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Multivariate regression splines

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Abstract

Multivariate regression splines of arbitrary order assuming known knots using the additional function are developed. Model description and possible parameter tests for obtaining regression splines are also stated in detail for the triplicate case. A simulation study of drawn data from the Lubricant nonlinear regression model, where "Lubricant" is referred to lubricant data that we use in application, to compare the mean squares errors for the multivariate regression spline models and the multivariate polynomial models show the need of employing the multivariate regression splines in the approximation of the nonlinear regression models. © 1997 Elsevier Science B.V.

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1. Introduction

A problem common to many disciplines is that of adequately approximating a regression function of one or several independent variables, given only the value of the function perturbed by noise at various points in the dependent variable space. Smoothing techniques are an important approach to approximating the regression function with a minimum of preconceptions and assumptions as to what this function should be.

There are three main approaches to spline fitting. The roughness penalty approximations minimize a criterion that depends on a least-squares-like term plus a term penalizing roughness, where a parameter λ that regulates the tradeoff between the roughness of the regression function and its smoothness to the data has to be predetermined. Interesting work on this topic includes Kimeldorf and Wahba (1971), Wahba (1985, 1990), and Gu and Wahba (1993); Wahba (1985) and Gu and Wahba (1993) presented the multivariate thin-plate splines. Although techniques have been proposed for computing the smoothness parameter λ (see Cleveland, 1979; Wahba, 1979), there is no satisfactory general method for computing λ.

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The locally weighted regression method estimates the regression function to data by locally weighted least-squares fitting. Recent work on this topic includes Cleveland and Devlin (1988) and Cleveland et al. (1993). Algorithms for computing this spline function has been proposed by Cleveland et al. (1988). A weight function that weights the mass of observations of independent variables must be selected. However, the choice of an appropriate weight function in high dimensions is still difficult, and this is a computer intensive method.

The so-called regression spline or the least-squares spline approximates the regression function by piecewise polynomials, each defined over a different subregion of the domain of the spline. The approximation is constrained to be everywhere continuous, and sometimes it has continuous lower order derivatives or partial derivatives for the multivariate case as well. Several approaches to constructing regression splines have been presented in the literature. Poirier introduced the cubic spline (1973) and the bilinear spline (1975). Buse and Lim (1977) proved that the cubic spline can be computed by the restricted least-squares method. Later, Smith (1979) showed that the univariate regression splines of any degree of regression function may be represented in the additional function. This enables us to compute univariate regression splines simply by the least squares method. As a bivariate generalization, the bilinear spline presented by Poirier (1975) is a model of continuous piecewise bivariate polynomial function of order two. Eubank (1988, p. 372) pointed out that multivariate regression splines have received only cursory attention and further research is required before multivariate regression splines can become a standard method of multivariate surface fitting. Although recently Chen (1996) proposed a bivariate regression spline of arbitrary finite polynomial order by the restricted least-squares method, this method is difficult in generalization to higher dimensional model and is very complicated in constructing statistical inferences such as variables elimination for determining spline model because of complicated restriction method. Besides the three approaches stated above to spline fitting, there are some other multivariate fitting approaches in the literature; for example, Friedman (1991) and Stone (1994).

This paper provides a unified study of the multivariate regression splines of arbitrary finite dimension and polynomial order using the convenient additional function. This spline function not only generalize the regression spline to higher dimension but also greatly simplifies the statistical inferences, using, for example, F-test and t-test, for selecting regression spline models. We develop the multivariate regression splines by deriving bases of the smoothing regression functions. Various regression splines can also be obtained simply by removing terms from a piecewise multivariate polynomial function. A model description in detail and parameter tests for determining the spline model are given in the triplicate case. A simulation of the Lubricant nonlinear regression approximating by the multivariate polynomial and the multivariate regression splines reveals the advantages of fitting the data drawn from an unknown nonlinear regression model by the multivariate regression splines.

We will proceed as follows. In Section 2 we introduce and derive the multivariate regression splines. A detail discussion on statistical inferences of spline model selection in triplicate case is given in Section 3. Section 4 provides the simulation result. Finally, the proofs of lemmas and theorems are given in the Appendix.

