An estimation procedure with knot selection for multivariate regression splines

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Abstract. Knot selection for regression splines is crucial to the approximation power of splines. For univariate splines, many knot selection algorithms are available. However, extending those univariate algorithms to the multivariate case can be challenging. In this work, an estimation procedure with knot selection for multivariate regression splines is proposed, where the knot selection part is adapted from an existing univariate knot selection algorithm. Simulation results are included to demonstrate the performance of the proposed method.

1. Introduction
In nonparametric regression, one common approach for estimating the regression function is to approximate the regression function using known basis functions and then estimate the coefficients of basis functions using the method of least squares. Some examples of basis functions that have good approximation properties and have been used in nonparametric regression are wavelets [1] and spline functions [2]. Approximation based on fuzzy transforms is also a tool for function approximation (e.g. [3] and [4]). However, to apply this tool in nonparametric regression, an estimation procedure needs to be proposed and its statistical properties are to be investigated. In this paper, the focus is on nonparametric regression using spline approximation with least squares estimation.

In nonparametric regression, when the regression function is approximated using a spline function, the knot locations of the spline function have a significant effect on the approximation accuracy. There are different approaches for knot determination for regression splines. For instance, one can use equally spaced knots and determine the number of knots based on criteria such as the Bayesian information criterion (BIC) or Akaike information criterion (AIC). When using equally spaced knots splines to approximate a smooth regression function to obtain a regression function estimator, Stone [5] showed that the rate of convergence is optimal in the sense of [2] if the number of knots grows at a proper rate as the sample size increases.

In addition to the equally-spaced knot approach, another approach is to estimate the knot locations as unknown parameters, such as in [6] and [7]. While this approach offers great flexibility for determining knot locations, it is often time consuming to search for the best knot locations. When the regression function is multivariate, it is expected that the optimization of knot locations become even more challenging.

An alternative to the knot estimation approach is to perform knot selection. See [8] and [9] for example. Huang [10] proposed an algorithm for knot selection for univariate regression splines based on statistical testing. In this work, an extension of Huang’s algorithm to the multivariate case is
considered, and an estimation procedure based on the algorithm is proposed. The rest of the paper is organized as follows. The proposed estimation procedure for multivariate regression splines is given in Section 2. Results of simulation experiments are given in Section 3. Conclusions are given in Section 4.

2. Methodology

In this section, the problem set-up will be described and the proposed estimation procedure will be introduced. In addition, another estimation method that is compared with the proposed method in Section 3, will also be introduced. Suppose that \( (X_i, Y_i) : i = 1, \ldots, n \) are \( n \) independent observations from the following nonparametric regression model:

\[
Y_i = f(X_i) + \varepsilon_i, i = 1, \ldots, n, \tag{1}
\]

where \( f \) is the regression function to be estimated and \( \varepsilon_i \)s are errors. Let \( d \) be the dimension of each \( X_i \). The knot selection problem arise when one tries to approximate \( f \) using a spline function. For the univariate case where \( d = 1 \), if the regression function \( f \) in (1) can be approximated well using a spline of order \( m \) and knots \( \xi_1, \ldots, \xi_k \). Then an approximate model for (1) is

\[
Y_i = \sum_{j=0}^{m-1} \alpha_j p_j(X_i) + \sum_{j=1}^k \beta_j B_{m-1,k}(X_i) + \varepsilon_i, i = 1, \ldots, n, \tag{2}
\]

where \( \alpha_j \)s and \( \beta_j \)s are coefficients, \( p_j(x) = x^j \) for \( j = 0, \ldots, m-1 \) and for a real number \( \xi \),

\[
B_{m-1,k}(x) = \begin{cases} (x - \xi)^{m-1} & \text{if } x > \xi; \\ 0 & \text{otherwise.} \end{cases}
\]

