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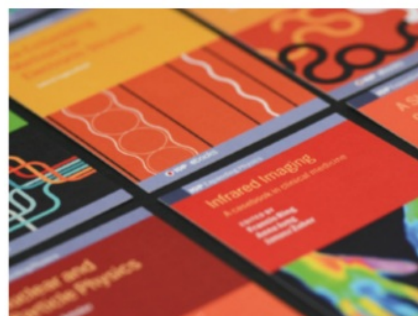
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Smoothing parameter selection method for multiresponse nonparametric regression model using smoothing spline and Kernel estimators approaches

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Abstract. The principle problem in multiresponse nonparametric regression model is how we estimate the regression functions which draw association between some dependent (response) variables and some independent (predictor) variables where there are correlations between responses. There are many techniques used to estimate the regression function. Two of them are spline and kernel smoothing techniques. Speaking about smoothing techniques, not only in uniresponse spline and kernel nonparametric regression models but also in multiresponse spline and kernel nonparametric regression models, the estimations of regression functions depend on smoothing parameters. In the previous researches the covariance matrices were assumed to be known. Matrix of covariance is not assumed known in this research. The goals of this research are selecting of optimal smoothing parameters for the model we consider through spline and kernel smoothing techniques. Optimal smoothing parameters can be obtained by taking the solution to generalized cross validation (GCV) optimization problem. The obtained results of this research are the optimal smoothing parameter for smoothing spline estimator approach and the optimal smoothing parameter namely optimal bandwidth for kernel estimator approach.

1. Introduction

In statistical analysis we frequently involve a building mathematical model which examines the functional association between one or more than one dependent (response) and one or more than one independent (predictor) variables. Discussing about association between some dependent (response) variables and some independent (predictor) variables which is drawn by a function, we may not neglect an usual model namely a regression model. In analysis of regression which uses parametric and nonparametric regression models approaches we often meet to principle problem, i.e., estimate functions of regression. For approaching model of nonparametric regression where it has no specific pattern of the regression function, we can use some estimators to estimate function of regression in the model, for example spline, kernel, local linear, etc. In this approach, spline estimator is more flexible to estimate regression function than other estimators. Researchers who have used spline estimator in



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various cases of models of nonparametric regression with single response are [1-21]. Next, [22-28] used this estimator to estimate functions of regressions in models of nonparametric regression with two responses and more than two responses. On the other hand, [29-35] have proposed kernel estimator to estimate models of nonparametric regression with single response. Furthermore, [36-38] have studied these estimators, i.e., spline and kernel, for estimating functions of regression in models of nonparametric regression with both single response and multi-responses.

Estimate regression functions in models of nonparametric regression with single response that uses smoothing techniques, either spline estimator or kernel estimator, depends on smoothing parameters [2, 10, 20, and 39]. In single response spline nonparametric regression, if smoothing parameter value is very small then it will give a very rough estimator of nonparametric regression function [20]. In contrary, if smoothing parameter value is very large then it will give a very smooth estimator of nonparametric regression function [20]. Therefore, we need to select optimal smoothing parameter in order to obtain estimator that is suitable with data. For this need, some researchers have proposed some selection methods for selecting the optimal smoothing parameters, for instance [2] proposed cross validation (CV) method, [10] proposed unbiased risk (UBR) method, and [20 and 39-40] proposed generalized cross validation (GCV) methods.

All researchers who have been mentioned previously, discussed the estimating methods of regression functions in either uniresponse or multiresponse nonparametric regression models only [1-38]. These researchers have not discussed the selecting of smoothing parameters methods. Further, although [2, 10, 20, and 39-40] have discussed the selecting of smoothing parameters methods, but these researchers have not discussed the selecting of smoothing parameters methods for the multiresponse nonparametric regression model by using kernel estimator. Also, previous researchers have not estimated the covariance matrix. Therefore, in this research we discuss method to select optimal smoothing parameters for the considered model by using both smoothing spline and kernel techniques.