2. Multivariate regression splines

Let $x_1,\dots,x_p$, $p>1$, be independent variables that are related to the response variable y. Consider the joint-points $\{\delta^i_{s_i}: s_i=0,1,\dots,a_i\}$, with $a_i \geq 1$, $i=1,\dots,p$, the elements of which are known as knots. These joint-points define a p-dimensional rectangular grid in the space of variables $x_1,\dots,x_p$ consisting of $a_1,\dots,a_p$ multivariate rectangles as the region set:

$$\{(x_1,\dots,x_p):\ \delta^i_{s_i} < x_i \leq \delta^i_{s_{i+1}},\ i=1,\dots,p\},\quad s_i=0,1,\dots,a_i,\ i=1,\dots,p. \tag{2.1}$$

Here $\delta^i_0, \delta^i_{a_i+1}$ are set such that the region $\{(x_1,\dots,x_p): \delta^i_0 < x_i < \delta^i_{a_i+1},\ i=1,\dots,p\}$ is the bounded domain of the regression function. The regression function has order k, which defines on each multivariate rectangle a multivariate polynomial of the following form:

$$\sum_{c_1+\cdots+c_p=0}^{k} \beta_{c_1\dots c_p} \prod_{i=1}^{p} x_i^{c_i}, \tag{2.2}$$

where $c_1,\dots,c_p$ are nonnegative integers and $\prod$ denotes for product of polynomial functions. In the following, we state the setting of the piecewise multivariate polynomial regression model.

Definition 2.1. (a) An order k piecewise multivariate polynomial function is a function defined on the region of (2.1) such that each multivariate rectangle $\{(x_1,\dots,x_p)$: $\delta^i_{s_i-1} < x_i \leq \delta^i_{s_i},\ i=1,\dots,p\}$ has an order k multivariate polynomial defined on it.

(b) An order k piecewise multivariate polynomial regression model is the following:

$$y=f(x_1,\dots,x_p)+\varepsilon \tag{2.3}$$

for which f is an order k piecewise multivariate polynomial function and ε is the error term.

The class of order k piecewise multivariate polynomial function is a vector space with dimension $\binom{p+k}{p}\prod_{i=1}^{p}(a_i+1)$. The multivariate regression spline is then a model (2.3) for which the regression function f satisfies some continuity condition of partial derivatives.

Definition 2.2. (a) An order k piecewise multivariate polynomial function of model (2.3) is said to be a multivariate regression spline if it has some continuous partial derivatives.

(b) A multivariate regression spline is said to have continuity-degree $j, 0 \leq j \leq k-1$, if its $(j_1,\dots,j_p)$-th partial derivative is continuous for $0 \leq j_1+\cdots+j_p \leq j$.

We now state an equivalent form of the order k piecewise multivariate polynomial function, which generalizes the formulation of the piecewise univariate polynomial function in Nurnberger (1989) to the multivariate case.

Lemma 2.3. *The order k piecewise multivariate polynomial function can be formulated in the form,*

$$P+\sum_{s=1}^{p}\sum_{t_s=1}^{a_s} P^{t_s} I(x_s>\delta^s_{t_s})$$

$$\sum_{1\le s_1<s_2\le p}\sum_{t_{s_2}=1}^{a_{s_2}}\sum_{t_{s_1}=1}^{a_{s_1}} P^{t_{s_1}t_{s_2}} I(x_{s_1}>\delta^{s_1}_{t_{s_1}},\ x_{s_2}>\delta^{s_2}_{t_{s_2}})$$

$$\vdots$$

$$+\sum_{t_p=1}^{a_p}\cdots\sum_{t_1=1}^{a_1} P^{t_1\dots t_p} I(x_1>\delta^1_{t_1},\dots,x_p>\delta^p_{t_p}),$$

where $P^{\cdots}$ are multivariate polynomials with the form of (2.2).

Denote the additional function "+" by $x_+=\max\{x,0\}$. The next result provides a basis based on additional function for the space of order k piecewise multivariate polynomial functions that guides an easy way to construct multi-variate regression splines.

