ELSEVIER Computational Statistics & Data Analysis 21 (1996) 399–418

COMPUTATIONAL STATISTICS & DATA ANALYSIS

Bivariate regression splines

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Received May 1993; revised May 1995

Abstract

Towards the construction of multivariate spline functions, we introduce a way to set linear restrictions in the generation of bivariate regression splines. The hyperplanes in $\mathbb{R}^2$ are used in the role of "knot" to slice the domain of explanatory variables; hence, we have the flexibility in domain partition which includes rectangle, parallelogram, trapezoid and trapezium.

Keywords: Bivariate regression spline; Hyperplane; Linear restriction; Piecewise polynomial

1. Introduction

A standard way to approximate the cause-and-effect relationship is a single model over the entire range of explanatory variables, for example, models for linear or polynomial regression. In practice, it might be more realistic to partition the range of explanatory variables as disjoint regimes and to approximate the relationship by a sequence of submodels which is smoothly connected, in some sense, at the boundaries of neighboring regimes. A useful technique for this purpose is the spline function.

Among many approaches to define spline functions, three are widely used. The first is the interpolating spline function, a piecewise polynomial generated completely by interpolating the data points and satisfying conditions of continuous derivatives up to a required order. This method is useful only for fitting nonnoisy data and is then unsuitable for statistical data analysis. The second is the smoothing spline, a solution to an optimization problem of minimizing a sum of a least-squares-like term and a term penalizing roughness. The other is the regression spline which is a piecewise polynomial calculating its parameters by least-squares technique with imposed conditions of continuous derivatives up to a required order. For general accounts of splines, the paper by Wegman and Wright (1983)

SSDI 0167-9473(94)00026-7

provides a clear review of splines of these and other kinds; the book by Eubank (1988) provides a good introduction of the theory of smoothing splines.

Being a smooth piecewise polynomial, the regression spline has received much attention from statisticians. Several approaches have been studied to generate regression splines. Poirier (1973) introduced a cubic regression spline with an excellent discussion of basic theory. Buse and Lim (1977) developed linear restrictions on parameter space such that the regression cubic spline is obtained by the restricted least-squares technique. Smith (1979) showed that the cubic regression spline can be obtained by using the " + " function.

About extensions of smoothing splines to the multivariate case, Meingnet (1979), Dyn and Wahba (1982), Cox (1984) and Barry (1986) investigated the multivariate smoothing splines by the method of penalized least squares. Poirier (1975) considered in two articles bilinear splines by the method of " + " function; one article has a good application of a bilinear spline to formulate the Cobb–Douglas production function.

Our objective is to propose a class of bivariate regression splines by the technique of restricted least squares. This topic is motivated by several reasons. Buse and Lim (1977) pointed out that formulating a regression cubic spline by the restricted least-squares technique is more general than the approach by Poirier (1973), in that the number of restrictions can be varied and the validity of the restrictions can be tested. However, the regression spline by the technique of restricted least squares has been done for only the case of a cubic single-variable spline. An extension of regression spline to the multivariate case is only the bilinear regression spline of Poirier (1975). The regression regime considered in spline is mostly the rectangular type, but Hamermesh (1970) and Otto et al. (1966) pointed out that many economic structural changes happen only on the axis of a single variable. In Hamermesh's paper he considered estimation of a wage equation for which the consumer price index is the factor affecting the structure. Otto et al. attempted to explain the budgetary process of US government agencies where time is considered as the index of structural changes.

Based on the development of restriction matrices that impose restrictions on the space of regression parameters, we can design regression splines of many types and can extend the polynomial order to arbitrary "k". Of course, the bivariate regression spline that has changed on the axis of a single variable is considered.

The bivariate regression splines to be defined are piecewise bivariate polynomials defined on domain of connected regime sets with continuity condition of partial derivatives on neighborhoods of regime sets. The regime set is a partition of $\mathbb{R}^2$ by the slicing tool of hyperplanes that generate regression splines of many types, including rectangle, trapezoid, trapezium and parallelogram.

In general, a hyperplane in $\mathbb{R}^2$ can be formulated as

$$\Gamma_c(\delta_1, \delta_2) = \{x = (x_1, x_2)' \colon \delta_1 x_1 + \delta_2 x_2 = c\} \tag{1.1}$$

with $c = 0$ or 1. For specification, pairs $(\Gamma_1(\delta_1, 0), \Gamma_0(\delta_1, 0))$ and $(\Gamma_1(0, \delta_2), \Gamma_0(0, \delta_2))$ with $\delta_1 \neq 0$ and $\delta_2 \neq 0$ include vertical and horizontal hyperplanes, and the pair $(\Gamma_1(\delta_1, \delta_2), \Gamma_0(\delta_1, \delta_2))$ with $\delta_1, \delta_2 \neq 0$ include slant hyperplanes. With various hyperplanes, we can choose to construct regression splines in many ways. Besides our proposal of regression splines of some types by the restricted least-squares technique, an important part of this work is to find linear restrictions that fulfil the continuity conditions. In contrast to a knot in the role of a change point in a single-variable spline function, we call the hyperplane in $\mathbb{R}^2$ the knot space also.

In Section 2, we introduce monotone and bivariate quadrilateral regression splines for which the knot space $\Gamma_1(\delta_1, \delta_2)$ with $\delta_1, \delta_2 \neq 0$ is used as a slicing tool. In Section 3, rectangle-type bivariate regression spline with knot spaces $\Gamma_1(\delta_1, 0)$ with $\delta_1 \neq 0$ and $\Gamma_1(0, \delta_2)$ with $\delta_2 \neq 0$ is introduced. The linear restrictions that fulfil the required continuity conditions are derived for all cases. A Bayesian technique for estimating the hyperplanes is introduced in Section 4.