2. Results of research and discussion

Here, we provide a mathematical statistics method for selecting the smoothing parameters for the model that we consider through both smoothing spline and kernel techniques.

2.1. Smoothing parameters selection method by using smoothing spline estimator approach

Firstly, suppose (y_{ij}, x_{ij}) is data set which accords with the following multiresponse nonparametric regression model:

$$y_{ij} = g_i(x_{ij}) + \varepsilon_{ij}, \quad a_i \leq x_i \leq b_i, \quad i=1,2,\dots,p, \quad j=1,2,\dots,n_i \quad (1)$$

where y_{ij} represents i^{th} response of j^{th} observation, unknown smooth regression functions g_1, g_2, \dots, g_p are included in Sobolev space $W_2^m[a_i, b_i]$, and independent random errors ε_{ij} have zero-mean and variance σ_{ij}^2 [28 and 37].

Secondly, based on (1) we have $\underline{y} = (y_1, y_2, \dots, y_p)'$, $\underline{f} = (f_1, f_2, \dots, f_p)'$, $\underline{\varepsilon} = (\varepsilon_1, \varepsilon_2, \dots, \varepsilon_p)'$, and $\underline{x} = (x_1, x_2, \dots, x_p)'$ where $\underline{y}_i = (y_{i1}, y_{i2}, \dots, y_{in_i})'$, $\underline{g}_i = (g_i(x_{i1}), g_i(x_{i2}), \dots, g_i(x_{in_i}))'$, $\underline{\varepsilon}_i = (\varepsilon_{i1}, \varepsilon_{i2}, \dots, \varepsilon_{in_i})'$, $\underline{x}_i = (x_{i1}, x_{i2}, \dots, x_{in_i})'$. So, for $j=1,2,\dots,n_i$ and $i=1,2,\dots,p$, the equation (1) can be expressed in the following vector notation:

$$\underline{y} = \underline{g} + \underline{\varepsilon} \quad (2)$$

where $\underline{\varepsilon}$ have zero-mean and covariance of $[W(\sigma^2)]^{-1} = \text{diag}(W_1(\sigma_1^2), W_2(\sigma_2^2), \dots, W_p(\sigma_p^2))$ [28]. Estimation of regression functions \underline{g} in (2) through smoothing spline method occurs as a solution to

minimization problem of penalized weighted least-square (PWLS). Thus, we must find \hat{g} that can make the following PWLS minimum:

$$\text{Min}_{g_1, \dots, g_p \in W_p^2} \{ (\sum_{i=1}^p n_i)^{-1} (y_1 - g_1)' W_1(\sigma_1^2) (y_1 - g_1) + \dots + (y_p - g_p)' W_p(\sigma_p^2) (y_p - g_p) + \lambda_1 \int_{a_1}^{b_1} (g_1^{(2)}(x_1))^2 dx_1 + \dots + \lambda_p \int_{a_p}^{b_p} (g_p^{(2)}(x_p))^2 dx_p \} \quad (3)$$

for pre-specified value of $\underline{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_p)'$. Equation (3) shows that the first expression represents sum squares of errors (MSE) which penalizes lack of fit, and the second expression with its weight $\underline{\lambda}$ represents penalty of roughness. Thus, the penalty of roughness penalizes the curvature of g . Further, we call λ_i ($i=1, 2, \dots, p$) as parameter of smoothing. If $0 < \lambda_i < +\infty$ then the solution of (3) will be different from interpolation to a linear model. Next, equation (3) will be dominated by the roughness penalty, and estimating of smoothing spline will lead to be a constant, if $\lambda_i \rightarrow +\infty$. On the other hand, the penalty of roughness will not occur in (3) if $\lambda_i \rightarrow 0$, and the data will be interpolated by estimating of smoothing spline. It means that smoothing parameter λ_i controls the trade-off between the goodness of fit:

$$(\sum_{i=1}^p n_i)^{-1} (y_1 - g_1)' W_1(\sigma_1^2) (y_1 - g_1) + \dots + (y_p - g_p)' W_p(\sigma_p^2) (y_p - g_p)$$

and smoothness of the estimate:

$$\lambda_1 \int_{a_1}^{b_1} (g_1^{(2)}(x_1))^2 dx_1 + \dots + \lambda_p \int_{a_p}^{b_p} (g_p^{(2)}(x_p))^2 dx_p.$$

