A Novel PM_{2.5} Concentrations Probability Density Prediction Model Combines The Least Absolute Shrinkage And Selection Operator With Quantile Regression

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1 **A novel PM2.5 concentrations probability density prediction model combines the least absolute**
2 **shrinkage and selection operator with quantile regression**

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9 **Abstract:** PM2.5 has a significant negative impact on human health and atmospheric quality, and
10 accurate prediction of its concentration is necessary. PM2.5 concentration is influenced by a
11 combination of factors from both meteorological conditions and air quality. It is essential to identify the
12 significant factors influencing PM2.5 concentrations in the prediction process. To address this issue,
13 this paper proposes the quantile regression (QR) model based on the least absolute shrinkage and
14 selection operator (LASSO), combined with kernel density estimation (KDE) for probabilistic density
15 prediction of PM2.5 concentrations. The model uses LASSO regression to select the influential factors,
16 and then the quartiles of daily PM2.5 concentrations obtained using the QR model are imported into the
17 KDE model to obtain the probability density curves of PM2.5 concentrations. In this paper, empirical
18 analysis is performed with the data sets of Beijing, China, and Jinan, China, and the accuracy of the
19 model is evaluated using the mean absolute percentage error (MAPE) and the relative mean square error
20 (RMSE). The simulation results reveal that the LASSO-QR-KDE model has a higher accuracy than
21 the traditional prediction models and the currently used research models. The model provides a novel
22 and excellent tool for policy makers to predict PM2.5 concentrations.

23 **Keywords:** PM2.5 concentration prediction; probability density prediction; the least absolute

24 shrinkage and selection operator; quantile regression; Air pollution; Hybrid models

25 **1. Introduction**

26 PM2.5 refers to the particulate matter in the ambient air with an aerodynamic equivalent diameter
27 less than or equal to 2.5 microns, which has a small particle size and can be used as a carrier of toxic
28 substances. These fine particles can be inhaled into the human body through the respiratory system and
29 adhere to the upper and lower respiratory tracts and lung lobes, causing damage to the nervous system,
30 cardiovascular and cerebrovascular systems, and respiratory systems. People who have been exposed to
31 fine particulate pollution for a long time are more likely to face cardiovascular and respiratory diseases
32 (Geng et al. 2015; Lee et al. 2017; Mukhopadhyay and Sahu 2018). At the same time, PM2.5 pollution
33 has a negative impact on the normal development of agriculture, industry, and cultural tourism. It will
34 also affect traffic order and cause major economic losses. By predicting the concentration of PM2.5 and
35 accurately forecasting it, it is possible to issue early warnings for heavily polluted weather in order to
36 take targeted protective measures. Therefore, in order to maintain the order of production activities,
37 reduce public health risks, and provide meaningful reference for relevant policy makers, the prediction
38 of PM2.5 concentration is of great significance.

39 Currently, prediction models for air pollutant concentrations such as PM2.5 can be divided into
40 three main categories: deterministic models, classical statistical models, and machine learning models
41 (Jiang and Qiao 2021). Deterministic methods mainly include weather research forecasting model
42 (WRF) (Cao et al. 2018), community multiscale air quality model (CMAQ) (Yang et al. 2019), and
43 coupled WRF-CMAQ meteorological-chemical model (Syraikov et al. 2016). The above methods use
44 relevant meteorological data and pollutant source data to simulate the process of pollutants from

emission to accumulation to dispersion and transfer, so as to predict and analyze the concentration of pollutants. According to Lightstone et al. (2017), such methods are more complex and do not have a significant advantage in prediction accuracy over other models. At the level of statistical models, autoregressive integrated moving average model (ARIMA) and multiple linear regression model (MLR) are more used among scholars in the problem of PM_{2.5} concentration prediction (Zhang et al. 2018). However, the concentration of PM_{2.5} is affected by a variety of variable factors and has strong nonlinearity and complexity. Statistical models are not satisfactory in processing nonlinear time series data. Machine learning has the advantage of covering knowledge of probability theory, statistics, approximate theory and knowledge of complex algorithms, and can simulate the way of human learning. Machine learning has superior predictive performance and is widely used in air pollutant concentration prediction. At the same time, the hybrid model is also widely used in the prediction of the concentration of air pollutants such as PM_{2.5}. Huang and Kuo (2018) combined convolutional neural network (CNN) and long short-term memory (LSTM) and applied it to the PM_{2.5} prediction system. This method effectively improved the prediction accuracy of the LSTM model. Huang et al. (2021) used empirical mode decomposition (EMD) to decompose the PM_{2.5} concentration series. They input the multiple stationary sub-sequences and meteorological features obtained after decomposition into the constructed gated recurrent unit neural network (GRU) in order to train and predict them. The results showed that the accuracy of the EMD-GRU model is much higher than that of the single GRU model. Li et al. (2017) introduced the co-integration theory in order to solve the problem of the lack of evaluation of the possible correlation between different variables in the current research. He used the Flower Pollination Algorithm (FPA) to optimize the parameters of the Support Vector Machine (SVM) model, and made high-precision predictions of the PM_{2.5} and PM₁₀ concentrations in two important

cities in Yunnan Province, China.

The concentration of PM_{2.5} is affected by many factors, not only related to meteorological factors, but also closely related to economic development mode, industrial structure, and energy efficiency. In the big data environment, related data sources are extensive and the characteristics are different, making the prediction of PM_{2.5} concentration more complicated. Reviewing the existing literature related to the prediction of PM_{2.5} and other air pollutant concentrations, it is found that most of the prediction methods obtain deterministic point prediction results, which can hardly reflect the uncertainty of their fluctuations. To solve the above problems, a probability density prediction method for PM_{2.5} concentration can be used to overcome the shortcomings of the traditional point prediction and interval prediction methods. In this way, the future PM_{2.5} concentration values and the concentration fluctuation intervals under the corresponding confidence intervals can be obtained, and the probability of occurrence of each point within the interval can also be visualized. With the probability density function of the predicted PM_{2.5} concentration, more detailed and effective information can be obtained than the traditional prediction methods. It is extremely helpful for the accurate prediction of PM_{2.5} concentration.

However, due to the complexity and variability of factors affecting PM_{2.5} concentration, the probability density function that accurately portrays the uncertainty of PM_{2.5} concentration is difficult to obtain. Therefore, in order to predict PM_{2.5} concentration more accurately, valuable information needs to be extracted from the wide range of influencing factors first, so as to filter out the influencing factors that have significant explanatory significance on PM_{2.5} concentration. The traditional classical method of variable selection is mainly represented by the subset selection method. This method compared $2^p - 1$ non-empty subsets of all p -dimensional variables with a certain criterion to find the

optimal subset. Here the most representative selection criteria are mainly the Akaike information criterion (AIC) based on information theory proposed by Hirotugu Akaike in 1974 (Hoerl and Kennard 2000), the BIC criterion based on Bayes' method proposed by Schwarz (1978), and the cross-validation criterion. But for the information age where high-dimensional data are proliferating in various fields, the complexity and high cost of computation make the traditional variable selection methods no longer applicable to these high-dimensional data structures. Therefore, statisticians have started to focus on variable selection methods for high-dimensional data. In the field of variable selection for high-dimensional data, Tibshirani's 1996 proposal of the LASSO algorithm (Least Absolute Shrinkage and Selection Operator) under the ordinary linear model was of epoch-making significance (Tibshirani 1996). It was inspired by two algorithms, ridge Regression (Hoerl and Kennard 2000) and Nonnegative Garrote (Breiman 1995).

LASSO was essentially a coefficient compression method that compressed the coefficients of non-significantly influential variables to zero, achieving both variable selection and parameter estimation at the same time. This method can be seen as an improvement of ridge regression, but it is milder in compressing the coefficients of significant variables with significant effects, thus ensuring the accuracy of parameter estimation. In a previous study, Koen et al. (2021) used a LASSO regression model to select variables closely related to four common chronic diseases in the Netherlands to predict disease prevalence. The results showed that the use of the LASSO algorithm significantly improved the predictive performance of the model. Jasleen and Mamta (2021) used a correlation-based adaptive LASSO algorithm to identify potentially important influences while studying pollutant concentrations and meteorological factors in Delhi and its surrounding cities. Evaluation of the model revealed better performance of this approach in extracting subset of features. In an empirical study, Li et al. (2021)

found that real surplus management (REM) was strongly selected as a key crisis predictor by the LASSO algorithm, developing an updated distress forecasting model with surplus management considerations for the Chinese market. In addition, the method has been applied to the variable selection process of quantile regression models.