2. Bivariate regression spline with slant knot space $\Gamma_1(\delta_1, \delta_2)$

Let k be a positive integer. The class of degree k bivariate polynomials is formulated as

$$\boldsymbol{P} = \left\{P\colon P(\boldsymbol{x}, \boldsymbol{\beta}) = \sum_{l=0}^{k} \sum_{j_1+j_2=l} \beta_{j_1 j_2} x_1^{j_1} x_2^{j_2},\ \beta_{j_1 j_2}\text{'s are real}\right\}, \tag{2.1}$$

where $\boldsymbol{x} = (x_1, x_2)'$ is a vector of explanatory variables and the vector $\boldsymbol{\beta}$ contains coefficients $\beta_{j_1 j_2}$ of the bivariate polynomial.

We introduce monotone and bivariate quadrilateral regression splines based on slant knot space. Before this, we discuss a spline model for bivariate two-phase regression.

Definition 2.1. Let $\delta = (\delta_1, \delta_2)'$ with $\delta_1, \delta_2 \neq 0$. The bivariate two-phase regression model

$$y = P(\boldsymbol{x}, \boldsymbol{\beta}^a) I(\boldsymbol{x}'\delta \leq 1) + P(\boldsymbol{x}, \boldsymbol{\beta}^b)) I(\boldsymbol{x}'\delta > 1) + \varepsilon \tag{2.2}$$

is a bivariate two-phase slant regression spline model if it satisfies the following continuity conditions:

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^a) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^b) \quad \text{for } \boldsymbol{x} \in \Gamma_1(\delta) \text{ and } 0 \leq j_1 + j_2 \leq k-1, \tag{2.3}$$

where

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}) = \frac{\partial^{j_1+j_2}}{\partial^{j_1} x_1 \partial^{j_2} x_2} P(\boldsymbol{x}, \boldsymbol{\beta}).$$

The condition $P_{jk-j}(\boldsymbol{x}, \boldsymbol{\beta}^a) = P_{jk-j}(\boldsymbol{x}, \boldsymbol{\beta}^b)$ is not considered because it would result in the fact that $\beta^a_{jk-j} = \beta^b_{jk-j}$, $j = 0, \ldots, k$, where β^a_{jk-j} and β^b_{jk-j} are coefficient parameters of $\boldsymbol{P}(., \boldsymbol{\beta}^a)$ and $\boldsymbol{P}(., \boldsymbol{\beta}^b)$ corresponding to the term $x_1^j x_2^{k-j}$.

To fulfil the continuity conditions for this regression spline, we derive a sufficient condition represented by some linear restrictions on the parameter space. The representation of a differentiated bivariate polynomial on knot space $\Gamma_1(\delta_1, \delta_2)$ leads us to find those linear restrictions.

Lemma 2.2. *Let* $\mathbf{P} \in \boldsymbol{P}$ *and* $0 \le j_1 + j_2 \le k - 1$; *the* (j_1, j_2)*th partial derivative of bivariate polynomial P on hyperplane* $\Gamma_1(\delta_1, \delta_2)$ *with* $\delta_2 \ne 0$ *is formulated*:

$$P_{j_1 j_2}(x_1, \boldsymbol{\beta}) = \sum_{0 \le c \le k-(j_1+j_2)} \left[\sum_{l=c}^{k-(j_1+j_2)} \sum_{0 \le d \le c} \times \frac{(-1)^{c-d}(j_1+d)!\,(j_2+l-d)!}{\delta_2^{l-d}\; d!\;\; (l-d)!} \binom{l-d}{c-d} \beta_{j_1+d\, j_2+(l-d)} \delta_1^{c-d} \right] x_1^c. \tag{2.4}$$

Consider the vector $\boldsymbol{\beta}$ in a fixed permutation of parameters $\beta_{j_1 j_2}$. For this permutation there are vectors $L_{j_1 j_2}(c)$, $c = 0, 1, \ldots, k - (j_1 + j_2)$ such that

$$L_{j_1 j_2}(c) \cdot \boldsymbol{\beta} = \sum_{l=c}^{k-(j_1+j_2)} \sum_{0 \le d \le c} \frac{(-1)^{c-d}(j_1+d)!\,(j_2+l-d)!}{\delta_2^{l-d}\; d!\;\; (l-d)!} \binom{l-d}{c-d} \times \beta_{j_1+d\, j_2+(l-d)} \delta_1^{c-d}. \tag{2.5}$$

The permutation is specified in a convenient way according to its corresponding knot space. With the above vector representation.

$$P_{j_1 j_2}(x_1, \boldsymbol{\beta}) = \sum_{0 \le c \le k-(j_1+j_2)} L_{j_1 j_2}(c) \cdot \boldsymbol{\beta}\, x_1^c. \tag{2.6}$$

Let the parameter vectors $\boldsymbol{\beta}^a$ and $\boldsymbol{\beta}^b$ be arranged associated with the same permutation of indices. Then the condition $P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^a) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^b)$ for $0 \le j_1 + j_2 \le k - 1$ on $\Gamma_1(\delta_1, \delta_2)$ is

$$\sum_{0 \le c \le k-(j_1+j_2)} L_{j_1 j_2}(c) \cdot (\boldsymbol{\beta}^a - \boldsymbol{\beta}^b) x_1^c = 0 \quad \text{for } x_1 \in \mathbb{R} \text{ and all } 0 \le j_1 + j_2 \le k-1, \tag{2.7}$$

which is equivalent to

$$L_{j_1 j_2}(c) \cdot (\boldsymbol{\beta}^a - \boldsymbol{\beta}^b) = 0, \quad 0 \le c \le k-(j_1+j_2) \text{ and } 0 \le j_1 + j_2 \le k-1. \tag{2.8}$$