Theorem 2.4. *The following set is a basis for the space of order k piecewise multivariate polynomial functions,*

$$\prod_{i=1}^{p} x_i^{c_i},\ \prod_{i\ne s} x_i^{c_i}(x_s-\delta^s_{t_s})_+^{c_s},\quad \prod_{i\ne s_1,s_2} x_i^{c_i}(x_{s_1}-\delta^{s_1}_{t_{s_1}})_+^{c_{s_1}}(x_{s_2}-\delta^{s_2}_{t_{s_2}})_+^{c_{s_2}},\dots,\quad \prod_{i=1}^{p}(x_i-\delta^i_{t_i})_+^{c_i}, \tag{2.4}$$

where nonnegative integers $c_1,\dots,c_p$ satisfy that $0\le\sum_{i=1}^{p}c_i\le k$, and domain of t_i is $1,\dots,a_i$ for $i=1,\dots,p,s,s_1$ and s_2, etc.

We can easily check that the number of basis functions above is exactly the necessary integer $\binom{p+k}{p}\prod_{i=1}^{p}(a_i+1)$. With Theorem 2.4, any linear combination of the functions in the basis of (2.4) provides some kind of multivariate regression spline. However, the interesting regression spline might be the one with continuity-degree $j\in\{0,1,\dots,k-1\}$. We now state it in the following theorem.

Theorem 2.5. *Let $b=\min\{b^*,p\}$, where $b^*=\max\{b_0: b_0(j+1)\le k,\ b_0$ is integer$\}$. The set of the following functions is a basis of the space of order k multivariate* *regression splines with continuity-degree j*:

$$\prod_{i=1}^{p} x_i^{c_i}, \quad (x_s - \delta_{t_s}^s)_+^{c_s} \prod_{i \neq s} x_i^{c_i}, \quad (x_{s_1} - \delta_{t_{s_1}}^{s_1})_+^{c_{s_1}} (x_{s_2} - \delta_{t_{s_2}}^{s_2})_+^{c_{s_2}} \prod_{i \neq s_1, s_2} x_i^{c_i}, \ldots,$$

$$\prod_{i=1}^{b} (x_{s_i} - \delta_{t_{s_i}}^{s_i})_+^{c_{s_i}} \prod_{i \neq s_1, \ldots, s_b} x_i^{c_i}, \tag{2.5}$$

where c_s, c_{s_i} *are restricted on the set* $\{j+1,\ j+2, \ldots, k\}$ *and* $c_1, \ldots, c_p$ *satisfy* $\sum_{i=1}^{p} c_i \leq k$. *Also, domain of* t_i *is* $1, \ldots, a_i$.

In the particular case where $j = k-1$, the smoothest multivariate regression spline might be of great interest.

Corollary 2.6. *The smoothest multivariate regression spline can be formulated as*

$$y = \sum_{c_1 + \cdots + c_p = 0}^{k} \beta_{c_1 \cdots c_p} \prod_{i=1}^{p} x_i^{c_i} + \sum_{s=1}^{p} \sum_{t_s=1}^{a_s} \beta_k^{t_s} (x_s - \delta_{t_s}^s)_+^k + \varepsilon.$$

3. Triplicate regression spline and statistical inferences for model selection

This representation of regression spline based on basis is clearly a very useful one since it casts the spline problem into an ordinary multiple regression context. Moreover, many of the F-test, t-test, and nonparametric test procedures for determining whether some of the polynomial coefficients should be zeros carry over directly. For explanation, we consider in this section the case of $p = 3$ in detail including bases in various continuity degrees and possible parameter tests. For this triplicate case, let the joint-points be redenoted by δ_s, γ_t and α_u where $s = 0, 1, \ldots, a+1$, $t = 0, 1, \ldots, b+1$ and $u = 0, 1, \ldots, d+1$. Define triplicate spline function sets:

$$B_0 = \{x_1^{c_1} x_2^{c_2} x_3^{c_3}\},$$

$$B_1 = \{(x_1 - \delta_s)_+^{c_1} x_2^{c_2} x_3^{c_3} : j+1 \leq c_1 \leq k,\ (x_2 - \gamma_t)_+^{c_2} x_1^{c_1} x_3^{c_3} : j+1 \leq c_2 \leq k,$$
$$(x_3 - \alpha_u)_+^{c_3} x_1^{c_1} x_2^{c_2} : j+1 \leq c_3 \leq k\},$$