Quantile regression was first proposed by Koenker and Bassett (1978). Due to its unique explanatory power, it has become one of the key tools for data analysis and is widely used in various data analysis fields (Koenker 2015). Quantile regression can give a more comprehensive picture of the conditional distribution of the explanatory variables. Instead of analyzing only the conditional expectation (mean) of the explanatory variable, the method can also analyze how the explanatory variables affect the median, quantile, etc. of the explanatory variable. Kang et al. (2021) used quantile regression to study the impact of macroprudential policies on the level of bank financing of Chinese firms, and pointed out that the intensity of the impact of macroprudential policies was different at different quantile points. salari et al. (2021) combined the idea of quantile regression in the study of the impact of multiple factors on the ecological footprint of emerging countries, and discussed the significant impact of different quantile factors. Sun et al. (2021) used quantile autoregressive models to analyze return and volatility series on multiple time scales using the crude oil market as an example. It was found that the autoregressive coefficients vary with quantile. The above study further demonstrates the advantages of quantile regression. Namely, the method can explain the effect of each input variable on the corresponding variable at different quartiles and obtain a more detailed relationship between the input and response variables.

The approach of combining the LASSO algorithm with quantile regression has been applied to the power, financial, and medical sectors. he et al. (2019) predicted electricity consumption based on

LASSO-quantile regression for Guangdong Province, China, and California, USA. Simulation results showed that the method provided better performance for electricity consumption forecasting. Cao et al. (2021) studied the optimal portfolio problem based on the LASSO-quantile regression method and showed that the results obtained by this method were close to the given value at risk under certain canonical conditions, demonstrating the robustness and effectiveness of this method. Taha et al. (2018) reduced the data dimensionality by LASSO and used quantile regression method to study and analyze the prostate cancer dataset. The results validated the superiority of this combined method.

There are no studies that have applied LASSO quantile regression to air pollutant concentration prediction. In this paper, the LASSO-QR-KDE model is proposed to combine LASSO quantile regression with kernel density estimation. Firstly, this paper will apply the LASSO variable selection method to extract the factors that have significant effects on PM_{2.5} concentrations from the high-dimensional external influences data to obtain a lower dimensional data set. Subsequently, the quantile regression model is combined with the quantile regression method to obtain the conditional quantile of PM_{2.5} concentrations at different quantile points. Finally, the kernel density estimation method was employed to obtain the probability density prediction curves of PM_{2.5} concentrations on any consecutive day in the future month.

The main innovations and contributions of this paper can be divided into the following two aspects:

(1) The LASSO-QR-KDE model proposed in the paper reduces the uncertainty of the prediction by downscaling the influencing factors of PM_{2.5} concentration and selecting the factors that have a significant influence on it. Moreover, it is able to obtain different probability distributions of PM_{2.5}

concentrations at different quantile points and further obtain probability density curves. Compared with the common point prediction, the probability density prediction expands the prediction range and provides a more detailed and informative explanation for the prediction of PM_{2.5} concentrations.

(2) This paper demonstrates the superiority of the method through experiments on two real data sets in Beijing and Jinan, China. Three different scenarios are investigated and compared in this paper: without considering external factors, considering external factors without variable selection, and using the LASSO algorithm to filter external factors. The results show that the proposed LASSO-QR-KDE model has superior performance, and its MAPE and RMSE are both taken to the minimum value. Moreover, when comparing five models commonly used to predict PM_{2.5} concentrations, namely ARIMA, BP, RBF, CNN-LSTM and EMD-GRU, the LASSO-QR-KDE model was found to achieve higher accuracy.

The rest of the paper is organized as follows: the second part describes the theoretical basis and methodology involved in the model proposed in the paper. The third part presents the constructed neural network model and its evaluation criteria. The fourth part gives an empirical analysis and discussion of the two cases and shows how the data are handled. Finally, the conclusions of the paper are given in the fifth part.

2.Methodology

2.1 LASSO method

The LASSO method adds a penalty term to optimize the traditional objective function to produce a sparse solution. The method avoids the problem of overfitting caused by excessive explanatory variables (He et al. 2021). It proceeds by extracting the key variables from the high-dimensional

variables. The method is effectively solving the problem of multicollinearity among variables and improving the explanatory accuracy of the model, which is highly evaluated and widely used. In addition, compared with ridge regression, the Lasso method can directly compress the regression coefficients of redundant predictor variables to zero, obtaining a more streamlined set of predictor variables. Over-compression of important regression coefficients can also be avoided.

Given a matrix of independent variables $X = (x_1, x_2, \dots, x_n)$, where $X_j = (x_{1j}, x_{2j}, \dots, x_{mj})^T$, $j = 1, 2, \dots, n$, the dependent variable $Y = (y_1, y_2, \dots, y_m)^T$. It is assumed that the data have been standardized, $\sum_{i=1}^m x_{ij} = 0$, $\sum_{i=1}^m x_{ij}^2 = 1$, $\sum_{i=1}^m y_i = 0$, then the linear model between Y and X is established as Eq. (1).

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n + \varepsilon \quad (1)$$

where β_0 is the constant term, β_i is the coefficient of each variable, and ε is the random disturbance term.

Suppose $\beta = (\beta_1, \beta_2, \dots, \beta_n)^T$, then the LASSO estimation of β is as in Eq. (2).

$$\hat{\beta}^{LASSO} = \operatorname{argmin} \sum_{i=1}^m \left(y_i - \beta_0 - \sum_{j=1}^n x_{ij} \beta_j \right)^2$$

$$s. t. \quad \sum_{j=1}^n |\beta_j| \leq \lambda \quad (2)$$

where the penalty parameter is λ and $\lambda \geq 0$. If $\hat{\beta}^0$ is the least squares estimation of β_j , then $\lambda_0 = \sum_{j=1}^n |\hat{\beta}^0|$. When $\lambda < \lambda_0$, the absolute value of the LASSO estimation of the regression coefficient β_j in the model is smaller than the absolute value of $\hat{\beta}^0$. As λ decreases gradually, the LASSO estimation of certain β_j decreases or even goes to zero. The variable can be eliminated if its estimation is zero, which indicates that it has little association with the dependent variable Y , and thus

the variable selection function can be achieved. The commonly used estimation and testing methods regarding the penalty parameter λ are the cross-validation criterion, the generalized validation method, and the AIC (Hoerl and Kennard 2000).

For the solution of the LASSO problem, the least angle regression (LARS) significantly enhances the computational efficiency of LASSO. Suppose $A = \{j_1, j_2, \dots, j_k\} \subseteq \{1, 2, \dots, n\}$ is the indicator set, and define the matrix of $m \times k$ as $X_A = (\lambda_{j_1} x_{j_1}, \lambda_{j_2} x_{j_2}, \dots, \lambda_{j_k} x_{j_k})$, where the value of λ can be determined by Eq. (3).

$$\lambda_{jl} \begin{cases} 1, & x_{jl} \text{ is positively correlated with } Y \\ 0, & x_{jl} \text{ is not correlated with } Y \\ -1, & x_{jl} \text{ is negatively correlated with } Y \end{cases} \quad (3)$$

Subsequently, suppose that $G_A = X_A' X_A$ and $A_A = (I_A' G_A^{-1} I_A)^{-\frac{1}{2}}$, $u_A = X_A w_A$ is the angular component vector in X_A , $w_A = A_A G_A^{-1} I_A$, where I_A is a K-dimensional column vector and all elements are equal to 1. It can be shown that the angular component vector u_A is a unit vector and $X_A' u_A = A_A I_A$.

Establish the LARS estimation as $\hat{\mu} = X \hat{\beta}$. Assuming that the current estimate is $\hat{\mu}_A$, $\hat{e} = X'(Y - u_A)$ indicates that the respective variable is currently correlated with Y . From the previous assumptions, the variables in A are maximally correlated with Y , and the relationship can be expressed by Eq. (4).

$$\begin{cases} |\hat{e}_j| = \widehat{C}, j \in A \\ |\hat{e}_j| < \widehat{C}, j \notin A \end{cases} \quad (4)$$

where $\widehat{C} = \max_j \{|\hat{e}_j|\}$.

(1) Calculate the value of $\widehat{C}$.

(2) Calculate X_A , A_A , u_A by taking $\lambda_j = \text{sign}\{\hat{e}_j\}$ ($j \in A$).

(3) Calculate $a = X'u_A$, with X being the full matrix of independent variables.

(4) Calculate $\hat{\mu}_{A+} = u_A + \hat{\gamma}u_A$, where $\hat{\gamma} = \min_{j \notin A}^+ \left\{ \frac{\bar{c} - \hat{c}_j}{A_A - a_j} + \frac{c + c_j}{A_A + a_j} \right\}$. $\min^+$ means that only the

smallest positive value in the set is selected for calculation.