The continuity condition (2.3) can be replaced by linear restrictions in (2.8). The bivariate two-phase regression spline is then the restricted least-squares estimator of which the restriction matrix is the vertical joining of all vectors $L_{j_1 j_2}(c)$, $0 \le c \le k - (j_1 + j_2)$ and $0 \le j_1 + j_2 \le k - 1$. However, unlike the single-variable case (see Buse and Lim, 1977), the class of $L_{j_1 j_2}(c)$ in (2.8) is a linearly dependent set having numerous numbers. We seek a maximum set of linear independent vectors that greatly simplifies the task of finding regression splines.

Definition 2.3. Any maximum set of linearly independent vectors in set $\{L_{j_1 j_2}(c)$: $0 \le c \le k - (j_1 + j_2)$ and $0 \le j_1 + j_2 \le k - 1\}$ is called a $\Gamma_1(\delta_1, \delta_2)$-based restriction basis.

For this knot space $\Gamma_1(\delta_1, \delta_2)$, the following theorem exactly explains the dependence and gives a restriction basis.

Theorem 2.4. *Suppose $\delta_1 \neq 0$. (a) Fix (r, j), $1 \le r \le k-1$ and $1 \le j \le r$. For b, $0 \le b \le k-r$, $L_{r-jj}(b) = (-(b+1) \times L_{r-jj-1}(b+1) + L_{r-j+1j-1}(b)) \times (\delta_1/\delta_2)$. (b) The set $\{L_{i0}(c)\colon 0 \le c \le k-i,\ i = 0, 1, \ldots, k-1\}$ of number $\binom{k+2}{2} - 1$ vectors forms a $\Gamma_1(\delta_1, \delta_2)$-based restriction basis.*

Assume that we have n observations $(y_i, \boldsymbol{x}_i)$ with $\boldsymbol{x}_i'\delta \le 1$ for $i \le n_1$ and $\boldsymbol{x}'\delta > 1$ for $i > n_1$. Let

$$\boldsymbol{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad \boldsymbol{X}^a = \begin{pmatrix} x_1' \\ \vdots \\ x_{n_1}' \end{pmatrix}, \quad \boldsymbol{X}^b = \begin{pmatrix} \boldsymbol{x}_{n_1+1}' \\ \vdots \\ \boldsymbol{x}_n' \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\beta}^a \\ \boldsymbol{\beta}^b \end{pmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} \boldsymbol{X}^a & 0 \\ 0 & \boldsymbol{X}^b \end{bmatrix}. \tag{2.9}$$

Moreover, let $\boldsymbol{R}$ be the vertical joinings of vectors of $\Gamma_1(\delta_1, \delta_2)$-based restriction basis. Then the restricted least-squares estimator of the bivariate two-phase regression spline is

$$\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}_{\text{ls}} - (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{R}'(\boldsymbol{R}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{R}')^{-1}\boldsymbol{R}\hat{\boldsymbol{\beta}}_{\text{ls}}, \tag{2.10}$$

where $\hat{\boldsymbol{\beta}}_{\text{ls}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$, the ordinary least-squares estimator of β.
The estimated bivariate-two phase regression spline is

$$y = P(\boldsymbol{x}, \hat{\boldsymbol{\beta}}^a) I(\boldsymbol{x}'\delta \le 1) + P(\boldsymbol{x}, \hat{\boldsymbol{\beta}}^b) I(\boldsymbol{x}'\delta > 1), \tag{2.11}$$

where $\hat{\boldsymbol{\beta}}^a$ and $\hat{\boldsymbol{\beta}}^a$ satisfy $\hat{\boldsymbol{\beta}} = (\hat{\boldsymbol{\beta}}^a / \hat{\boldsymbol{\beta}}^b)$.

The number of parameters of a bivariate polynomial of order k is $\binom{k+2}{2}$. With a continuity condition imposing $\binom{k+2}{2} - 1$ linear restrictions, the degrees of freedom of the parameter space of the bivariate two-phase regression spline is then $\binom{k+2}{2} + 1$. We extend this idea to a multiphase case.

Definition 2.5. (a) If a set of slant knot spaces $\{\Gamma_1(\delta^r), \delta_1^r, \delta_2^r \neq 0,\ r = 0, 1, \ldots, a\}$ such that the class of sets

$$\{\boldsymbol{x}\colon \boldsymbol{x}'\delta^j \ge 1, 0 \le j \le r-1 \text{ and } \boldsymbol{x}'\delta^r < 1\}, \quad r = 1, \ldots, a \tag{2.12}$$

forms a partition of the domain of explanatory variables x_1 and x_2, that is, they are mutually exclusive, then we call them slant monotone regime sets.

(b) A bivariate slant regression spline with regime sets (2.12) is defined as

$$f(\boldsymbol{x}) = \sum_{r=1}^{a} P(\boldsymbol{x}, \boldsymbol{\beta}^r) I(\boldsymbol{x}\colon \boldsymbol{x}'\delta^j \ge 1,\ 0 \le j \le r-1 \text{ and } \boldsymbol{x}'\delta^r < 1), \tag{2.13}$$

with continuity conditions

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{r-1}) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^r) \quad \text{on } \Gamma_1(\delta^{r-1}) \tag{2.14}$$

for $0 \le j_1 + j_2 \le k-1$ and $r = 2, \ldots, a$.