The solution to optimization in (3) is a smoothing spline estimator. Function basis of this estimator is a spline of natural cubic where its knots are x_1, x_2, \dots, x_{n_i} ($i=1, 2, \dots, p$). It means that interpolation of special structured spline which depends on the smoothing parameter λ_i value selection gets turn into a representative approach of the regression functions g_i ($i=1, 2, \dots, p$) in model (1). Next, by applying reproducing kernel Hilbert space (RKHS) method, we determine regression function estimate, and its result is:

$$\hat{g}_{\underline{\lambda}}(x) = (\hat{g}_{1, \lambda_1}(x_1), \hat{g}_{2, \lambda_2}(x_2), \dots, \hat{g}_{p, \lambda_p}(x_p))' = K\hat{d} + \Sigma\hat{c} = A(\underline{\lambda})y \quad (4)$$

where

$$A(\underline{\lambda}) = K[K'M^{-1}W(\underline{\sigma}^2)K]^{-1} K'M^{-1}W(\underline{\sigma}^2) + \Sigma M^{-1}W(\underline{\sigma}^2)[I - K(K'M^{-1}W(\underline{\sigma}^2)K)^{-1} K'M^{-1}W(\underline{\sigma}^2)]$$

is called as "hat matrix" and a non-singular matrix, so it is a invertible matrix [28 and 37], and $\hat{g}_{\underline{\lambda}}(x)$ is estimated regression function based on smoothing spline estimator where its function basis is natural cubic spline with knots x_1, x_2, \dots, x_{n_i} ($i=1, 2, \dots, p$), for a fixed parameter of smoothing $\underline{\lambda} > 0$. So, $A(\underline{\lambda})$ is a smoother matrix that is positive-definite (symmetrical), and it does not depend on y , but it depends on parameter of smoothing $\underline{\lambda}$ and knots x_1, x_2, \dots, x_{n_i} ($i=1, 2, \dots, p$) [28, 37 and 40].

Furthermore, we may express the estimated regression function of model in (4) as follows:

$$\hat{g}_{\underline{\lambda}}(x) = A(\lambda_1, \dots, \lambda_p; \underline{\sigma}^2)y \quad (5)$$

where $\underline{\sigma}^2 = (\sigma_1^2, \dots, \sigma_p^2)'$. Mean square error (MSE) of (5) can be determined as follows:

$$MSE(\lambda_1, \dots, \lambda_p; \underline{\sigma}^2) = \frac{(y - \hat{g}_{\underline{\lambda}}(x))' W(\underline{\sigma}^2) (y - \hat{g}_{\underline{\lambda}}(x))}{\sum_{i=1}^p n_i}$$

$$\begin{aligned}
 &= \frac{\left(\underline{y} - A(\lambda_1, \dots, \lambda_p; \sigma^2) \underline{y} \right)' W(\sigma^2) \left(\underline{y} - A(\lambda_1, \dots, \lambda_p; \sigma^2) \underline{y} \right)}{N} \\
 &= \frac{\left[\left(W(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \underline{y} \right]' \left[\left(W(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \underline{y} \right]}{N} \\
 &= \frac{\left\| \left(W(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \underline{y} \right\|^2}{N}
 \end{aligned}$$

where norm $\|a\|$ is defined as $\|a\| = \sqrt{a_1^2 + a_2^2 + \dots + a_p^2}$ for $a = (a_1, a_2, \dots, a_p)'$, $N = \sum_{i=1}^p n_i$, I_N is an identity matrix, and $W(\sigma^2)$ is a diagonal matrix that has been given by [28, 37 and 40], so that $\left(W(\sigma^2) \right)^{\frac{1}{2}}$ is also a diagonal matrix and it has the square root .