For the multivariate case, one may use the tensor product of univariate basis functions for splines as multivariate basis functions. However, if all tensor basis functions are used, the number of basis functions can be quite large, especially when many knots are used for each dimension. The tensor basis functions used in the proposed method only include basis functions of one the two forms: \( B_{a_1,\ldots,a_d} \), and \( p_{j_1,\ldots,j_d} \), where for real numbers \( a_1,\ldots,a_d \) and integers \( j_1,\ldots,j_d \in \{0,\ldots,3\} \),

\[
B_{a_1,\ldots,a_d}(x_1,\ldots,x_d) = \prod_{i=1}^d B_{a_i}(x_i)
\]

and

\[
p_{j_1,\ldots,j_d}(x_1,\ldots,x_d) = \prod_{i=1}^d p_{j_i}(x_i)
\]

for real numbers \( x_1,\ldots,x_d \). For the proposed method, the basis functions are selected from a collection of basis functions determined by some knot vectors \( \xi_1,\ldots,\xi_k \), where \( \xi_j = (\xi_{j_1},\ldots,\xi_{j_d}) \) is a \( d \)-dimensional vector for \( j = 1,\ldots,k \). Let \( S_{\xi_1,\ldots,\xi_k} \) denote the collection of basis functions determined by knot vectors \( \xi_1,\ldots,\xi_k \), then

\[
S_{\xi_1,\ldots,\xi_k} = S_0 \cup \{ B_{i_1,\ldots,i_d} : j \in \{1,\ldots,k\} \}
\]

(3)

where \( S_0 = \{ p_{j_1,\ldots,j_d} : j_1,\ldots,j_d \in \{0,\ldots,3\} \} \). Thus the approximation model for (1) considered in this study is

\[
Y = \sum_j \alpha_j B^*_j(X) + \varepsilon_i, i = 1, \ldots, n, \tag{4}
\]

where \( B^*_j \)s are some basis functions selected from \( S_{\xi_1,\ldots,\xi_k} \) and \( \alpha_j \)s are the coefficients. Next, we will give the details of the proposed estimation procedure in Section 2.1.

2.1. The proposed estimation procedure and the BIC-Backward algorithm
As mentioned before, for the proposed method, the basis functions are selected from \( S_{\xi_1, \ldots, \xi_k} \), which is defined in (3), where \( \xi_1, \ldots, \xi_k \) are knot vectors of dimension \( k \). In this section, we will give details of how to select the knot vectors.

To determine whether a knot vector \((\xi_1, \ldots, \xi_d)\) is needed, we construct a random test \((\xi, \delta, \psi, \xi, \delta, \psi)\), which is an extension of the test in [10]. The test \((\xi, \delta, \psi, \xi, \delta, \psi)\) is based on \((X_i, Y_i)\) s such that \( ||X_i - \xi|| < \delta \) and \( b^T(X_i - \xi) > 0 \). To obtain the test statistic, we generate IID coefficients \((X_i, \ldots, X_d)\) from the uniform distribution on \([-1,1]\). Let \( b = (b_1, \ldots, b_d) \) be the vector of the generated coefficients. The hyperplane \( \{x : b^T(x - \xi) = 0\} \) splits the \( X_i \) s such that \( ||X_i - \xi|| < \delta \) into two groups \( \{X_i : i \in \Lambda_1\} \) and \( \{X_i : i \in \Lambda_2\} \), where \( \Lambda_1 = \{i \in \{1, \ldots, n\} : ||X_i - \xi|| < \delta \text{ and } b^T(X_i - \xi) > 0\} \) and \( \Lambda_2 = \{i \in \{1, \ldots, n\} : ||X_i - \xi|| < \delta \text{ and } b^T(X_i - \xi) < 0\} \).

For \( j = 1, 2 \), let \( n_j \) be the number of elements in \( \Lambda_j \). If both \( n_1 \) and \( n_2 \) are at least 40, regress \( Y_i \) on tensor products of univariate linear functions of \( \{X_i : i \in \Lambda_j\} \), using linear regression and let \( \hat{a}_j \) be the \( 2d \times 1 \) least squared estimator of regression coefficient vector and \( RSS_j \) be the residual sum of squares. Then, compute the conditional covariance matrix of \( \hat{a}_1 - \hat{a}_2 \) given \( X_i \) s: \( i \in \Lambda_1 \cup \Lambda_2 \), assuming that the regression errors are \( \varepsilon_i \) s, and \( \varepsilon_i \) s are IID \( \mathcal{N}(0, \sigma^2) \) and are independent of \( X_i \) s. Under the above assumption, the conditional covariance matrix of \( \hat{a}_1 - \hat{a}_2 \) given \( X_i \) s: \( i \in \Lambda_1 \cup \Lambda_2 \) is \( \sigma^2 \) multiplied by a known matrix. Let \( \Sigma \) denote the matrix such that \( \sigma^2 \Sigma \) is the conditional covariance matrix of \( \hat{a}_1 - \hat{a}_2 \) given \( X_i \) s: \( i \in \Lambda_1 \cup \Lambda_2 \). Then the test statistic is given by