$$B_2 = \{(x_1 - \delta_s)_+^{c_1} (x_2 - \gamma_t)_+^{c_2} x_3^{c_3} : j+1 \leq c_i \leq k,\ i = 1, 2,$$
$$(x_1 - \delta_s)_+^{c_1} (x_3 - \alpha_u)_+^{c_3} x_2^{c_2} : j+1 \leq c_i \leq k,\ i = 1, 3,$$
$$(x_2 - \gamma_t)_+^{c_2} (x_3 - \alpha_u)_+^{c_3} x_1^{c_1} : j+1 \leq c_i \leq k,\ i = 2, 3\},$$

$$B_3 = \{(x_1 - \delta_s)_+^{c_1} (x_2 - \gamma_t)_+^{c_2} (x_3 - \alpha_u)_+^{c_3} : j+1 \leq c_i \leq k,\ i = 1, 2, 3\}.$$

where c_1, c_2 and c_3 are nonnegative integers also satisfy $0 \leq c_1 + c_2 + c_3 \leq k$, and s, t, and u are positive integers with $1 \leq s \leq a$, $1 \leq t \leq b$, and $1 \leq u \leq d$.

The following corollary specifies the bases for triplicate regression spline in various continuity degrees.

Corollary 3.1. *The followings indicate bases for the vector spaces of triplicate regression splines in various continuity degrees*:

$$\{B_0, B_1, B_2, B_3\} \quad \text{if } 0 \le j \le k/3 - 1,$$
$$\{B_0, B_1, B_2\} \quad \text{if } k/3 - 1 < j \le k/2 - 1,$$
$$\{B_0, B_1\} \quad \text{if } k/2 - 1 < j \le k - 1,$$
$$\{B_0\} \quad \text{if } j = k. \tag{3.1}$$

We now state some possible parameter tests for determining various triplicate regression splines. A piecewise triplicate polynomial regression model can be formulated as

$$\begin{aligned} y = &\sum_{c_1+c_2+c_3=0}^{k} \beta_{c_1c_2c_3} x_1^{c_1} x_2^{c_2} x_3^{c_3} + \sum_{s=1}^{a} \sum_{c_1+c_2+c_3=0}^{k} \beta^{s}_{c_1c_2c_3} (x_1 - \delta_s)_+^{c_1} x_2^{c_2} x_3^{c_3} \\ &+ \sum_{t=1}^{b} \sum_{c_1+c_2+c_3=0}^{k} \beta^{t}_{c_1c_2c_3} (x_2 - \gamma_t)_+^{c_2} x_1^{c_1} x_3^{c_3} + \sum_{u=1}^{d} \sum_{c_1+c_2+c_3=0}^{k} \beta^{u}_{c_1c_2c_3} (x_3 - \alpha_u)_+^{c_3} x_1^{c_1} x_2^{c_2} \\ &+ \sum_{s=1}^{a} \sum_{t=1}^{b} \sum_{c_1+c_2+c_3=0}^{k} \beta^{st}_{c_1c_2c_3} (x_1 - \delta_s)_+^{c_1} (x_2 - \gamma_t)_+^{c_2} x_3^{c_3} + \sum_{s=1}^{a} \sum_{u=1}^{d} \sum_{c_1+c_2+c_3=0}^{k} \\ &\times \beta^{su}_{c_1c_2c_3} (x_1 - \delta_s)_+^{c_1} (x_3 - \alpha_u)_+^{c_3} x_2^{c_2} + \sum_{t=1}^{b} \sum_{u=1}^{d} \sum_{c_1+c_2+c_3=0}^{k} \beta^{tu}_{c_1c_2c_3} (x_2 - \gamma_t)_+^{c_2} (x_3 - \alpha_u)_+^{c_3} x_1^{c_1} \\ &+ \sum_{s=1}^{a} \sum_{t=1}^{b} \sum_{u=1}^{d} \sum_{c_1+c_2+c_3=0}^{k} \beta^{stu}_{c_1c_2c_3} (x_1 - \delta_s)_+^{c_1} (x_2 - \gamma_t)_+^{c_2} (x_3 - \alpha_u)_+^{c_3} + \varepsilon. \end{aligned}$$

The dimension of the piecewise triplicate polynomial function is

$$6^{-1}(k+3)(k+2)(k+1)(a+1)(b+1)(d+1).$$

The dimension could be a very large number when any of k, a, b, and d is large. Then, in addition to the consideration of smoothness, some kind of smoother regression spline with smaller number of parameters we might want to use for analyzing the data with number of observations not large enough.