Next, we define a quantity (further it is called as GCV function) as follows:

$$G(\lambda_1, \dots, \lambda_p; \sigma^2) = \frac{N^{-1} \left\| \left(W(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \underline{y} \right\|^2}{\left[N^{-1} \text{trace} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \right]^2}$$

where $(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2))$ is a non-zero matrix, because $\lambda_i > 0, i = 1, 2, \dots, p$.

Finally, we obtain optimal smoothing parameter, namely $\lambda_{optimal} = (\lambda_{1(optimal)}, \dots, \lambda_{p(optimal)})'$ by taking the solution to the following optimization:

$$\begin{aligned}
 G_{optimal}(\lambda_{1(optimal)}, \dots, \lambda_{p(optimal)}; \sigma^2) &= \underset{\lambda_1 \in R^+, \dots, \lambda_p \in R^+}{Min} \left\{ G(\lambda_1, \dots, \lambda_p; \sigma^2) \right\} \\
 &= \underset{\lambda_1 \in R^+, \dots, \lambda_p \in R^+}{Min} \left\{ \frac{N^{-1} \left\| \left(W(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \underline{y} \right\|^2}{\left[N^{-1} \text{trace} \left(I_N - A(\lambda_1, \dots, \lambda_p; \sigma^2) \right) \right]^2} \right\}. \tag{6}
 \end{aligned}$$

2.2. Smoothing parameters selection method by using Kernel estimator approach.

In analysis of nonparametric regression, to estimate the function g in model (1) through kernel smoothing technique, basically we use a decreasing distance function in x -space that is a weighted raw data average.

For model given in (1), according to [37] for predicting at x_{ij} , the weighted raw data average scheme by relating it with i^{th} -response observations, namely y_{ik} , is given by:

$$v_{(i)jk} = \frac{K_i \left(\frac{t_{ij} - t_{ik}}{h_i} \right)}{\sum_{k=1}^{n_i} K_i \left(\frac{t_{ij} - t_{ik}}{h_i} \right)} = \frac{K_i(u)}{\sum_{k=1}^{n_i} K_i(u)}, \quad i = 1, 2, \dots, p \tag{7}$$

where $K(u)$ is called as kernel function which is a decreasing function of u , and $h_i > 0$ is a parameter of smoothing called as bandwidth. The kernel function $K(u)$ should be a symmetric function. It usually give a probability density function for example Gaussian function [34-35].

By considering equation (7), we get the estimated regression function of model given in (1) to estimate function of regression at point of fit x_{ij} which is expressed as:

$$\hat{g}_k(x_{ij}) = \hat{y}_{ij} = \sum_{k=1}^{n_i} v_{(i)jk} y_{ik} = v'_{ik} \underline{y}_i, \quad i=1,2,\dots,p, \quad j=1,2,\dots,n_i. \quad (8)$$

where each point of n_i points is given by a unequal weight $v_{(i)jk}$, $k=1,2,\dots,n_i$ for any point of fit x_{ij} . Thus, we can express the estimated regression function in (8) as:

$$\hat{g} = Vy \quad (9)$$

where $V = \text{diag}(V_{i1}, V_{i2}, \dots, V_{in_i})$, and

$$V_{ij} = \begin{pmatrix} v_{(i)11} & v_{(i)12} & \cdots & v_{(i)1n_i} \\ v_{(i)21} & v_{(i)22} & \cdots & v_{(i)2n_i} \\ \vdots & \vdots & \ddots & \vdots \\ v_{(i)n_i1} & v_{(i)n_i2} & \cdots & v_{(i)n_in_i} \end{pmatrix}.$$

Therefore, we can determine estimator of regression function of model given in (1) based on kernel estimator, and its result is [37]:

$$\hat{g}(x) = (\hat{g}_1(x_1), \hat{g}_2(x_2), \dots, \hat{g}_p(x_p))' = \text{diag}(V_{i1}, V_{i2}, \dots, V_{in_i}) (y_1, y_2, \dots, y_p)'. \quad (10)$$