We add knot spaces $\Gamma_1(\delta^0)$ and $\Gamma_1(\delta^r)$ only for convenience. In fact, we assume that there is no observation falling under the hyperplane $\delta^{0\prime}\boldsymbol{x} = 1$ and falling above the hyperplane $\delta^{r\prime}\boldsymbol{x} = 1$. The $\binom{k+2}{2} - 1$ linear restrictions are imposed associated with each neighboring knot space and the continuity requirement does not apply on the boundary knot spaces $\Gamma_1(\delta^r)$ for $r = 0, a$. The knot spaces and the number "a" (or "b" that is used later) are assumed to be known. Explicit formulation of the bivariate slant regression spline is an analogous extending of (2.10) and (2.11) to the case of "a" polynomials that we neglect.

As the parameters for the bivariate slant regression spline numbers $a\binom{k+2}{2}$ in total, so (b) of Theorem 2.4 implies that this spline has degrees of freedom $\binom{k+2}{2} + (a-1)$. A refinement of slant monotone regime sets is the quadrilateral set.

Definition 2.6. (a) Let $\{\delta_u^r\}$ and $\{\delta_v^h\}$ represent nonzero knot vectors. If the set of slant knot spaces $\{\Gamma_1(\delta_u^r), \Gamma_1(\delta_v^h\}; r = 0, 1, \ldots, a, h = 0, 1, \ldots, b\}$ such that the class of sets

$$\{\boldsymbol{x}: \boldsymbol{x}'\delta_u^{r-1} \geq 1, \boldsymbol{x}'\delta_u^r < 1, \boldsymbol{x}'\delta_v^{h-1} \geq 1 \text{ and } \boldsymbol{x}'\delta_v^h < 1\}, \quad r = 1, \ldots, a \text{ and } h = 1, \ldots, b \tag{2.15}$$

forms a partition of the domain of explanatory variables x_1 and x_2, then we call them a quadrilateral regime set.

(b) A bivariate quadrilateral regression spline with regime sets (2.15) is defined as

$$y = \sum_{h=1}^{b}\sum_{r=1}^{a} P(x, \beta^{rh}) I(\boldsymbol{x}'\delta_u^{r-1} \geq 1, \boldsymbol{x}'\delta_u^r < 1, \boldsymbol{x}'\delta_v^{h-1} \geq 1 \text{ and } \boldsymbol{x}'\delta_v^h < 1) + \varepsilon, \tag{2.16}$$

with the following continuity conditions.

Fixed h:

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{r-1\,h}) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{rh}) \quad \text{on } \Gamma_1(\delta_u^{r-1}),\ r = 2, \ldots, a \tag{2.17}$$

Fixed r:

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{r\,h-1}) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{rh}) \quad \text{on } \Gamma_1(\delta_v^{h-1}),\ h = 2, \ldots, b \tag{2.18}$$

for $0 \leq j_1 + j_2 \leq k - 1$.

This quadrilateral regression spline has the property that each piece of polynomial includes all regressor terms $x_1^{j_1} x_2^{j_2}$ for which $j_1 + j_2 \leq k$ is satisfied. However, the rectangle regression spline, to be introduced in the next section, has to sacrifice some regressor terms to fulfil continuity conditions in (2.17) and (2.18). With Theorem 2.4, we have an explicit form of the bivariate regression spline.

Let $\boldsymbol{R}_u^r$, $\boldsymbol{R}_v^h$ be the vertical joinings' of $\Gamma_1(\delta^r)$ and $\Gamma_1(\delta^h)$-based restriction basis', $r = 1, \ldots, a-1$ and $h = 1, \ldots, b-1$, respectively. For these ab polynomials, to fulfil the continuities of the polynomials on the jth row regimes the restriction matrix includes the submatrix that has nonzero elements on the following matrix, of which its corresponding parameter vectors are also listed:

$$\tilde{\boldsymbol{R}}_u^j = \begin{bmatrix} \boldsymbol{\beta}^{1j} & \boldsymbol{\beta}^{2j} & \boldsymbol{\beta}^{3j} & \cdots & \boldsymbol{\beta}^{a-1j} & \boldsymbol{\beta}^{aj} \\ \boldsymbol{R}_u^1 & -\boldsymbol{R}_u^1 & & & & \\ & \boldsymbol{R}_u^2 & -\boldsymbol{R}_u^2 & & & \\ & & & \ddots & & \\ & & & & \boldsymbol{R}_u^{a-1} & -\boldsymbol{R}_u^{a-1} \end{bmatrix}, \quad j = 1, \ldots, b. \tag{2.19}$$

The restriction matrix includes a submatrix that has a nonzero subset for continuities of polynomials on the kth column regimes as

$$\tilde{\boldsymbol{R}}_v^k = \begin{bmatrix} \boldsymbol{\beta}^{k1} & \boldsymbol{\beta}^{k2} & \boldsymbol{\beta}^{k3} & \cdots & \boldsymbol{\beta}^{k\,b-1} & \boldsymbol{\beta}^{kb} \\ \boldsymbol{R}_v^1 & -\boldsymbol{R}_v^1 & & & & \\ & \boldsymbol{R}_v^2 & -\boldsymbol{R}_v^2 & & & \\ & & & \ddots & & \\ & & & & \boldsymbol{R}_v^{b-1} & -\boldsymbol{R}_v^{b-1} \end{bmatrix}, \quad k = 1, \ldots, a. \tag{2.20}$$