To be specific, let us illustrate the possible parameter tests by the use of the additional function to determine triplicate regression splines. Presence of the term $\beta^{s}_{c_1c_2c_3}$ allows a discontinuity on the hyperplane $x_1 = \delta_s$ in the $(c_1c_2c_3)$-th partial derivative of the spline function, and the presence of the term $\beta^{st}_{c_1c_2c_3}$, for any $(s,t), s, t \ne 0$, further allows discontinuity on both hyperplanes $x_1 = \delta_s$ and $x_2 = \gamma_t$ in the $(c_1c_2c_3)$-th partial derivative of the spline function. On the other hand, the absence of $\beta^{stu}_{c_1c_2c_3}$ for all t and u forces the $(c_1c_2c_3)$-th partial derivative of the spline function on $x_1 = \delta_s$ to be continuous.

Additional smoother surfaces can be obtained by removing appropriate terms from the piecewise triplicate polynomial function. Because most regression functions are very smooth, multivariate polynomials are infinitely differentiable on every hyperplane, thus it is not unreasonable to assume as much smoothness as possible in a spline model. Therefore, testing the importance of j continuity-degree for the model in (3.1) may be of interest to obtain a smoother regression surface. However, we should know that the more parameter terms we delete from the regression function the worse the fit will be, although the fitting surface will be smoother.

4. Numerical example

Linssen (1975) studied the kinematic viscosity of a lubricant as a function of temperature and pressure in atmosphere. In his study, the viscosity is suitable represented by the following, called Lubricant nonlinear regression model,

$$y = \theta_1(\theta_2 + x_1)^{-1} + \theta_3 x_2 + \theta_4 x_2^2 + \theta_5 x_2^3 + (\theta_6 + \theta_7 x_2^2)x_2 \\ \times \exp(-x_1(\theta_8 + \theta_9 x_2^2)^{-1}) + \varepsilon,$$

where y, x_1 and x_2 represent viscosity, temperature and pressure, respectively. We now pretend that the true regression model is unknown and we are going to fit the data from the Lubricant model by the multivariate polynomial regression model and the bivariate regression spline model. In this simulation, the computer facility include the S^+ simulated on the Sparc 20 Sun Work Station. With setting $\theta_i = 1$, $i = 1, \dots, 9$, we randomly generate 160 observations for each replication from the region $\{0 < x_1 < 20, 0 < x_2 < 20\}$ with $\varepsilon \sim N(0,1)$. For each data we apply the least squares method to compute the bivariate polynomial estimate from order 1 to 12 and the 4 pieces bivariate regression spline with knots $\delta_1 = 10$, and $\gamma_1 = 10$ from order 1 to 3. The replication is 1000. Here the bivariate regression spline is based on the following basis:

$$\{x_1^{c_1} x_2^{c_2},\ (x_1 - 10)_+^{c_1} x_2^{c_2},\ (x_2 - 10)_+^{c_2} x_1^{c_1},\ (x_1 - 10)_+^{c_1}(x_2 - 10)_+^{c_2}\},$$

where c_1 and c_2 are with $0 \le c_1 + c_2 \le k$.

Tables 1 and 2 provide the mean squares errors (MSE) where the values in the brackets represent the numbers of variables in the polynomial model or the regression spline.