(4) Set $\hat{\mu}_A = u_{A+}$, and then returns to step (1) to continue the loop until all the independent

variables are used for the operation.

2.2 Quantile regression

Quantile regression is a linear model that describes the relationship between the explanatory variable X and the conditional quantile of the response variable Y . The formula is given in Eq.(5).:

$$Q(\tau|X) = \alpha_0(\tau) + \alpha_1(\tau)X_1 + \alpha_2(\tau)X_2 + \cdots + \alpha_m(\tau)X_m = X'\alpha(\tau) \quad (5)$$

where $Q(\tau|X)$ is the estimate of the response variable Y corresponding to the explanatory variable $X = [X_1, X_2, \cdots, X_m]$ under the τ th quantile condition. $\alpha(\tau) = [\alpha_0(\tau), \alpha_1(\tau), \cdots, \alpha_m(\tau)]^T$ is the model parameter associated with the quantile τ , which is estimated and solved by Eq. (6).

$$\begin{aligned} & \min \sum_{i=1}^N \rho_{\tau}(Y_i - X_i\alpha(\tau)) \\ & = \min \left[\sum_{i|Y_i \geq X_i\alpha(\tau)} \tau(Y_i - X_i\alpha(\tau)) + \sum_{i|Y_i < X_i\alpha(\tau)} (\tau - 1)(Y_i - X_i\alpha(\tau)) \right] \end{aligned} \quad (6)$$

where N is the number of samples and $\rho_{\tau}(\cdot)$ is the loss function of the model, which is expressed as in Eq. (7)

$$\rho_{\tau}(u) = \begin{cases} \tau u, & u \geq 0 \\ (\tau - 1)u, & u < 0 \end{cases} \quad (7)$$

After the obtained estimate of $\alpha(\tau)$, the estimate of the response variable at the τ th quantile can be solved according to Eq. (5).

2.3 Kernel density estimation

The solution of the density function of a random variable can be solved by parametric estimation methods and nonparametric estimation methods. However, the parametric estimation method requires prior estimation of the density function form of the random variable, which often leads to a large discrepancy between the actual density function and the estimated density function.

The kernel density estimation (KDE) method can overcome the drawbacks of the parameter estimation methods. KDE is used in probability theory to estimate unknown density functions and was proposed by Rosenblatt and Emanuel Parzen (1991). The method enables to employ a set of random variables from the same unknown distribution function to estimate its density function. KDE has no requirement to know the prior distribution of the data in question or to make any assumptions about the data in question. The method requires only input variables, kernel density estimation function and optimal bandwidth to perform the predictions.

$f(x)$ is the density function of the random variable x , $f(x) = F'(x)$. According to the principle of KDE, a simple estimate of $f(x)$ can be obtained as in Eq. (8).

$$f(x) = \frac{F(x+k) - F(x-k)}{2k} \quad (8)$$

where k is a non-negative series of constants and $F(x)$ is the sample distribution function of the random variable x . $x_1, x_2, \dots, x_n$ are n sample points of an independent identically distributed one-dimensional continuous overall sample. Its probability density function is $f(x)$ and the kernel density estimate is as in Eq. (9).

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^n K_h(x - x_i) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - x_i}{h}\right) \quad (9)$$

where $K(\cdot)$ is the kernel function, which is essentially the weight function. h is called the bandwidth, and its choice determines the smoothness and accuracy of the estimated density function.

3. LASSO-QR-KDE model

3.1 Quantile regression model based on LASSO

The precision of PM2.5 concentration prediction is influenced by various external factors, and the impact of different factors on the prediction results varies in degrees. According to the description of quantile regression and the LASSO method in the previous section, the quantile regression model is constructed as Eq. (10).

$$Y_t = r(\tau) + \sum_{c=1}^p \alpha_c(\tau) Y_{t-c} + \sum_{d=1}^m \left(\sum_{j=1}^q \beta_j^d(\tau) X_{t-j}^d \right) + \varepsilon_t \quad (10)$$

where Y_t is the prediction series and X_t is the sequence of influencing factors. m indicates the number of influencing factors and c indicates the maximum number of lags of the prediction series, $c = 1, 2, \dots, p$. τ is the quantile, $\tau \in (0, 1)$. The regression coefficient vector for the prediction target of the τ th quantile is $\alpha_c(\tau)$, and the regression coefficient vector for the τ th quantile is $\beta_j^d(\tau)$, $d = 1, 2, \dots, m$. q indicates the maximum number of lags of the influence factor. $r(\tau)$ is the intercept term and ε_t is the error term. The predicted value of PM2.5 concentration y_t at the τ th quantile can be further obtained, which is calculated as Eq. (11)

$$Q_{Y_t}(\tau | Y_t, X_t) = r(\tau) + \sum_{c=1}^p \alpha_c(\tau) Y_{t-c} + \sum_{d=1}^m \left(\sum_{j=1}^q \beta_j^d(\tau) X_{t-j}^d \right) \quad (11)$$

According to Eqs. (10) and (11), it can be observed that there is heterogeneity in $r(\tau)$, $\alpha_c(\tau)$, and $\beta_j^d(\tau)$, which indicates the discrepancy in the importance of the studied samples. This reflects the impact of the selected influence factors on the PM2.5 concentration prediction results under different

quantile points. The parameters $\alpha_c(\tau)$ and $\beta_j^d(\tau)$ in Eq. (11) can be solved by Eq. (12).

$$\min \sum_{t=1}^n \rho_\tau(Y_t - r(\tau) - \sum_{c=1}^p \alpha_c(\tau) Y_{t-c} - \sum_{d=1}^m (\sum_{j=1}^q \beta_j^d(\tau) X_{t-j}^d)) \quad (12)$$

where $\rho_\tau(u)$ is the check function with the following Eq. (13).

$$\rho_\tau(u) = (\tau - I(u < 0))u \quad (13)$$

$I(u < 0)$ is called the indicator function and $u < 0$ is the conditional relation. When $u < 0$ is true, $I(u < 0) = 1$, and vice versa $I(u < 0) = 0$. To improve the speed of operation, the interior point algorithm is applied to solve the equation (Portnoy and Koenker 1997).

Since the influence of multiple factors on PM2.5 concentration is considered, this paper will apply the LASSO method to filter a large number of influence factors. The penalty parameter L1 is added to the original objective function, and Eq. (14) is obtained as follows.

$$\min \sum_{t=1}^n \rho_\tau \left(Y_t - r(\tau) - \sum_{c=1}^p \alpha_c(\tau) Y_{t-c} - \sum_{d=1}^m \left(\sum_{j=1}^q \beta_j^d(\tau) X_{t-j}^d \right) \right) + \lambda (\|\alpha(\tau)\|_1 + \|\beta(\tau)\|_1) \quad (14)$$

where λ is the penalty parameter and its penalty enhances as the value taken increases. $\|\alpha(\tau)\|_1$ and $\|\beta(\tau)\|_1$ are the 1-norm. $\|\alpha(\tau)\|_1$ is the loss function that measures the effectiveness of the quantile regression model to fit the data. $\|\beta(\tau)\|_1$ is the penalty function, which can be used to achieve variable selection by constraining the insignificant coefficients to zero. To facilitate the solution of the LASSO-QR model, Eq. (14) can be transformed into Eq. (15).

$$\begin{aligned}
& \min \sum_{t=1}^n \rho_{\tau} \left(Y_t - r(\tau) - \sum_{c=1}^p \alpha_c(\tau) Y_{t-c} - \sum_{d=1}^m \left(\sum_{j=1}^q \beta_j^d(\tau) X_{t-j}^d \right) \right) \\
& \text{s. t.} \quad \|\alpha(\tau)\|_1 + \|\beta(\tau)\|_1 < \delta
\end{aligned} \tag{15}$$

where δ is the constraint parameter corresponding to λ . The degree of constraint on the coefficients increases as the value of δ is taken to decrease. The LASSO-QR model is used to demonstrate the distribution of PM2.5 concentrations at different quantiles, and to filter out the influencing factors that are significant to its interpretation. In this way, the effect of reducing the data dimensionality and optimizing the prediction model can be achieved.