The restriction matrix is $\boldsymbol{R}$ with $\boldsymbol{R}' = (\tilde{\boldsymbol{R}}_u^{1\prime}, \tilde{\boldsymbol{R}}_u^{2\prime}, \ldots, \tilde{\boldsymbol{R}}_u^{b\prime}, \tilde{\boldsymbol{R}}_v^{1\prime}, \ldots, \tilde{\boldsymbol{R}}_v^{a\prime})$. The matrices in (2.19) and (2.20) contain zeros for which the corresponding parameter vectors are not listed. Consider an arrangement, the set joining vector $\tilde{\boldsymbol{\beta}}^j$ with $\tilde{\boldsymbol{\beta}}^{j\prime} = (\boldsymbol{\beta}^{1j\prime}, \ldots, \boldsymbol{\beta}^{aj\prime}), j = 1, \ldots, b$ and further joining $\boldsymbol{\beta}$ with $\boldsymbol{\beta}' = (\tilde{\boldsymbol{\beta}}^{1\prime}, \ldots, \boldsymbol{\beta}^{b\prime})$. Let the corresponding observation vectors and matrices be $(\boldsymbol{y}^{rh}, \boldsymbol{X}^{rh})$, $r = 1, \ldots, a$ and $h = 1, \ldots, b$. Define the extending observation vectors and matrices, $\boldsymbol{y}$ with $\boldsymbol{y}' = (\boldsymbol{y}^{1\prime}, \ldots, \boldsymbol{y}^{b\prime})$ where $\boldsymbol{y}^j$ satisfies $\boldsymbol{y}^{j\prime} = (\boldsymbol{y}^{1j\prime}, \ldots, \boldsymbol{y}^{aj\prime})$ and $\boldsymbol{X} = \mathrm{diag}(\boldsymbol{X}^1, \ldots, \boldsymbol{X}^b)$ where $\boldsymbol{X}^j = \mathrm{diag}(\boldsymbol{X}^{1j}, \ldots, \boldsymbol{X}^{aj})$. The restricted least-squares estimator of the bivariate quadrilateral regression spline has the form of (2.10) where matrices $\boldsymbol{y}$, $\boldsymbol{X}$, and $\boldsymbol{R}$ are the versions listed above.

The remaining important task is to list explicitly the matrix form of the $\Gamma_1(\delta_1, \delta_2)$-based restriction basis. Before this, we consider a simple permutation of the index set $\{(j_1, j_2)\colon 0 \le j_1 + j_2 \le k\}$. Define a suborder set

$$S(m)\colon \quad (k-m, 0)\,(k-m-1, 1)\,(k-m-2, 2), \ldots, (k-m-i, i), \ldots, (0, k-m), \tag{2.20}$$

where $0 \le i \le k - m$. $S(m)$ is an ordered set of $\{(j_1, j_2)\colon j_1 + j_2 = k - m\}$. We define the permutation of the index set as the horizontal joining of suborder set $S(m)$ with sequence $m = k, k-1, \ldots, 0$; that is,

$$S(k)\,S(k-1), \ldots, S(0). \tag{2.21}$$

With this index permutation, we set $\boldsymbol{\beta}$ as a vector of parameters $\beta_{j_1 j_2}$ permuted according to the order (2.20), (2.21). As an example, we list the matrix form of $\Gamma_1(\delta_1, \delta_2)$-based restriction basis for $k = 2, 3$ and 4 in the following where permutation of vectors is set by way of vertical joining of subvectors:

$$\begin{bmatrix} L_{io}(0) \\ L_{io}(1) \\ \vdots \\ L_{io}(k-i) \end{bmatrix} \quad i = 0, 1, \ldots, k-1.$$

The empty cells in the following three matrices represent zero elements and their corresponding parameters according to a linear restriction are also listed.

Case 1: $k = 2$

β_{20}	β_{11}	β_{02}	β_{10}	β_{01}	β_{00}
1	$\frac{\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$			
	$\frac{1}{\delta_2}$	$\frac{2\delta_1}{\delta_2^2}$	1	$\frac{\delta_1}{\delta_2}$	
		$\frac{1}{\delta_2^2}$		$\frac{1}{\delta_2}$	1
2	$\frac{\delta_1}{\delta_2}$				
	$\frac{1}{\delta_2}$		1		

Case 2: $k = 3$

β_{30}	β_{21}	β_{12}	β_{03}	β_{20}	β_{11}	β_{02}	β_{10}	β_{01}	β_{00}
1	$\frac{-\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$	$\frac{-\delta_1^3}{\delta_2^3}$						
	$\frac{1}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	$\frac{3\delta_1^2}{\delta_2^3}$	1	$\frac{-\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$			
		$\frac{1}{\delta_2^2}$	$\frac{-3\delta_1}{\delta_2^3}$		$\frac{1}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	1	$\frac{-\delta_1}{\delta_2}$	
			$\frac{1}{\delta_2^3}$			$\frac{1}{\delta_2^2}$		$\frac{1}{\delta_2}$	1

3	$\frac{-2\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$			
	$\frac{2}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	2	$\frac{-\delta_1}{\delta_2}$	
		$\frac{1}{\delta_2^2}$		$\frac{1}{\delta_2}$	1
6	$\frac{-2\delta_1}{\delta_2}$				
	$\frac{2}{\delta_2}$		2		

Case 3: $k = 4$ (matrix is horizontally separated into two parts)

Part 1:

β_{40}	β_{31}	β_{22}	β_{13}	β_{04}	β_{30}	β_{21}	β_{12}	β_{03}
1	$\frac{-\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$	$\frac{-\delta_1^3}{\delta_2^3}$	$\frac{\delta_1^4}{\delta_2^4}$				
	$\frac{1}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	$\frac{3\delta_1^2}{\delta_2^3}$	$\frac{-4\delta_1^3}{\delta_2^4}$	1	$\frac{-\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$	$\frac{-\delta_1^3}{\delta_2^3}$
		$\frac{1}{\delta_2^2}$	$\frac{-3\delta_1}{\delta_2^3}$	$\frac{6\delta_1^2}{\delta_2^4}$		$\frac{1}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	$\frac{3\delta_1^2}{\delta_2^3}$
			$\frac{1}{\delta_2^3}$	$\frac{-4\delta_1}{\delta_2^4}$			$\frac{1}{\delta_2^2}$	$\frac{-3\delta_1}{\delta_2^3}$
				$\frac{1}{\delta_2^4}$				$\frac{1}{\delta_2^3}$
4	$\frac{-3\delta_1}{\delta_2}$	$\frac{2\delta_1^2}{\delta_2^2}$	$\frac{-\delta_1^3}{\delta_2^3}$					
	$\frac{3}{\delta_2}$	$\frac{-4\delta_1}{\delta_2^2}$	$\frac{3\delta_1^2}{\delta_2^3}$		3	$\frac{-2\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$	
		$\frac{2}{\delta_2^2}$	$\frac{-3\delta_1}{\delta_2^3}$			$\frac{2}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	
			$\frac{1}{\delta_2^3}$				$\frac{1}{\delta_2^2}$	
12	$\frac{-6\delta_1}{\delta_2}$	$\frac{2\delta_1^2}{\delta_2^2}$						
	$\frac{6}{\delta_2}$	$\frac{-4\delta_1}{\delta_2^2}$			6	$\frac{-2\delta_1}{\delta_2}$		
		$\frac{2}{\delta_2^2}$				$\frac{2}{\delta_2}$		

24	$\frac{-6\delta_1}{\delta_2}$				
	$\frac{6}{\delta_2}$			6	

Part 2:

β_{20}	β_{11}	β_{02}	β_{10}	β_{01}	β_{00}
		zero subvector			
		zero subvector			
1	$\frac{-\delta_1}{\delta_2}$	$\frac{\delta_1^2}{\delta_2^2}$			
	$\frac{1}{\delta_2}$	$\frac{-2\delta_1}{\delta_2^2}$	1	$\frac{-\delta_1}{\delta_2}$	
		$\frac{1}{\delta_2^2}$		$\frac{1}{\delta_2}$	1
		zero subvector			
		zero subvector			
2	$\frac{-\delta_1}{\delta_2}$				
	$\frac{1}{\delta_2}$		1		
		zero subvector			
		zero subvector			
2					
		zero subvector			
		zero subvector			

where "zero subvector" is a vector of zeros.

We give the restriction basis of order k in a matrix form. The following matrices list only the nonzero parts of which the corresponding parameters are also listed. Let

$$\boldsymbol{R} = \begin{bmatrix} L(0) \\ L(1) \\ \vdots \\ L(k) \end{bmatrix}, \tag{2.22}$$

where

$$L(0)=\begin{bmatrix} L_{k-10}(1)\\ L_{k-20}(2)\\ \vdots\\ L_{00}(k)\end{bmatrix},\qquad L(s)=\begin{bmatrix} L_{k-s0}(1)\\ L_{k-s-10}(2)\\ \vdots\\ L_{00}(k-s+1)\end{bmatrix},\quad s=1,\dots,k.$$

Submatrix $L(0)$ is

$$\begin{array}{llllll}
\beta_{k0} & \beta_{k-1\,1} & \beta_{k-2\,2}\cdots\beta_{k-i-1\,i-1} & \beta_{k-i\,i}\cdots\beta_{1\,k-1} & \beta_{0k} & \\
k! & -(k-1)!\dfrac{\delta_1}{\delta_2} & & & & \\
\dfrac{k!}{2!} & \dfrac{-(k-1)!\delta_2}{\delta_1} & (k-2)!\dfrac{\delta_1^2}{\delta_2^2} & & & \\
\vdots & & \vdots & & & \\
\dfrac{k!}{i!} & \dfrac{-(k-1)!\delta_1}{(i-1)!\delta_2} & \dfrac{(k-2)!\delta_1^2}{(i-2)!\delta_2^2}\cdots & \dfrac{(-1)^{i-1}(k-i+1)!\delta^{i-1}}{1!\;\;\delta^{i-1}} & (-1)^i(k-i)!\dfrac{\delta_1^i}{\delta_2^i} & \\
\vdots & & & & & \\
1 & \dfrac{-\delta_1}{\delta_2} & \dfrac{\delta_1^2}{\delta_2^2}\cdots & \dfrac{(-1)^{k-1}\delta_1^{k-1}}{\delta_2^k} & \dfrac{(-1)^k\delta_1^k}{\delta_2^k} &
\end{array}\tag{2.23}$$

where index $i=1,\dots,k$.