Table 1
MSE for fitting Lubricant model by polynomial regression

Polynomial order	MSE	Polynomial order	MSE
1	3 103 486	9	946
3	2590	11	1086
5	1580	13	1148
7	980		

Table 2
MSE for fitting Lubricant model by regression spline

Spline order	MSE
1(12)	248 684
2(24)	1168
3(40)	1.325

Table 3
Variables which occurred more than 200 times and their corresponding MSEs

$\begin{pmatrix}\text{Spline order}\\ \text{MSE}\end{pmatrix}$	Variables
$\begin{pmatrix}3\\ 13.740\end{pmatrix}$	$x_2, x_1^2, x_2^2, x_1x_2, x_2^3, x_1x_2^2,$ $(x_2-10)_+^0, (x_2-10)_+, x_1(x_2-10)_+,$ $(x_2-10)_+^2, x_1(x_2-10)_+^2, (x_1-10)_+^3, (x_2-10)_+^3$
$\begin{pmatrix}4\\ 13.976\end{pmatrix}$	$x_1, x_2, x_2^2, x_1x_2, x_1^3, x_2^2, x_1x_2^2, x_1x_2^3,$ $x_1(x_2-10)_+^0, x_1(x_2-10)_+, x_1(x_2-10)_+^2,$ $x_1(x_2-10)_+^3, (x_1-10)_+^4$

Although the true regression function is smooth, the large mean squares errors imply that the polynomial function is not adequate in fitting the data from the Lubricant nonlinear regression model. However, a four-piece bivariate regression spline of order 3 is already adequate in approximating the data from the nonlinear regression model.

It is then concluded that the regression splines of order 3 or 4 are appropriate to approximate the Lubricant nonlinear regression model. Since the true model contains only 9 unknown parameters, the 4-piece bivariate regression splines of order 3 and 4 contain parameters of number 40 and 60, respectively. It is then interesting to see if there is a still smaller scale of bivariate regression splines which can adequately interprete the Lubricant nonlinear regression model. For this purpose, we perform a simulation of 500 replications of data drawn from the Lubricant model. For each replication, Efroymson's forward stepwise method is used for selecting the variable sets from the orders 3 and 4 bivariate regression spline models. We then collect the variables that appear more than 200 and 400 times as listed in Tables 3 and 4.

A simulation of 1000 replications for data drawn from the Lubricant model and using the selected models in Tables 3 and 4 to fit the data is then further conducted. Their corresponding mean squares errors are also listed in Tables 3 and 4.

Table 4
Variables which occurred more than 400 times and their corresponding MSEs

$\binom{\text{Spline order}}{\text{MSE}}$	Variables
$\binom{3}{37.725}$	$x_2, x_2^2, x_1x_2, x_2^3, x_1x_2^2, (x_2-10)_+,$ $x_1(x_2-10)_+, (x_2-10)_+^2, x_1(x_2-10)_+^2, (x_2-10)_+^3$
$\binom{4}{352.61}$	$x_2^3, x_1x_2^2, x_1x_2^3, x_1(x_2-10)_+^2, x_1(x_2-10)_+^3$

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Appendix

Proof of Lemma 2.3. Let $m_{pq} = \min\{p,q\}$. For $0 \le q \le \sum_{i=1}^{p} a_i - 1$, denote order k piecewise multivariate polynomial

$$f_q = f_q^1 + f_q^2, \tag{A.1}$$

where

$$\begin{aligned} f_q^1 = {} & P_0 + \sum_{s=1}^{p} \sum_{t_s}^{\min\{q,a_s\}} P_{t_s}^{t_s} I(x_s > \delta_{t_s}^s) \\ & + \sum_{1 \le s_1 < s_2 \le p} \sum_{\substack{t_{s_1}+t_{s_2}=2 \\ 1 \le t_{s_i} \le a_{s_i}}}^{q} P_{t_{s_1}+t_{s_2}}^{t_{s_1} t_{s_2}} I(x_{s_1} > \delta_{t_{s_1}}^{s_1}, x_{s_2} > \delta_{t_{s_2}}^{s_2}) \\ & \vdots \\ & + \sum_{1 \le s_1 < \cdots < s_{m_{pq}} \le p} \sum_{\substack{t_{s_1}+\cdots+t_{s_{m_{pq}}}=q \\ 1 \le t_{s_i} \le a_{s_i}}} P_{t_{s_1}+\cdots+t_{s_{m_{pq}}}}^{t_{s_1} t_{s_2} \ldots t_{s_{m_{pq}}}} \\ & I(x_{s_i} > \delta_{t_{s_i}}^{s_i},\ i = 1, \ldots, m_{pq}) \end{aligned}$$

and

$$f_q^2 = \sum_{t_1+\cdots+t_p=q+1}^{a_1+\ldots+a_p} P_q^{t_1 \ldots t_p} I(\delta_{t_i}^i < x_i \le \delta_{t_i+1}^i,\ i = 1, \ldots, p),$$

where $P_q^{\cdots}$ has the form of (2.2). We further let

$$f_q^{20} = \sum_{t_1+\cdots+t_p=q+1} P_q^{t_1\cdots t_p} I(\delta_{t_i}^i < x_i \le \delta_{t_i+1}^i,\ i = 1,\ldots,p).$$