3.2 Probability density prediction of PM2.5 concentration

From the above method, the conditional quantile of PM2.5 concentration at different quantile points can be obtained, and each quantile is the prediction result of PM2.5 concentration at different quantile points. The mean square error performance of the Epanechnikov kernel function is optimal and its efficiency loss is small. In this paper, Epanechnikov kernel function is used to predict the PM2.5 concentration at each quantile as its input value, and the prediction result of the probability density of PM2.5 concentration is then obtained. The expression of the Epanechnikov kernel function is as follows.

$$k(x) = \frac{3}{4} (M - x^2) M \quad (|x| \leq 1) \tag{16}$$

where $M(\cdot)$ is an indicative function. When $|x| \leq 1$ is true $M(\cdot)$ takes the value of 1, and vice versa $M(\cdot)$ takes the value of 0.

3.3 LASSO-QR-KDE neural network model

Neural networks employ nonlinear kernel functions that can provide a better way to deal with complex nonlinear objects. In the paper, a quantile regression neural network is used to predict the quantile corresponding to random variables at different quantile levels based on the single hidden layer neural network model proposed by Taylor (Madsen and Nielsen 1993). The hyperbolic tangent Sigmoid function is used as the hidden layer basis function of the neural network in solving the problem utilizing quantile regression neural network. First a stable network structure is established between the input and response variables to achieve the prediction of different quartiles of the predicted object, and then the probability density can be estimated by using the kernel density estimation of nonparametric estimation. The expression of the quantile regression neural network model used in the paper is as follows.

$$Q_Y(\theta|X) = f[x, u(\theta), v(\theta)] = \sum_{j=1}^J \left\{ \frac{2v_j(\theta)}{1 + e^{-2 \sum_{i=1}^n u_{ij}(\theta) X_i}} - v_j(\theta) \right\} \quad (17)$$

where θ is the quantile, $u(\theta) = \{u_{ij}(\theta)\}$ is the weight matrix to be estimated between the input layer and the implied layer, and $V(\theta) = \{v_j(\theta)\}$ is the connection weight vector between the implied layer and the output layer. To achieve the parameter estimation of Eq. (17), which can be achieved by solving the optimization objective function Eq. (18).

$$\bar{E}_\theta = \frac{1}{N} \sum_{i=1}^N \rho_\theta \{Y_i - f[X, U(\theta), V(\theta)]\} \quad (18)$$

To prevent the neural network model from falling into the process-fitting state, the corresponding penalty term is added to the objective function. The new objective function is as follows

$$E_\theta(U(\theta), V(\theta)) = \tilde{E}_\theta + \lambda_1 \sum_{i,j} u_{ij}(\theta) + \lambda_2 \sum_{i,j} v_j(\theta) \quad (19)$$

where λ_1 and λ_2 are the penalty parameters of the model. By determining the optimal penalty parameters, the model can be effectively prevented from over-fitting to the empirical data, which can reduce the prediction error and improve the prediction accuracy. The optimal estimate of $U(\theta)$ and $V(\theta)$ can be obtained by optimizing Eq. (19) after getting the value of $\min_{[U(\theta), V(\theta)]} E_{\theta}(U(\theta), V(\theta))$. Bringing the estimated values into Eq. (17), the conditional quantile estimation function of the response variable can be obtained. The structural flow chart of the model is shown in Fig. 1.

Figure.1. Flow chart of the model

3.4 Evaluation Criteria

For testing the prediction performance of the method in the paper, a comprehensive and reasonable analysis and evaluation of the prediction results is required. In this paper, mean absolute percentage error(MAPE) and relative mean square error (RMSE) are used to evaluate the accuracy of the model. MAPE measures the relative magnitude of the prediction error, while RMSE is more

sensitive to outlier data and can highlight error values with large effects, and the expressions are as follows.

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{A_i - F_i}{A_i} \right| \quad (20)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (A_i - F_i)^2}{n}} \quad (21)$$

where n indicates the number of days of PM2.5 concentration being used for prediction, A_i is the actual value, and F_i is the predicted value. The closer the values of MAPE and RMSE to zero indicates the better model performance.

4. Empirical analysis

4.1 Case 1: Beijing, China

Beijing is located in the north of China and has 12 national automatic air quality monitoring sites. 21 century, Beijing has developed rapidly and made great achievements in industrial construction. However, along with the economic boom, the air quality in Beijing has also been affected, and it is far from the national standard and the expectation of the people, especially the foggy weather makes the whole society pay extra attention to the fine particulate matter PM2.5 pollution which is more difficult to prevent and control. In recent years, Beijing has vigorously promoted clean energy and strengthened environmental supervision, enabling pollutant concentrations to drop significantly. However, the first quarter still has a high PM2.5 concentration, as shown in Fig.2. In order to continuously promote the environmental construction, the prediction of PM2.5 is essential.

In this case, the data were selected from January 1, 2018 to January 31, 2019 for Beijing, China. The data were obtained from the National Meteorological Data Center of China (<http://data.cma.cn/>),

and all data were normalized in advance. From the experience of previous studies, the concentration of PM2.5 is influenced not only by air quality but also by meteorological factors. In this paper, five air quality indicators and five meteorological factor indicators were selected as influencing factors to investigate the implications on PM2.5 concentration prediction.

Fig.2. The PM2.5 concentration in Beijing from 2018 to 2020

According to the previous Eq. (11), the sequence of PM2.5 concentrations to be predicted is $(y_1, y_2, \dots, y_n)$, where n is the number of samples to be predicted. The sequence of influencing factors is X_t and $X_t = (X_t^1, X_t^2, \dots, X_t^m)$, m is taken as 10 in this paper. X_t^d is the d th influencing factor, and $X_t^d = (x_{t-1}^d, x_{t-2}^d, \dots, x_{t-q}^d)$. In this paper, X_t^1 indicates daily PM10 concentration ($\mu\text{g}/\text{m}^3$), X_t^2 indicates daily SO2 concentration ($\mu\text{g}/\text{m}^3$), X_t^3 indicates daily CO concentration (mg/m^3), X_t^4 indicates daily NO2 concentration ($\mu\text{g}/\text{m}^3$), and X_t^5 indicates daily O3 concentration ($\mu\text{g}/\text{m}^3$); X_t^6 indicates daily average temperature (0.1°C), X_t^7 indicates the daily relative humidity (%), X_t^8 indicates the daily average air pressure (0.1hPa), X_t^9 indicates the daily average wind speed (0.1m/s), and X_t^{10} indicates the wind direction of daily maximum wind speed (16 directions). The details of each

influencing factor are shown in Table 1. $Y_t = (y_{t-1}, y_{t-2}, \dots, y_{t-c})$ is used to indicate the historical PM2.5 concentration with lag c period. Both c and q are taken as 4 in the paper.

Data from January 1, 2018 to December 31, 2018 in Beijing were used as training data, and data from January 1, 2019 to January 31, 2019 were used as test data. Through the rolling prediction method, the data of the four days before the prediction day were used as input variables to predict the PM2.5 concentration values on that day. As shown in Table 1, a total of 44 factors are included in the obtained training data.

The LASSO method was applied to the training data for variable filtering, and the LASSO compressed path diagram is shown in Fig. 3. The colored dashed lines indicate the route of the factor selection process, the horizontal coordinates represent the constraint coefficients, and the vertical coordinates represent the regression coefficients. From Appendix A (Table A.1), it can be seen that Lasso proceeds to the 38th step with the smallest cp value, and then the optimal number of steps for Lasso regression is 38. Eight factors with non-zero coefficients were retained, as shown in the part marked with an asterisk in Table 1. The selected factors are those that have significant explanations for PM2.5 concentrations in Beijing. The above output shows that PM2.5 concentration in Beijing is influenced by its historical concentration, SO2 concentration, CO concentration, average temperature, wind speed and wind direction.