We set $L(s)=[M_{(s)}^{(0)},M_{(s)}^{(1)},\dots,M_{(s)}^{(s)}]$ where, for $m=0,1,\dots,s$, $M_{(s)}^{(m)}$ is

$$\begin{array}{llll}
\beta_{k-s-1\,s-m}\dfrac{1}{\delta_2^{s-m}}(k-s)! & \beta_{k-s-1\,s-m+1} & \cdots\;\beta_{k-s-i\,s+i-m} & \cdots\;\beta_{0\,k-m}\\
\dfrac{(k-s)!}{\delta_2^{s-m}1!} & \dfrac{-(k-s-1)!}{\delta_2^{s-m+1}}\dbinom{s-m-1}{1}\delta_1 & & \\
\vdots & \vdots & & \\
\dfrac{(k-s)!}{\delta_2^{s-m}1!} & \dfrac{-(k-s-1)!}{\delta_2^{s-m+1}}\dbinom{s-m-1}{1}\delta_1 & \cdots\;\dfrac{(-1)^i(k-s-i)!}{\delta_2^{s+i-m}}\dbinom{s+i-m}{i}\delta_1^i & \\
\vdots & \vdots & & \\
\dfrac{1}{\delta_2^{s-m}} & \dfrac{-1}{\delta_2^{s-m+1}}\dbinom{s-m-1}{1}\delta_1 & \cdots\;\dfrac{(-1)^{k-s}}{\delta_2^{k-m}}\dbinom{k-m}{k-s}\delta_1^{k-s} &
\end{array}\tag{2.24}$$

3. Patial bivariate regression spline constructed by knot spaces $\Gamma_1(\delta_1, \mathbf{0})$ and $\Gamma_1(\mathbf{0}, \delta_2)$

The vertical and horizontal knot spaces include $\Gamma_1(\delta_1, 0)$, $\Gamma_1(0, \delta_2)$, $\Gamma_0(\delta_1, 0)$ and $\Gamma_0(0, \delta_2)$. Without cancellation of some polynomial terms the continuity requirement on knot spaces $\Gamma_0(\delta_1, 0)$ and $\Gamma_0(0, \delta_2)$ produces unwanted regression splines. To see this, we consider only the knot space $\Gamma_0(0, \delta_2)$. The (j_1, j_2)th derivative of the bivariate polynomial on $\Gamma_0(0, \delta_2)$ is

$$P_{j_1 j_2}(x_1, \boldsymbol{\beta}) = \sum_{c=0}^{k-(j_1+j_2)} \frac{(j_1+c)!\ j_2!}{c!} \beta_{j_1+c j_2} x_1^c. \tag{3.1}$$

For fixed (j_1, j_2), the continuity conditions

$$P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^{r-1}) = P_{j_1 j_2}(\boldsymbol{x}, \boldsymbol{\beta}^r) \quad \text{on } \Gamma_0(0, \delta_2) \tag{3.2}$$

imply that

$$\beta^r_{j_1+cj_2} = \beta^{r-1}_{j_1+cj_2} \quad \text{for } 0 \le c \le k-(j_1+j_2). \tag{3.3}$$

Hence, the continuity condition (3.2) of partial derivatives induces an unpleasant result of equating neighboring parameters. By verifying implication of (3.3) for all $0 \le j_1 + j_2 \le k-1$, all parameters of neighboring polynomials $P(.,\boldsymbol{\beta}^r)$ and $P(.,\boldsymbol{\beta}^{r-1})$ except β^r_{0k} and β^{r-1}_{0k} (the term β_{0k} corresponding to $P(.,\boldsymbol{\beta}^r)$ and $P(.,\boldsymbol{\beta}^{r-1})$) are equal. Because of this unpleasant property, we consider only those regression splines with knot spaces $\Gamma_1(\delta_1, 0)$ and $\Gamma_1(0, \delta_2)$ as the slicing tools. There remain unpleasant implications of the use of these two knot spaces. The unpleasant one is avoided by slight relaxation in deleting some polynomial terms. We will study for only the knot space $\Gamma_1(0, \delta_2)$, the case of knot space $\Gamma_1(\delta_1, 0)$ is similar and is skipped.

Lemma 3.1. *The (j_1, j_2)th partial derivative of a bivariate polynomial P in $\boldsymbol{P}$ on knot space $\Gamma_1(0, \delta_2)$ with $\delta_2 \neq 0$ has the form*

$$P_{j_1 j_2}(x_1, \boldsymbol{\beta}) = \sum_{c=0}^{k-(j_1+j_2)} (L_{j_1 j_2}(c) \cdot \boldsymbol{\beta}) x_1^c, \tag{3.4}$$

where

$$L_{j_1 j_2}(c) \cdot \boldsymbol{\beta} = \sum_{l=c}^{k-(j_1+j_2)} \frac{(j_1+c)!(l-c+j_2)!}{\delta_2^{l-c} c!(l-c)!} \beta_{j_1+cj_2+l-c} \quad \textit{and}$$

$$0 \le j_1 + j_2 \le k-1.$$

Definition 3.2. Generated by knot spaces $\Gamma_1(0, \delta_2)$, the maximum set of linearly independent vectors in set $\{L_{j_1 j_2}(c)\colon 0 \le c \le k-(j_1+j_2),\ 0 \le j_1+j_2 \le k-1\}$ is called a $\Gamma_1(0, \delta_2)$-based restriction basis.

The following theorem states a relation of linear dependence of vector $L_{j_1 j_2}(c)$ and gives a basis set.

Theorem 3.3. *Suppose* $\delta_1 = 0$. (a) *Fix* (j, b) *where* $1 \le j \le k - b - 1$ *and* $0 \le b \le k - 2$. *If* $0 \le s \le k - (j + b)$, *then vector* $L_{jb}(k - (b + j) - s)$ *is proportional to vector* $L_{0b}((k - b) - s)$. (b) *The set* $\{L_{0b}(c)\colon 0 \le c \le k - b, 0 \le b \le k - 1\}$ *is the* $\Gamma_1(0, \delta_2)$*-based restriction basis.*

The vector $L_{0k-c}(c)$ has only one nonzero element of the form

$$\frac{\beta_{ck-c}}{(k-c)!} \tag{3.5}$$

To set restriction $L_{0k-c}(c)\cdot(\boldsymbol{\beta}^r - \boldsymbol{\beta}^{r-1}) = 0$ implies that $\beta^r_{ck-c} = \beta^{r-1}_{ck-c}$. The simple way to avoid this unpleasant property is to delete all vectors $L_{0k-c}(c)$ from the restriction basis.