\[
W_k = \frac{(\hat{a}_1 - \hat{a}_2)^T \Sigma^{-1} (\hat{a}_1 - \hat{a}_2)}{\sigma^2},
\]

where

\[
\sigma^2 = \frac{RSS_1 + RSS_2}{n_1 + n_2 - 2}.
\]

The above process of generating \( b \) to obtain \( W_k \) is repeated until three \( W_k \) s are obtained. However, the number of repetitions is limited to 10. Let \( W \) be the maximum of the \( W_k \) s. The maximum is defined as \(-\infty\) if there is not any \( W_k \) obtained. Then \( W \) is the test statistic for \( \psi_{0.05, \delta, d} \). If \( W \) is greater than the 95% quantile of the \( \chi^2 \) distribution with \( 2d \) degrees of freedom, then \( \xi \) is considered as an important knot vector. The proposed estimation procedure for \( f \) is given below.

**Algorithm 2.**

- For \( j = 1, \ldots, 5 \), take \( \delta = 1/2^j \) and carry out Steps (i) and (ii).
  - (i) For \( i = 1, \ldots, n \), conduct the test \( \psi_{0.05, \delta, d} \). Select \( X_i \) as a knot vector if the \( p \)-value is less than 0.05.
  - (ii) Let \( \mathcal{X}_j \) be the set of selected knot vectors from (i). Take the regression model in (4) as the full model and then perform backward elimination of variables to obtain a sequence of reduced models. Choose the reduced model with the smallest BIC value. Let \( \text{BIC}_j \) denote the smallest BIC value.
Let $BIC_j$ be the smallest BIC value among $BIC_1, \ldots, BIC_5$. The estimated regression function in the model corresponding to $BIC_j$ is the final estimator of the regression function $f$.

For comparison purpose, another estimation method based on equally-spaced knots with backward elimination is considered. The method will be referred as BIC-Backward. The details of BIC-Backward are given below.

**Algorithm for BIC-Backward.**
- For $j = 1, \ldots, 4$, take $\delta = 1/2^j$. Let $(\xi_0, \ldots, \xi_k) = (\delta, 2\delta, \ldots, 1-\delta)$ be the $k$ equally spaced knot points in $(0, 1)$ with $k = 2^j - 1$. Let $S_{\mu,\delta}$ be the set of tensor basis functions, where for each dimension, the univariate basis functions are $p_0, \ldots, p_5, B_{3,\delta}, \ldots, B_{5,\delta}$.

  (i) Take the regression model in (4) as the full model with the basis functions $B_j$’s replaced by the basis functions in $S_{\mu,\delta}$ and then perform backward elimination of variables to obtain a sequence of reduced models. Choose the reduced model with the smallest BIC value. Let $BIC_j$ denote the smallest BIC value.
- Let $BIC_5$ be the smallest BIC value among $BIC_1, \ldots, BIC_5$. The estimated regression function in the model corresponding to $BIC_5$ is the final estimator of the regression function $f$.

Note that $j = 5$ is not used in the algorithm for BIC-Backward since the number of basis functions exceeds the sample size $n = 1000$ in such case.

### 3. Simulation results

A simulation experiment has been carried out to examine the performance of the proposed estimation procedure and the results are given in this section.