Table 1

The statement of influencing factors of PM2.5 concentration in Beijing

Name(Codename)	Lags			
Daily PM2.5 concentration(Y_t)	Y_{t-1}^*	Y_{t-2}	Y_{t-3}	Y_{t-4}
Daily PM10 concentration(X_t^1)	X_{t-1}^1	X_{t-2}^1	X_{t-3}^1	X_{t-4}^1
Daily SO2 concentration(X_t^2)	$X_{t-1}^2^*$	X_{t-2}^2	X_{t-3}^2	X_{t-4}^2
Daily CO concentration(X_t^3)	$X_{t-1}^3^*$	X_{t-2}^3	$X_{t-3}^3^*$	X_{t-4}^3
Daily NO2 concentration(X_t^4)	X_{t-1}^4	X_{t-2}^4	X_{t-3}^4	X_{t-4}^4
Daily O3 concentration(X_t^5)	X_{t-1}^5	X_{t-2}^5	X_{t-3}^5	X_{t-4}^5

Daily average temperature(X_t^6)	X_{t-1}^6	$X_{t-2}^6 *$	$X_{t-3}^6 *$	X_{t-4}^6
Daily relative humidity(X_t^7)	X_{t-1}^7	X_{t-2}^7	X_{t-3}^7	X_{t-4}^7
Daily average air pressure(X_t^8)	X_{t-1}^8	X_{t-2}^8	X_{t-3}^8	X_{t-4}^8
Daily average wind speed(X_t^9)	$X_{t-1}^9 *$	X_{t-2}^9	X_{t-3}^9	X_{t-4}^9
The wind direction of daily maximum wind speed(X_t^{10})	$X_{t-1}^{10} *$	X_{t-2}^{10}	X_{t-3}^{10}	X_{t-4}^{10}

Fig.3. The procedure chart of compressing factors(Beijing)

Three situations are considered in the paper to make the empirical analysis more objective and to verify the validity of the LASSO-QR-KDE method for probability density prediction. They are probability density prediction without considering external factors, probability density prediction with considering external factors but without variable selection, and probability density prediction with applying LASSO for variable selection. After training, the neural network structures for the three cases are shown in Table 2. The number of times the neural network was trained was set to 1000, and the penalty parameters λ_1 and λ_2 in Eq. (19) were set to 0.5. The quartiles range from 0.05 to 0.95 with an interval of 0.05. With the trained neural network model, the continuous quartiles for each day in January 2019 can be obtained. The obtained PM2.5 concentration quantile is then used as an input variable and imported into the Epanechnikov kernel function to obtain the probability density curve of PM2.5 concentration for each day in January 2019.

Table 2

Structure of neural network in three situations(Beijing)

Situation (Codename)	Input layer- Hidden layer- Output layer
without considering external factors (A)	7-3-1
considering external factors without variable selection (B)	53-3-1
LASSO-QR-KDE(C)	10-3-1

Fig. 4, Fig.5, and Fig.6 show the probability density curves of PM2.5 concentrations in Beijing for eight days in January under three scenarios in turn. The horizontal coordinate value corresponding to the red dashed line in the figure indicates the actual PM2.5 concentration in Beijing on that day, while the solid blue line is the probability density curve and the highest point is the mode of the predicted value. The comparison of the three plots shows that the highest probability point (highest point) of the probability density curve often deviates from the actual value when no external factors are considered. On days 1, 17, and 25 in Fig. 4, the actual values appear at the tail of the probability density curve, and the predicted values deviate significantly from the actual values. With external factors taken into account but not selected, the prediction situation improved. According to Figure 5, the prediction value that deviates significantly from the actual value is significantly improved, and only on day 13 the actual value is at the tail of the probability density curve. In the case of using LASSO to select the variables, according to Figure 6, the actual values are basically near the highest probability point of the probability density curve, and there is no case that the actual values are at the tail of the probability density curve. It can be seen that the LASSO-QR-KDE model has a good performance in predicting the probability density of PM2.5 concentration, and the predicted values have a higher probability of being close to the actual values.

Appendix B (Table B.1) gives the predicted values and relative errors of PM2.5 concentrations at the highest point of the probability density curve (mode) for January 2019 in Beijing under three situations. Combining with Fig. 7, it can be seen that the maximum relative errors in the three situations

are 15.64%, 13.29%, and 11.42%, and the minimum relative errors are 0.88%, 0.99%, and 0.08%. The performance of the LASSO-QR-KDE model is significantly better than the other two situations. The results in Table 3 demonstrate that the best prediction results are obtained using the LASSO-QR-KED model, where the MAPE is 2.40% and the RMSE is 1.63. In addition, the probability density prediction considering external factors but without variable selection also performs better than the probability density prediction without considering external factors.

Fig.4. Probability density curve of Beijing without considering external factors

Fig.5. Probability density curve of Beijing considering external factors but without variable selection

Fig.6. Probability density curve of Beijing with LASSO-QR-KDE model

In the prediction of PM2.5 concentrations with quantile regression neural networks, the prediction results using the LASSO-QR-KDE model outperformed the prediction results without considering external factors and without variable selection. This indicates that the probability density prediction of PM2.5 concentration should adequately consider the influence of external environment, and the optimal prediction model can be obtained by filtering multiple external factors.

Fig. 7. Relative error of prediction results for three situations in Beijing (%)

Table 3

Prediction errors for three situations in Beijing

Situation (Codename)	MAPE(%)	RMSE
without considering external factors (A)	6.04	4.11
considering external factors without variable selection (B)	3.41	2.74
LASSO-QR-KDE(C)	2.40	1.63

4.2 Case 2: Jinan, China

Jinan is located in East China and has built 8 national automatic air environment quality

monitoring points. Jinan used to be a heavy industrial production base, and heavy industrial enterprises have made outstanding contributions to the economic development of Jinan. However, the development of heavy industries has brought pollution in various aspects such as air and water. In addition, due to the high topography around Jinan, its air mobility is poor and dust is easily accumulated over the city. According to Fig. 8, it can be seen that its annual PM2.5 concentration has a U-shaped distribution. Accurate prediction of PM2.5 concentrations is essential to promote the local environment and to reduce public health risks.

Fig.8. The PM2.5 concentration in Jinan from 2018 to 2020

In this case, data from January 1, 2020 to January 31, 2021 were selected from the National Meteorological Data Center of China (<http://data.cma.cn/>) for Jinan, China, and all data were pre-normalized. Consistent with Case 1, m is taken as 10 and $c = q = 4$. The data from January 1, 2020 to December 31, 2020 in Jinan were treated as training data and the data from January 1, 2021 to January 31, 2021 were treated as test data using the rolling prediction method. From Appendix A (Table

A.2), it can be seen that the cp value at step 32 is the smallest, and the optimal number of steps for Lasso regression is obtained as 32. The LASSO compression path diagram is shown in Fig. 9. Ten factors were selected, as shown in the variables marked with an asterisk in Table 4. The results show that the PM2.5 concentration in Jinan is influenced by its historical concentration, PM10 concentration, CO concentration, NO2 concentration, O3 concentration, as well as wind speed and wind direction.

Table 4

The statement of influencing factors of PM2.5 concentration in Jinan

Name(Codename)	Lags			
Daily PM2.5 concentration(Y_t)	Y_{t-1}^*	Y_{t-2}	Y_{t-3}	Y_{t-4}
Daily PM10 concentration(X_t^1)	$X_{t-1}^1^*$	X_{t-2}^1	X_{t-3}^1	X_{t-4}^1
Daily SO2 concentration(X_t^2)	X_{t-1}^2	X_{t-2}^2	X_{t-3}^2	X_{t-4}^2
Daily CO concentration(X_t^3)	$X_{t-1}^3^*$	$X_{t-2}^3^*$	$X_{t-3}^3^*$	X_{t-4}^3
Daily NO2 concentration(X_t^4)	$X_{t-1}^4^*$	X_{t-2}^4	X_{t-3}^4	X_{t-4}^4
Daily O3 concentration(X_t^5)	X_{t-1}^5	X_{t-2}^5	$X_{t-3}^5^*$	X_{t-4}^5
Daily average temperature(X_t^6)	X_{t-1}^6	X_{t-2}^6	X_{t-3}^6	X_{t-4}^6
Daily relative humidity(X_t^7)	X_{t-1}^7	X_{t-2}^7	X_{t-3}^7	X_{t-4}^7
Daily average air pressure(X_t^8)	X_{t-1}^8	X_{t-2}^8	X_{t-3}^8	X_{t-4}^8
Daily average wind speed(X_t^9)	$X_{t-1}^9^*$	X_{t-2}^9	$X_{t-3}^9^*$	X_{t-4}^9
The wind direction of daily maximum wind speed(X_t^{10})	X_{t-1}^{10}	$X_{t-2}^{10^*}$	$X_{t-3}^{10^*}$	X_{t-4}^{10}

Fig.9. The procedure chart of compressing factors(Jinan)

The same as Case 1, Case 2 also considered three cases. After training, the neural network structures for the three cases are shown in Table 5.

Table 5
Structure of neural network in three situations(Jinan)

Situation (Codename)	Input layer- Hidden layer- Output layer
without considering external factors (A)	6-5-1
considering external factors without variable selection (B)	40-5-1
LASSO-QR-KDE(C)	12-5-1

Fig. 10, Fig. 11, and Fig. 12 show the probability density curves of PM2.5 concentrations in Jinan for eight days in January under three scenarios in turn. The highest probability point of the probability density curve deviates from the actual value more often when the prediction is made without considering external factors, and the true value often appears at the end of the probability density curve. When external factors are taken into account, the prediction results are much better, especially when the LASSO method is used to select the variables and then make the prediction, the actual value basically appears at the highest point of the probability density curve. In this case, the LASSO-QR-KDE model also has a good performance in predicting the probability density of PM2.5 concentration.

