prediction performance. Specifically, the model is at the lowest level in both MSE and MAE dimensions, and the box-and-line plot has a compact distribution with no obvious outliers, indicating good stability and robustness. This result verifies the effectiveness of the model in the synergistic optimization of feature extraction and nonparametric regression modeling, highlighting its role in predicting meat proteins under the scenario. Among them, the three combined models, FPCA+XGBoost, FPCA+RF and FPCA+SVR, follow Kalman-FMGPR in terms of MSE and MAE, demonstrating low error values and relatively stable prediction ability. In contrast, FPCA+ElasticNet and FPCA+GPR perform poorly in both metrics, with higher errors and less stability, and suffer from a lack of adaptability. Especially in PCA+ElasticNet with PCA+GPR, the

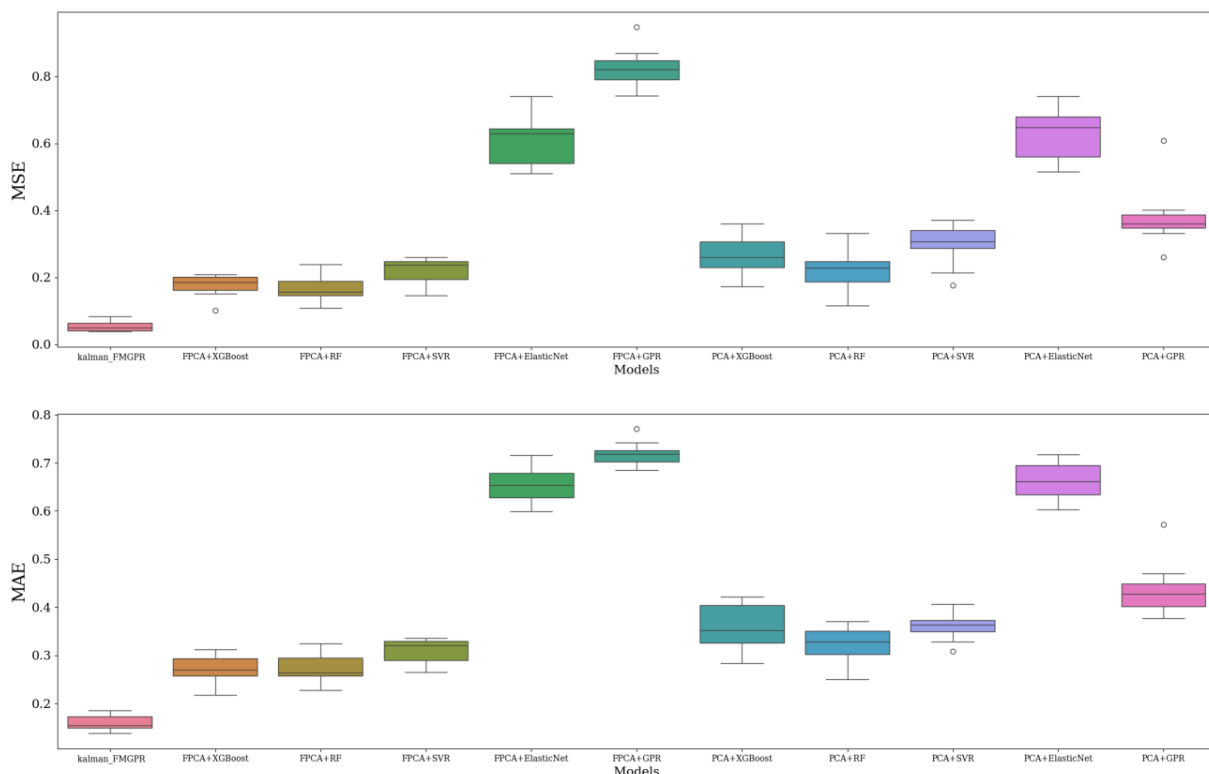
error metrics are significantly high, further indicating that FPCA is more advantageous in retaining critical information in functional data structures. In summary, the Kalman-FMGPR model performs optimally among all the participating models, with smaller error, higher stability, and stronger generalization ability.

In order to evaluate the performance of various modeling approaches in the task of predicting maize protein content in the maize dataset, this paper compares and analyzes ten different sets of model combinations, using the mean square error (MSE) and the mean absolute error (MAE) as evaluation metrics. The data results are shown in Table 3.

**Table 3.** Comparison of model prediction errors based on corn dataset

Model name	MSE	MAE
Kalman-FMGPR	0.1547	0.2936
FPCA+XGBoost	0.3153	0.4445
FPCA+RF	0.2860	0.4076
FPCA+SVR	0.3277	0.4469
FPCA+ElasticNet	0.6899	0.6618
FPCA+GPR	0.9218	0.7823
PCA+XGBoost	0.4775	0.5401
PCA+RF	0.4055	0.4928
PCA+SVR	0.2644	0.4013
PCA+ElasticNet	0.6899	0.6618
PCA+GPR	0.9218	0.7823

Figure 3 presents the distribution of box-and-line plots for each model on the two indicator dimensions.