For the simulation experiment, the data generating process is described below. 100 data sets are generated from model (1) with $n = 1000$, $X_1, \ldots, X_n$ are IID random vectors from the uniform distribution on $(0,1)^2$, $\xi$ s are IID random variables from $N(0, \sigma^2)$ with various $\sigma$ values, and $f \in \{f_1, f_2, f_3\}$. Here $f_1$ is the probability density function for the bivariate normal distribution with mean $(0.4, 0.4)$ and diagonal covariance matrix with diagonal vector $(0.05, 0.05)$,

$$f_2(u,v) = \begin{cases} c(u/2,v/2) & \text{if } (u,v) \in [0.2,0.8]^2; \\ 0 & \text{otherwise.} \end{cases}$$

where $c$ is the density function of the Joe copula with parameter 40, and $f_3$ is the two dimensional AMH copula density with parameter $-0.8$. The cumulative distribution function of the Joe copula with parameter $\theta$ is the function $C_1$ given by

$$C_1(u,v) = 1 - ((1-u)^\theta + (1-v)^\theta - (1-u)^\theta(1-v)^\theta)^{1/\theta}$$

for $(u,v) \in (0,1)^2$. The cumulative distribution function of the AMH copula with parameter $\theta$ is the function $C_2$ defined by

$$C_2(u,v) = \frac{uv}{1 - \theta(1-u)(1-v)}$$

for $(u,v) \in (0,1)^2$. The graphs of $f_1, f_2, f_3$ on $(0,1)^2$ are shown in the left, middle and right panels of figure 1 respectively.
Figure 1. Graphs of $f_1, f_2, f_3$.

For each of the generated data set, the proposed method (Algorithm 2) is applied to obtain an estimated regression function $\hat{f}$. The mean squared error

$$\frac{1}{n} \sum_{i=1}^{n} (\hat{f}(X_i) - f(X_i))^2$$

is computed to evaluate the estimation accuracy. For comparison purpose, the algorithm for BIC-Backward is also applied to generated data sets. For each of the three functions $f_1, f_2, f_3$ and for each $\sigma$, the mean and standard deviation of the 100 mean squared errors are reported in Table 1 for the BIC-Backward method and the proposed method. The $\sigma$ values are chosen so that the ratio

$$r = \frac{E|f(X)|}{\sigma}$$

is about 140 or 7 when the distribution of $X$ is the uniform distribution on $(0,1)^d$.

From the results in Table 1, for $f_1$ and $f_2$, which need to be approximated by splines with many knots, the proposed method performs better than the BIC-Backward method when $\sigma$ is small, and the BIC-Backward method performs better than the proposed method when $\sigma$ is large. For $f_3$, which is a smooth function, the proposed method performs better for the large $\sigma$ case, and the BIC-Backward method performs better for the small $\sigma$ case.

Table 1. Averages and standard deviations for mean squared errors.

| $\sigma$ | BIC-Backward | Algorithm 2 |
|---------|--------------|-------------|
| $f_1$   | 3.890 × 10^{-2} | 7.695 × 10^{-5} (2.629 × 10^{-5}) | 2.989 × 10^{-5} (1.023 × 10^{-5}) |
| $f_1$   | 7.781 × 10^{-1} | 2.316 × 10^{-1} (3.644 × 10^{-3}) | 2.911 × 10^{-1} (2.880 × 10^{-3}) |
| $f_2$   | 2.117 × 10^{-2} | 1.697 × 10^{-4} (8.929 × 10^{-5}) | 1.463 × 10^{-4} (7.026 × 10^{-5}) |
| $f_2$   | 4.234 × 10^{-1} | 2.2189 × 10^{-1} (8.949 × 10^{-2}) | 2.527 × 10^{-1} (6.812 × 10^{-2}) |
| $f_3$   | 1.636 × 10^{-3} | 1.322 × 10^{-7} (2.608 × 10^{-8}) | 1.271 × 10^{-6} (1.562 × 10^{-7}) |
| $f_3$   | 3.272 × 10^{-2} | 2.2534 × 10^{-5} (7.555 × 10^{-6}) | 2.100 × 10^{-5} (6.142 × 10^{-6}) |

4. Discussion and conclusions

In this article, an estimation procedure for nonparametric regression is proposed. The proposed procedure is based on spline approximation and a knot vector selection step is involved. The knot vector selection step is adapted from the univariate knot selection algorithm in [10]. One major modification is that the requirement that the distance between two knots is at least $\delta$ is removed so that knot vectors that are close to one another may be selected when necessary. To avoid the overfitting
problem when too many knot vectors are selected, the backward elimination step is included in the proposed procedure.

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