Fig.10. Probability density curve of Jinan without considering external factors

Fig.11. Probability density curve of Jinan considering external factors but without variable selection

Fig.12. Probability density curve of Beijing with LASSO-QR-KDE model

Appendix B (Table B.2) presents the predicted values of PM2.5 concentrations at the highest point of the probability density curve (mode) and the relative errors for Jinan in January 2021 under three situations. Fig. 13 shows that the maximum relative errors in the three cases are 14.77%, 11.46% and 6.52%, and the minimum relative errors are 1.02%, 1.53% and 0.05%. The overall performance using the LASSO-QR-KDE model is significantly improved over the other two situations. The experimental results in Table 6 show that the mode has the best prediction results when applying LASSO for variable selection, where MAPE is 2.36% and RMSE is 2.07. Similar to Case 1, probability density prediction

of PM2.5 concentration using LASSO-QR-KDE model can get more accurate results.

Fig. 13. Relative error of prediction results for three situations in Jinan (%)

Table 6

Prediction errors for three situations in Jinan

Situation (Codename)	MAPE(%)	RMSE
without considering external factors (A)	5.20	4.74
considering external factors without variable selection (B)	4.54	4.50
LASSO-QR-KDE(C)	2.36	2.07

4.3 Comparisons with other models

To demonstrate the superiority of the LASSO-QR-KDE method for PM2.5 concentration prediction, a variety of traditional prediction models and novel research models are introduced in this section for comparison with the proposed method. In this section, the prediction results are compared using the same data set. Five comparison models are presented below.

(1) ARIMA (Autoregressive Integrated Moving Average model), which achieves time series forecasting by fitting the observed time series into a parametric model (Ruby-Figueroa et al. 2016);

(2) BP (Back Propagation Neural Network), which continuously adjusts the weights and thresholds of the network through training, and thus learns the mapping relationships in the input and output data (Zhou and Qu 2017);

(3) RBF (Radical Basis Function), similar to BP, but with good ability to approximate arbitrary nonlinear functions and to express the intrinsic unresolved regularities of the system (He et al. 2013);

(4) CNN-LSTM (convolutional neural networks-long short termmemory), which uses CNN for

feature extraction, and then inputs the extracted feature values into the LSTM structure (Huang and Kuo 2018).

(5) EMD-GRU (Empirical Mode Decomposition- Gate Recurrent Unit), which uses EMD to decompose PM2.5 concentration sequences, and then the decomposed multiple smooth subsequences and meteorological features are sequentially input into the GRU neural network for training and prediction (Huang et al. 2021).

The prediction results of each model for PM2.5 concentrations in Beijing are shown in Fig. 14 and for Jinan City in Fig. 15. The prediction errors of the two cases are compared in Fig. 16. In addition, the daily forecast data for each model are shown in Appendix C along with the daily forecast relative errors.

Fig. 14 The comparison between the predicted and actual values of each model (Beijing)

Fig. 15 The comparison between the predicted and actual values of each model (Jinan)

Fig. 16 Prediction error for each model

Based on the experimental results of each model, the following observations are derived:

- (1) Compared with the traditional prediction model ARIMA and the classical machine learning methods BP and RBF, the evaluation indexes of the other three models are better, which reflects that the networks designed specifically for dealing with time series problems outperform the typical shallow machine learning methods in terms of time series prediction. Furthermore, for the task of PM2.5 concentration prediction, the prediction performance of the combined model is better than that of the

single model.

(2) In both cases, the RMSE and MAPE of the LASSO-QR-KDE model are taken to be the minimum values. Taking the data of the Beijing case as an example, the RMSE and MAPE of the proposed model decreased by 2.14 and 2.78%, respectively, compared to the better-performing EMD-GRU model.

4.4 Discussion

In this paper, a new hybrid model is proposed to accurately predict the short-term variation of PM_{2.5} concentrations. Based on previous studies, LASSO is used for the selection of factors influencing PM_{2.5} concentrations, which greatly improves the prediction accuracy of the model. Similar to the findings of Koen et al.(2021), the LASSO method does contribute to a larger effect in improving the accuracy of the model interpretation. In addition, due to the specific nature of quantile regression, the effect of each factor on PM_{2.5} concentrations can be explained at different quantile points. The QR model provides the overall distribution of the response variables corresponding to the explanatory variables, which gives more information than the widely used mean regression (Sun et al. 2021). After obtaining the predicted values of the daily PM_{2.5} concentrations at multiple quartiles, the KDE model was used to estimate the probability density function of the daily PM_{2.5} concentrations, and the value corresponding to the highest point of the probability density curve was the predicted value of the concentration .

In summary, compared with other commonly used prediction models, the LASSO-QR-KDE model proposed in the paper can effectively identify the sequences that are significant to the prediction target and can obtain the probability distribution of the predicted values. Both cases involved in the

paper are areas with poor air quality and high PM2.5 concentrations, however, their main causes are different. Pollution from industrial development is a major factor in the poor air quality in Beijing, China, and in Jinan, China, it is the deposition of air pollutants due to its topography. The LASSO-QR-KDE model is able to perform better in the prediction results of both cases, indicating that the method is suitable for the prediction of areas with high PM2.5 concentrations. In future research, extension of the model to prediction of PM2.5 concentrations in general could be considered, and better selection methods for influence factors are also a future research direction.

5. Conclusion

This paper proposes the LASSO-QR-KDE model to predict the probability density of PM2.5 concentrations. Based on two cases in the Chinese region, the important influencing factors of PM2.5 concentrations are firstly screened out, and then the data are processed using the proposed model. The LASSO-QR-KDE model is applied to obtain continuous probability density prediction curves, which can provide more information for PM2.5 concentration prediction. According to the empirical analysis, the main findings are as follows:

(1) The LASSO-QR-KDE model starts from the perspective of dealing with high-dimensional data and is able to select factors that have a significant impact on PM2.5 concentrations. The model can eliminate irrelevant variables and achieve the goal of effectively reducing the data dimensionality without affecting the prediction performance. This paper compares the probability density prediction without considering external factors, the probability density prediction with considering external factors but without variable screening, and the probability density prediction with variable screening using LASSO. We found that the prediction of PM2.5 concentration is significantly affected by

considering external factors or not. The LASSO-QR-KDE model can enhance the model prediction accuracy effectively when external factors are considered.

(2) Applying the LASSO-QR-KDE model to PM2.5 concentration data can obtain the probability density prediction curve for each consecutive day in a month, and the true value almost appears near the highest point of the probability density curve. The continuous probability density curve can provide more information for the prediction of PM2.5 concentration, and can obtain more abundant prediction results compared with other prediction methods.

(3) From the experimental results of the two cases in the paper, there are differences in the important factors affecting PM2.5 concentrations in different regions. The RMSE and MAPE of both cases can be maintained around 2 and 2%, which indicates the applicability and accuracy of the method for prediction in areas with high PM2.5 concentrations. The model can effectively identify important features from the high-dimensional data and make differentiated predictions for areas with high PM2.5 concentrations, which can provide meaningful references for relevant policy makers to effectively reduce and control air pollution and reduce public health risks.

CRediT authorship contribution statement

Shaomei Yang: Methodology, Resources, Writing - review & editing.

Haoyue Wu: Conceptualization, Software, Validation, Investigation, Data curation, Writing - original draft.