Consider the decomposition $f_q^{20} = B_q + (f_q^{20} - B_q)$, where

$$\begin{aligned} B_q = &\sum_{s=1}^{p} P_q^{q+1} I(x_s > \delta_{q+1}^s,\ q+1 \le a_s) \\ &+ \sum_{1\le s_1<s_2\le p} \sum_{\substack{t_{s_1}+t_{s_2}=q+1 \\ 1\le t_{s_i}\le a_{s_i}}} P_q^{t_{s_1}t_{s_2}} I(x_{s_i} > \delta_{t_{s_i}}^{s_i},\ i = 1,2) \\ &\vdots \\ &+ \sum_{1\le s_1<\cdots<s_{m_{pq}}\le p} \sum_{\substack{t_{s_1}+\cdots+t_{s_{m_{pq}}}=q+1 \\ 1\le t_{s_i}\le a_{s_i}}} P_q^{t_{s_1}\ldots t_{s_{m_{pq}}}} I(x_{s_i} > \delta_{t_{s_i}}^{s_i},\ i = 1,\ldots,m_{pq}). \end{aligned}$$

We will show that for each piecewise multivariate polynomial f and $0 \le q \le \sum_{i=1}^p a_i - 1$ there exists a piecewise multivariate polynomial f_q of (A.1) such that $f = f_q$. Let $q = 0$. Obviously,

$$f = P + \sum_{t_1+\cdots+t_p=1}^{a_1+\cdots+a_p} P_1^{t_1\ldots t_p} I(\delta_{t_i}^i < x_i \le \delta_{t_i+1}^i,\ i = 1,\ldots,p)$$

with $P_1^{t_1\ldots t_p} = P^{t_1\ldots t_p} - P$. Denote by $P_0 = P$. Then $f = f_0$. Suppose that $f = f_q$ $(= f_q^1 + f_q^2)$. Can check that $f_q^{20} - B_q$ and $f_q^2 - f_q^{20}$ are all piecewise multivariate polynomials defined on the region

$$\bigcup_{t_1+\cdots+t_p=q+2}^{a_1+\cdots+a_p} \{(x_1,\ldots,x_p) : \delta_{t_i}^i < x_i \le \delta_{t_i+1}^i,\ i = 1,\ldots,p\}.$$

We now define polynomials $P_{q+1}^{t_1\ldots t_p}$. Denote polynomial $P_q^{t_1\ldots t_p}$ by $P_{q+1}^{t_1\ldots t_p}$ for which $P_q^{t_1\ldots t_p}$ is the polynomial of B_q defined on region $\{(x_1,\ldots,x_p) : \delta_{t_i}^i < x_i,\ i = 1,\ldots,p\}$. For $(t_1,\ldots,t_p)$ be such that $\sum_{i=1}^p t_i \ge q+2$, let $P_{q+1}^{t_1\ldots t_p}$ be such that $f_{q+1}^2 = f_q^2 - B_q$. We can also see that $f_q^1 + B_{q+1} = f_{q+1}^1$. Then we have

$$f = f_q^1 + B_q + f_q^2 - B_q = f_{q+1}^1 + f_{q+1}^2 = f_{q+1}.$$

The proof is completed by setting $q = \sum_{i=1}^p a_i - 1$.