**Figure 3.** Box line plot of model prediction error based on meat dataset

Overall, the Kalman-FMGPR model has the most superior performance among all the participating models, as it achieves the lowest values in both MSE and MAE, and the error level is significantly lower than that of other models. Meanwhile, the boxplot of this model has a small fluctuation range and almost no outliers, showing high stability and robustness. The above performance indicates that

the Kalman-FMGPR model possesses excellent fitting accuracy and generalization ability in dealing with the problem of maize protein content prediction. The comparison reveals that the overall performance of the model with FPCA feature extraction strategy is better than that of the model based on traditional PCA. In particular, FPCA+XGBoost, FPCA+RF, and FPCA+SVR maintain low errors in MSE and MAE, which is the second best performance, and the prediction results are more stable. This indicates that FPCA can capture the functional change features in the data more effectively, thus providing a more discriminative feature space for regression modeling. On the other hand, FPCA+ElasticNet and FPCA+GPR perform poorly, with large errors in both metrics and poor stability, suggesting that their modeling approaches have limited adaptability under the current feature structure. The overall prediction errors of the models with traditional PCA combinations are generally high, especially PCA+ElasticNet and PCA+GPR, which are at a disadvantage in both MSE and MAE, which confirms that the advantages of FPCA are more obvious in this kind of high-dimensional and structurally complex data. In summary, the Kalman-FMGPR model shows optimal comprehensive performance in the protein content prediction task, which not only has significant advantages in error control, but also excels in model stability and generalization ability.

On both datasets, FPCA+GPR performs the worst, but when looking at the data as high dimensional data data, i.e., the PCA+GPR model performs relatively well, which suggests that when a single kernel is taken, it is difficult for GPR to adapt to the data structure and continuity, and moreover illustrates the necessity of combining kernel functions.

#### 4. Conclusion

In this paper, we focus on the complex data scenario in which the response variable is scalar and the predictor variable is functional, and innovatively construct a Kalman filter-based functional multikernel Gaussian process additivity model to address the uncertainty measure of the response variable and the difficulty of selecting the kernel function of the Gaussian process. In practical applications such as meat and corn datasets analyzed by near-infrared spectroscopy, this kind of functional data is common, and it is difficult for traditional regression methods to accurately capture the characteristics of the data, and this model is committed to achieving high-precision prediction of physical and chemical indicators.

In the process of model construction, functional principal component analysis (FPCA) is firstly used to deal with the function-based predictor variables. Approximating and reconstructing the original discrete observation data through basis function expansion not only eliminates the measurement noise effectively, but also ensures the continuity of the function. Specifically, the mean of the function is calculated to achieve data centering, and then the principal components are extracted by solving the Fredholm integral equation, and the principal component scores are used as the input variables of the additive model to complete the feature extraction and dimensionality reduction of the data. When constructing the functional additive model, each additive component is regarded as an independent Gaussian process with zero mean value, and multiple functional Gaussian process regression additive sub-models are constructed based on different kernel functions to fully explore the nonlinear features of the data. Finally, the prediction results (mean and variance) of the sub-models are fused using Kalman filtering algorithm to realize the efficient integration of the models, so as to output the accurate prediction results containing uncertainty measures.

From the perspective of application expansion, the model can be extended to more fields in the future, such as biomedicine, industrial testing, environmental science and so on. In biomedicine, it is used to analyze protein structure data and dynamic change curves of disease markers. The use of electroencephalography (EEG) signal analysis allows for real-life brainwave monitoring of epileptic patients and seizure prediction based on it.; in the field of industrial testing, it helps to diagnose abnormalities in the monitoring data of the operating status of equipment. In performing aircraft engine vibration monitoring and fault prediction, early warning of aero-engine blade cracks can be achieved through the vibration acceleration curves collected by multiple sensors.; and in



environmental science, it is used to deal with the long-term trend prediction of meteorological data and water quality monitoring data. The effectiveness and adaptability of the model is further verified through practical application in different scenarios.

At the level of model optimization, parameter selection and kernel function optimization need to be studied in depth. Different combinations of parameter settings and kernel functions can significantly affect the model performance, and the optimal parameter combinations can be explored through intelligent optimization algorithms such as Bayesian optimization and genetic algorithms; at the same time, new types of kernel functions can be designed by combining the data characteristics or adopting a multi-core fusion strategy in order to enhance the model's ability to fit the complex data. By systematically optimizing the key factors, the prediction accuracy, stability and generalization ability of the model can be improved, so that it can have stronger reliability in the complex data environment and provide more solid technical support for practical applications.

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