Data availability statement

The datasets analysed during the current study are available in the *the National Meteorological*

609 *Data Center of China* repository, <http://data.cma.cn/>

610 **Ethical Approval**

611 Not applicable.

612 **Consent to Participate**

613 Not applicable.

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620 The authors declare that they have no known competing financial interests or personal
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Appendix

Appendix A

Table A.1

LASSO regression results of Beijing data

Step	Df	Rss	Cp	Step	Df	Rss	Cp	Step	Df	Rss	Cp
0	1	4.76	419.17	19	16	2.24	70.00	38*	31	1.83	37.67
1	2	4.18	333.85	20	17	2.24	71.06	39	32	1.83	39.35
2	3	3.33	208.06	21	18	2.23	71.49	40	33	1.82	39.81
3	4	3.00	160.10	22	19	2.14	60.01	41	34	1.80	39.78
4	5	2.94	152.46	23	20	2.11	57.53	42	35	1.79	39.09
5	6	2.74	125.38	24	21	2.10	59.03	43	36	1.78	39.93
6	7	2.68	118.01	25	22	2.07	55.93	44	37	1.77	41.10
7	8	2.68	118.95	26	21	2.07	53.53	45	38	1.76	41.31
8	9	2.65	117.39	27	22	2.05	52.10	46	39	1.75	41.62
9	10	2.65	118.72	28	23	2.04	53.22	47	40	1.74	42.04
10	9	2.60	110.15	29	24	2.04	55.05	48	41	1.71	40.00
11	10	2.57	106.98	30	25	2.03	56.14	49	42	1.71	41.79
12	11	2.47	94.52	31	26	1.97	48.49	50	41	1.70	38.48
13	12	2.38	82.09	32	27	1.92	43.32	51	42	1.70	40.39
14	11	2.35	75.60	33	28	1.91	43.94	52	43	1.70	42.19
15	12	2.34	76.18	34	29	1.89	43.30	38	31	1.83	37.67
16	13	2.32	75.94	35	30	1.85	38.86	39	32	1.83	39.35
17	14	2.28	70.92	36	31	1.84	38.96	40	33	1.82	39.81
18	15	2.26	70.80	37	32	1.83	40.20	41	34	1.80	39.78

Table A.2

LASSO regression results of Jinan data

Step	Df	Rss	Cp	Step	Df	Rss	Cp	Step	Df	Rss	Cp
0	1	6.82	465.33	19	18	2.88	57.72	38	33	2.37	30.58
1	2	4.36	192.16	20	19	2.82	53.35	39	34	2.35	30.61
2	3	3.70	120.33	21	20	2.78	51.48	40	35	2.34	31.34
3	4	3.53	102.75	22	21	2.76	51.16	41	36	2.34	33.23
4	5	3.49	100.29	23	22	2.75	51.11	42	37	2.33	35.12
5	6	3.35	86.65	24	23	2.74	52.50	43	38	2.33	36.81
6	7	3.23	75.10	25	24	2.72	52.41	44	39	2.33	38.60
7	8	3.10	62.32	26	25	2.68	49.27	45	40	2.31	38.85
8	9	3.06	60.18	27	26	2.55	37.63	46	41	2.31	39.86
9	10	3.05	61.65	28	27	2.52	36.02	47	40	2.30	36.98
10	11	3.02	59.27	29	28	2.52	37.68	48	41	2.30	38.86
11	12	2.99	58.89	30	29	2.50	37.87	49	42	2.29	40.63
12	13	2.98	59.81	31	30	2.47	36.09	50	43	2.29	42.17
13	14	2.96	59.14	32*	31	2.40	30.20	51	44	2.28	43.33
14	15	2.91	55.42	33	32	2.39	31.45	52	45	2.28	45.00
15	16	2.90	56.63	34	33	2.39	33.28	38	33	2.37	30.58
16	17	2.89	57.62	35	34	2.37	33.14	39	34	2.35	30.61
17	16	2.88	54.48	36	33	2.37	31.10	40	35	2.34	31.34
18	17	2.88	55.97	37	34	2.37	32.69	41	36	2.34	33.23

Appendix B

Table B.1

Prediction results for three situations of Beijing data

Time /day	Actual value ($\mu\text{g}/\text{m}^3$)	A		B		C	
		Mode	RE(%)	Mode	RE(%)	Mode	RE(%)
		($\mu\text{g}/\text{m}^3$)		($\mu\text{g}/\text{m}^3$)		($\mu\text{g}/\text{m}^3$)	
1	28	23.62	15.64	24.28	13.29	24.80	11.42
2	57	48.83	14.33	50.36	11.65	52.79	7.39
3	123	119.63	2.74	119.00	3.25	120.08	2.37
4	18	17.20	4.43	19.07	5.95	17.32	3.78
5	17	15.76	7.31	17.40	2.34	16.68	1.88
6	64	70.25	9.76	67.67	5.74	62.66	2.09
7	34	35.17	3.43	33.64	1.07	34.03	0.08
8	10	9.50	5.01	10.12	1.23	9.71	2.92
9	41	40.21	1.92	41.43	1.04	41.14	0.35
10	75	72.85	2.87	77.27	3.03	77.35	3.13
11	103	108.57	5.41	100.38	2.54	105.29	2.22
12	217	218.91	0.88	221.36	2.01	214.63	1.09
13	128	113.51	11.32	118.49	7.43	129.29	1.01

14	104	100.32	3.54	101.32	2.58	108.19	4.03
15	9	8.46	6.03	9.43	4.77	8.76	2.72
16	38	39.85	4.87	37.46	1.43	36.69	3.45
17	45	47.58	5.73	44.41	1.32	44.69	0.69
18	64	72.95	13.98	62.35	2.58	63.18	1.28
19	11	12.05	9.51	11.24	2.14	10.83	1.54
20	9	9.35	3.88	8.91	0.99	9.05	0.60
21	24	24.63	2.63	23.39	2.55	23.17	3.47
22	28	30.06	7.34	28.58	2.08	27.71	1.02
23	23	21.15	8.05	22.71	1.26	23.30	1.32
24	58	60.45	4.22	60.00	3.45	56.91	1.88
25	10	10.58	5.82	10.77	7.69	9.54	4.61
26	25	24.04	3.86	25.36	1.43	24.77	0.93
27	49	50.97	4.02	49.98	2.00	49.37	0.76
28	35	36.97	5.63	33.91	3.11	35.46	1.31
29	106	104.61	1.31	104.03	1.86	107.64	1.55
30	28	29.31	4.69	27.50	1.78	28.57	2.02
31	13	12.07	7.18	13.40	3.07	13.20	1.57

712 **Table B.2**

713 Prediction results for three situations of Jinan data

Time /day	Actual value ($\mu\text{g}/\text{m}^3$)	A		B		C	
		Mode ($\mu\text{g}/\text{m}^3$)	RE(%)	Mode ($\mu\text{g}/\text{m}^3$)	RE(%)	Mode ($\mu\text{g}/\text{m}^3$)	RE(%)
1	46	39.21	14.77	41.25	10.33	43.00	6.52
2	65	70.17	7.96	72.45	11.46	68.66	5.63
3	142	129.76	8.62	128.33	9.63	136.65	3.77
4	133	141.55	6.43	139.28	4.72	135.78	2.09
5	28	30.62	9.34	26.36	5.87	27.34	2.34
6	37	39.18	5.88	35.93	2.88	35.86	3.08
7	16	15.16	5.24	16.39	2.43	16.23	1.45
8	29	28.48	1.79	28.50	1.71	29.67	2.32
9	30	32.60	8.66	28.10	6.32	31.14	3.81
10	32	33.20	3.74	33.73	5.42	30.59	4.41
11	38	37.13	2.29	38.58	1.53	39.77	4.67
12	58	53.57	7.63	61.17	5.46	56.20	3.11
13	70	66.42	5.12	72.88	4.11	69.67	0.47
14	93	98.04	5.42	87.36	6.06	93.05	0.05
15	95	90.27	4.98	100.12	5.39	93.97	1.08
16	46	47.68	3.65	44.42	3.43	44.92	2.34
17	49	47.90	2.25	50.89	3.85	48.33	1.36
18	43	41.53	3.41	44.24	2.88	44.00	2.32
19	56	59.48	6.22	53.89	3.76	57.10	1.97
20	93	97.93	5.3	88.47	4.87	91.55	1.56

21	148	138.97	6.1	141.50	4.39	144.54	2.34
22	212	217.94	2.8	220.67	4.09	216.43	2.09
23	107	101.91	4.76	103.05	3.69	104.51	2.33
24	139	132.01	5.03	141.61	1.88	140.08	0.78
25	168	162.72	3.14	163.68	2.57	170.39	1.42
26	135	133.62	1.02	130.37	3.43	133.27	1.28
27	77	79.07	2.69	79.15	2.79	78.86	2.42
28	34	32.35	4.84	35.52	4.46	32.69	3.84
29	44	45.31	2.98	42.01	4.52	44.09	0.21
30	64	61.27	4.26	61.73	3.54	63.66	0.53
31	83	87.17	5.03	85.71	3.26	84.23	1.48