Proof of Theorem 2.4. Denote by $\bar{y} = y_1, \ldots, y_p$ for any finite set $\{y_1, \ldots, y_p\}$. Define a set of polynomial functions and truncated polynomial functions ψ by

$$\psi_{\pi s_i, \pi c_i}(\bar{x}) = \left(\prod_{i=1}^{p} c_i\right)^{-1} \prod_{i=1}^{p} [(x_i - \delta^i_{s_i})_+^{c_i} I(s_i > 0) + x_i^{c_i} I(s_i = 0)],$$
$$0 \le c_i \le k, s_i = 0, 1, \ldots, a_i, i = 1, \ldots, p. \tag{A.2}$$

(A.2) also has number of elements $\binom{k+p}{p} \prod_{i=1}^{p}(a_i + 1)$ and each element of them can be formulated as a linear combination of functions in (2.4). So the proof of this theorem is finished if we can show that the functions ψ of (A.2) are linearly independent. For $t_i = -, +,\ i = 1, \ldots, p$, let the partial derivative be

$$\psi^{\pi c_i^0}(\delta^{t_1}_{s_1^0}, \ldots, \delta^{t_p}_{s_p^0}) = \frac{\partial \sum_{i=1}^{p} c_i^0}{\pi \partial x_i^{c_i^0}} \psi_{\pi s_i, \pi c_i}(\bar{x})\Big|_{x_i = \delta^{t_i}_{s_i^0}}, \quad i = 1, \ldots, p.$$

We also define the linear function $\lambda_{\pi s_i^0, \pi c_i^0}$ on ψ by

$$\lambda_{\pi s_i^0, \pi c_i^0}(\psi) = \sum_{t_p = -, +} \cdots \sum_{t_1 = -, +} (-1)^{\sum_{i=1}^{p} \ell(t_i)} \psi^{\pi c_i^0}(\delta^{t_1}_{s_1^0}, \ldots, \delta^{t_p}_{s_p^0}), \tag{A.3}$$

where ℓ is the binary function defined by $\ell(t) = 1$ if $t = +$ and 0 if $t = -$. If we let

$$h_m(x_m) = \sum_{\substack{t_i = -, + \\ i = 1, \ldots, p \\ i \ne m}} (-1)^{\sum_{i \ne m} \ell(t_i)} \psi^{\pi_{i \ne m} c_i^0}(\delta^{t_1}_{s_1^0}, \ldots, x_m, \ldots, \delta^{t_p}_{s_p^0})$$

has continuous c_mth derivative at $\delta_{s_m^0}$, then

$$\lambda_{\pi s_i^0, \pi c_i^0}(\psi) = -\frac{\partial^{c_m}}{\partial x_m^{c_m}} h_m(x_m)\Big|_{x_m = \delta^+_{s_m^0}} + \frac{\partial^{c_m}}{\partial x_m^{c_m}} h_m(x_m)\Big|_{x_m = \delta^-_{s_m^0}} = 0.$$

With careful inspection, it can be seen that

$$\lambda_{\pi s_i^0, \pi c_i^0}(\psi) = \begin{cases} 1 & \text{if } s_i^0 = s_i, c_i^0 = c_i,\ i = 1, \ldots, p, \\ 0 & \text{otherwise.} \end{cases} \tag{A.4}$$

Any zero linear combination of (A.2) will have zero coefficients by (A.4). This shows that the set $\{\psi_{\pi s_i, \pi c_i}(\bar{x})\}$ is linearly independent and then the set of functions in (2.4) is a basis of the space of order k piecewise multivariate polynomial functions.

Proof of Theorem 2.5. The functions in (2.5) is a subset of the basis in (2.4). Denote this subset by B_j. We then know that B_j is a linearly independent set. We can also check that each element in B_j is a j continuity-degree polynomial or truncated polynomial. We then need only to show that these functions in B_j forms a generator of multivariate regression splines of continuity-degree j. The proof is an analogue of the one for proving the linear independence of the set in (2.4). We here only briefly sketch it.

Suppose that we have a multivariate regression splines of continuity-degree j. Denote it by f. Obviously, f can be formulated as a linear function in elements of (2.4). We then need only to show that the coefficients associated with the elements not in (2.5) have to be zeros. Consider the linear function $\lambda_{\pi s_i \pi c_i}$ of (A.3) for those $(s_1,\ldots,s_p)$ and $(c_1,\ldots,c_p)$ not in (2.5). Then smoothness condition of continuity-degree j on f implies that (A.4) holds and then the coefficients corresponding to the elements not in (2.5) are zeros. So, the set of elements in (2.5) is a generator of the class of multivariate regression splines of continuity-degree j.

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