Since the estimated regression function given in (9) depends on smoothing parameter namely bandwidth $h_i > 0$, $i=1,2,\dots,p$ then we also may write (9) in the following equation:

$$\hat{g}_h(x) = B(h_1, \dots, h_p; \sigma^2) \underline{y} \quad (11)$$

Furthermore, based on equations (9)-(11) we can determine the mean square error (MSE) of (11) as follows:

$$\begin{aligned} \text{MSE}(h_1, \dots, h_p; \sigma^2) &= \frac{(\underline{y} - \hat{g}_h(x))' V(\sigma^2) (\underline{y} - \hat{g}_h(x))}{\sum_{i=1}^p n_i} \\ &= \frac{(\underline{y} - B(h_1, \dots, h_p; \sigma^2) \underline{y})' V(\sigma^2) (\underline{y} - B(h_1, \dots, h_p; \sigma^2) \underline{y})}{N} \\ &= \frac{\left[(V(\sigma^2))^{\frac{1}{2}} \left((I_N - B(h_1, \dots, h_p; \sigma^2)) \underline{y} \right) \right]' \left[(V(\sigma^2))^{\frac{1}{2}} \left((I_N - B(h_1, \dots, h_p; \sigma^2)) \underline{y} \right) \right]}{N} \\ &= N^{-1} \left\| (V(\sigma^2))^{\frac{1}{2}} \left(I_N - B(h_1, \dots, h_p; \sigma^2) \right) \underline{y} \right\|^2 \end{aligned}$$

where norm $\|a\|$ is defined as $\|a\| = \sqrt{a_1^2 + a_2^2 + \dots + a_p^2}$ for $a = (a_1, a_2, \dots, a_p)'$, $N = \sum_{i=1}^p n_i$, I_N is an identity matrix, and $V(\sigma^2)$ is a diagonal matrix that has been given by [28 and 37], so that $(V(\sigma^2))^{\frac{1}{2}}$ is also a diagonal matrix and it has the square root.

Next, we define a quantity as follows:

$$G(h_1, \dots, h_p; \sigma^2) = \frac{N^{-1} \left\| \left(V(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - B(h_1, \dots, h_p; \sigma^2) \right) y \right\|^2}{\left[N^{-1} \text{trace} \left(I_N - B(h_1, \dots, h_p; \sigma^2) \right) \right]^2}$$

where $(I_N - B(h_1, \dots, h_p; \sigma^2))$ is a non-zero matrix because $h_i > 0$, $i = 1, 2, \dots, p$.

Finally, we obtain the optimal smoothing parameter called as optimal bandwidth $\hat{h}_{optimal} = (h_{1(optimal)}, \dots, h_{p(optimal)})'$ by taking the solution to the following optimization:

$$\begin{aligned} G_{optimal}(h_{1(optimal)}, \dots, h_{p(optimal)}; \sigma^2) &= \underset{h_1 \in R^+, \dots, h_p \in R^+}{\text{Min}} \left\{ G(h_1, \dots, h_p; \sigma^2) \right\} \\ &= \underset{h_1 \in R^+, \dots, h_p \in R^+}{\text{Min}} \left\{ \frac{N^{-1} \left\| \left(V(\sigma^2) \right)^{\frac{1}{2}} \left(I_N - H(h_1, \dots, h_p; \sigma^2) \right) y \right\|^2}{\left[N^{-1} \text{trace} \left(I_N - H(h_1, \dots, h_p; \sigma^2) \right) \right]^2} \right\}. \end{aligned} \quad (12)$$

3. Conclusion

The estimated regression functions in model (1) by using both smoothing spline estimator and kernel estimator approaches depends on smoothing parameters ($\hat{\lambda}$) and bandwidths (\hat{h}), respectively. In addition, by minimizing GCV functions given in (6) and in (12) we obtained optimal smoothing parameter for smoothing spline estimator approach and optimal smoothing parameter called as optimal bandwidth for kernel estimator approach, respectively.

Acknowledgement 13

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