714 Appendix C

715 Table C.1.1

716 Predicted values under various models of Beijing data ($\mu\text{g}/\text{m}^3$)

Time/day	Actual value	LASSO-QR-KDE	ARIMA	BP	RBF	CNN-LSTM	EMD-GRU
1	24.80	31.66	22.15	30.08	26.57	29.58	24.80
2	52.79	75.88	48.76	58.70	49.06	58.42	52.79
3	120.08	97.35	109.97	107.47	104.16	131.36	120.08
4	17.32	21.32	14.88	20.40	18.90	17.30	17.32
5	17.32	21.04	19.62	15.56	18.27	16.35	17.32
6	62.66	53.18	52.24	59.35	59.56	65.24	62.66
7	34.03	41.57	38.51	40.83	38.47	31.69	34.03
8	9.71	12.92	8.99	8.66	10.36	9.66	9.71
9	41.14	36.59	43.71	34.10	45.35	38.58	41.14
10	77.35	70.12	68.60	82.55	71.96	78.59	77.35
11	105.29	70.62	85.16	81.75	109.08	95.95	105.29
12	214.63	155.48	175.70	259.99	225.22	204.08	214.63
13	129.29	160.92	155.42	134.66	150.35	137.06	129.29
14	108.19	122.76	127.12	95.41	88.65	107.02	108.19
15	8.76	7.43	10.42	7.97	8.19	9.45	8.76
16	36.69	47.78	30.97	43.21	33.74	35.42	36.69
17	45.31	35.75	53.01	54.40	42.92	41.12	45.31
18	63.18	52.06	79.40	55.17	56.25	61.60	63.18
19	10.83	8.86	12.37	9.83	11.52	10.26	10.83
20	9.05	11.12	7.93	8.24	8.50	9.42	9.05
21	23.17	27.51	28.76	27.50	22.04	22.41	23.17
22	27.71	24.72	22.25	31.82	24.50	25.91	27.71
23	23.30	24.15	27.58	25.93	24.51	25.61	23.30
24	56.91	62.00	51.74	44.56	51.85	52.41	56.91
25	9.54	6.97	10.76	11.64	11.10	9.14	9.54
26	24.77	28.46	20.14	21.17	22.60	24.42	24.77

27	49.37	55.32	37.00	54.63	54.08	49.73	49.37
28	35.46	26.02	42.02	38.84	37.89	37.04	35.46
29	107.64	144.94	85.87	99.27	100.62	116.27	107.64
30	28.57	33.98	21.60	24.02	23.36	26.26	28.57
31	13.20	9.65	15.53	11.72	11.36	13.55	13.20

717 **Table C.1.2**

718 Relative errors under various models of Beijing data (%)

Time/day	LASSO-QR-KDE	ARIMA	BP	RBF	CNN-LSTM	EMD-GRU
1	11.42	13.07	20.88	7.42	5.11	5.63
2	7.39	33.12	14.46	2.98	13.93	2.49
3	2.37	20.85	10.59	12.63	15.32	6.80
4	3.78	18.45	17.32	13.31	4.99	3.89
5	1.88	23.77	15.44	8.48	7.46	3.80
6	2.09	16.90	18.38	7.26	6.93	1.94
7	0.08	22.25	13.25	20.09	13.14	6.80
8	2.92	29.24	10.09	13.42	3.55	3.38
9	0.35	10.76	6.60	16.84	10.62	5.91
10	3.13	6.51	8.54	10.06	4.06	4.78
11	2.22	31.44	17.32	20.63	5.90	6.84
12	1.09	28.35	19.03	19.81	3.79	5.95
13	1.01	25.72	21.42	5.20	17.46	7.08
14	4.03	18.04	22.23	8.26	14.76	2.91
15	2.72	17.40	15.76	11.45	9.01	5.02
16	3.45	25.73	18.50	13.70	11.20	6.80
17	0.69	20.56	17.79	20.88	4.62	8.63
18	1.28	18.66	24.07	13.79	12.11	3.75
19	1.54	19.42	12.43	10.66	4.69	6.75
20	0.60	23.58	11.86	8.48	5.53	4.66
21	3.47	14.62	19.84	14.57	8.18	6.61
22	1.02	11.73	20.53	13.64	12.49	7.45
23	1.32	5.02	19.93	12.75	6.59	11.36
24	1.88	6.89	10.80	23.18	10.60	9.64
25	4.61	30.33	7.63	16.37	10.98	8.63
26	0.93	13.82	19.45	15.32	9.61	2.33
27	0.76	12.90	24.48	11.48	10.37	1.49
28	1.31	25.67	20.05	10.97	8.25	5.83
29	1.55	36.74	18.99	6.35	5.07	9.69
30	2.02	21.36	22.85	14.22	16.59	6.21
31	1.57	25.79	19.47	9.81	12.64	4.23

719 **Table C.2.1**

720 Predicted values under various models of Jinan data ($\mu\text{g}/\text{m}^3$)

Time/day	Actual	LASSO-QR-KDE	ARIMA	BP	RBF	CNN-LSTM	EMD-GRU
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	value						
1	46	43.00	36.65	38.90	49.37	47.60	40.88
2	65	68.66	52.15	57.93	61.16	61.17	60.94
3	142	136.65	159.07	124.32	154.55	161.06	130.78
4	133	135.78	112.45	111.48	148.07	146.57	138.88
5	28	27.34	24.25	31.82	24.63	24.79	30.06
6	37	35.86	30.47	45.90	40.46	34.17	39.12
7	16	16.23	18.90	13.24	17.37	15.09	16.78
8	29	29.67	30.28	33.81	30.13	30.40	28.10
9	30	31.14	30.46	33.26	25.81	26.23	30.65
10	32	30.59	34.81	27.29	27.93	29.09	31.28
11	38	39.77	42.14	30.66	33.62	35.20	39.42
12	58	56.20	49.18	50.19	51.67	61.47	59.93
13	70	69.67	83.12	78.88	74.07	74.29	68.56
14	93	93.05	112.21	104.38	85.14	86.26	87.89
15	95	93.97	123.91	108.10	88.16	88.51	99.05
16	46	44.92	57.08	51.20	51.79	44.04	42.37
17	49	48.33	59.23	43.63	44.36	51.76	43.84
18	43	44.00	34.77	48.04	38.67	45.67	44.00
19	56	57.10	46.13	62.96	50.47	58.42	54.84
20	93	91.55	75.11	80.31	84.65	98.33	89.80
21	148	144.54	175.25	166.57	131.22	138.75	138.90
22	212	216.43	246.75	246.13	234.75	220.88	205.09
23	107	104.51	139.12	91.24	94.71	113.23	110.57
24	139	140.08	174.56	155.64	160.00	158.11	145.70
25	168	170.39	134.22	147.49	185.34	158.73	175.41
26	135	133.27	108.04	119.41	153.13	128.74	142.24
27	77	78.86	90.75	85.26	86.36	81.71	74.77
28	34	32.69	40.29	30.67	37.19	32.09	35.71
29	44	44.09	52.79	39.60	49.02	41.10	45.02
30	64	63.66	50.85	69.27	72.86	66.39	60.81
31	83	84.23	98.54	89.08	95.97	87.17	78.01

721 **Table C.2.2**

722 Relative errors under various models of Jinan data (%)

Time/day	LASSO-QR-KDE	ARIMA	BP	RBF	CNN-LSTM	EMD-GRU
1	6.52	20.32	15.44	7.33	3.47	11.14
2	5.63	19.77	10.87	5.91	5.89	6.25
3	3.77	12.02	12.45	8.84	13.42	7.90
4	2.09	15.45	16.18	11.33	10.20	4.42
5	2.34	13.38	13.64	12.05	11.45	7.34
6	3.08	17.64	24.06	9.36	7.66	5.72
7	1.45	18.15	17.23	8.57	5.71	4.85
8	2.32	4.43	16.59	3.88	4.83	3.09

9	3.81	1.54	10.88	13.97	12.56	2.16
10	4.41	8.77	14.71	12.72	9.10	2.25
11	4.67	10.90	19.32	11.53	7.36	3.74
12	3.11	15.20	13.46	10.91	5.99	3.33
13	0.47	18.74	12.69	5.82	6.13	2.06
14	0.05	20.66	12.24	8.45	7.25	5.50
15	1.08	30.43	13.79	7.20	6.83	4.26
16	2.34	24.09	11.30	12.58	4.27	7.89
17	1.36	20.88	10.96	9.46	5.63	10.53
18	2.32	19.15	11.73	10.08	6.20	2.32
19	1.97	17.63	12.42	9.87	4.33	2.08
20	1.56	19.24	13.64	8.98	5.73	3.44
21	2.34	18.41	12.55	11.34	6.25	6.15
22	2.09	16.39	16.10	10.73	4.19	3.26
23	2.33	30.02	14.73	11.49	5.82	3.34
24	0.78	25.58	11.97	15.11	13.75	4.82
25	1.42	20.11	12.21	10.32	5.52	4.41
26	1.28	19.97	11.55	13.43	4.64	5.36
27	2.42	17.86	10.73	12.15	6.12	2.90
28	3.84	18.49	9.79	9.39	5.62	5.04
29	0.21	19.98	10.01	11.42	6.60	2.31
30	0.53	20.54	8.24	13.84	3.74	4.99
31	1.48	18.72	7.32	15.63	5.03	6.01

723