Definition 3.4. Generated by knot space $\Gamma_1(0, \delta_2)$, the set $\{L_{0b}(c)\colon 0 \le c \le k - 1, 0 \le b \le k - c - 1\}$ is called a $\Gamma_1(0, \delta_2)$-based partial restriction basis and the set which corresponds to knot space $\Gamma_1(\delta_1, 0)$ is called a $\Gamma_1(\delta_1, 0)$-based restriction basis.

This partial restriction basis numbers $\binom{k+2}{2}$ elements.

First we consider a monotone regression spline when only the domain of a single variable is partitioned. Without loss of generality, we consider that single variable to be x_2.

Definition 3.5. Let R^h be the vertical joinings of vectors in $\Gamma_1(0, \delta_2)$-based partial restriction basis. A x_2-segmented bivariate regression spline is defined as

$$y = \sum_{h=1}^{b} P(\boldsymbol{x}, \boldsymbol{\beta}^h) I(\boldsymbol{x}\colon 1 \le x_2 \delta_2^{h-1}, x_2 \delta_2^h < 1) + \varepsilon \tag{3.6}$$

with continuity condition $R_y^{h-1}(\boldsymbol{\beta}^h - \boldsymbol{\beta}^{h-1}) = 0$, $h = 2, \ldots, a$.

Joining knot spaces $\Gamma_1(\delta_1, 0)$ and $\Gamma_1(0, \delta_2)$ produces rectangular regimes. We define rectangular regression splines as follows.

Definition 3.6. Let $\boldsymbol{R}_x^r$, $\boldsymbol{R}_y^h$ be vertical joinings' of vectors in $\Gamma_1(\delta_1, 0)$ and $\Gamma_1(0, \delta_2)$-based partial restriction basis'. A bivariate rectangular regression spline is defined as

$$y = \sum_{h=1}^{b} \sum_{r=1}^{a} P(\boldsymbol{x}, \boldsymbol{\beta}^{rh}) I(\boldsymbol{x}\colon x_1 \delta_1^{r-1} \ge 1, x_1 \delta_1^r < 1, x_2 \delta_2^{h-1} \ge 1 \text{ and } x_2 \delta_2^h < 1\} + \varepsilon \tag{3.7}$$

with: (a) For h, $R_x^{r-1}\boldsymbol{\beta}^{rh} = R_x^{r-1}\boldsymbol{\beta}^{r-1h}$, $r = 2, \ldots, a$ and
(b) for $R_y^{h-1}\boldsymbol{\beta}^{rh} = R_y^{h-1}\boldsymbol{\beta}^{rh-1}$, $h = 2, \ldots, b$.

The bivariate partial regression splines on regimes slicing on only one variable and the rectangular regimes can be analogously obtained in the form of (2.10). Poirier (1975) considered bilinear splines other than this restricted least-squares method. In one article he applied it to the Cobb–Douglas production function.

From examination of the linear restrictions of (a) and (b) above, the degree of freedom of the bivariate rectangle regession spline is "$ab(k+1)$". We list the partial restriction basis in a matrix form as

$$\boldsymbol{R}^* = \begin{bmatrix} R_0 \\ R_1 \\ \vdots \\ R_{k-1} \end{bmatrix} \quad \text{with } R_s = \begin{bmatrix} L_{00}(s) \\ L_{01}(s) \\ \vdots \\ L_{0k-s-1}(s) \end{bmatrix}, \quad s = 0, 1, \ldots, k-1, \tag{3.8}$$

and is

$$\begin{array}{llllllll}
\beta_{s\,k-s} & \beta_{s\,k-s-1} & \beta_{s\,k-s-2} \cdots \beta_{sh+1}\ \beta_{sh} & \cdots & \beta_{s2} & \beta_{s1} & \beta_{s0} \\
\frac{1}{\delta_2^{k-s}} & \frac{1}{\delta_2^{k-s-1}} & \frac{1}{\delta_2^{k-s-2}} \cdots & \cdots & \frac{1}{\delta_2^2} & \frac{1}{\delta_2} & 1 \\
\frac{k-s}{\delta_2^{k-s-1}} & \frac{k-s-1}{\delta_2^{k-s-2}} & \frac{k-s-2}{\delta_2^{k-s-3}} \cdots & \cdots & \frac{2}{\delta_2} & 1! & \\
\frac{(k-s)!}{\delta_2^{k-s-2}(k-s-2)!} & \frac{(k-s-1)!}{\delta_2^{k-s-3}(k-s-3)!} & \frac{(k-s-2)!}{\delta_2^{k-s-4}(k-s-4)!} \cdots & & 2! & & \\
\vdots & & & & & & \\
\frac{(k-s)!}{\delta_2^{k-s-h}(k-s-h)!} & \frac{(k-s-1)!}{\delta_2^{k-s-h-1}(k-s-h-1)!} & \frac{(k-s-2)!}{\delta_2^{k-s-h-2}(k-s-h-2)!} \cdots & \frac{(h+1)!}{\delta_2} & h! & & \\
\frac{(k-s)!}{\delta_2^2\, 2!} & \frac{(k-s-1)!}{\delta_2} & (k-s-2)! & & & & \\
\frac{(k-s)!}{\delta_2} & (k-s-1)! & & & & &
\end{array} \tag{3.9}$$

To obtain the restriction basis for a bivariate polynomial on knot space $\Gamma_0(\delta_1, \delta_2)$, we give a representation of the bivariate polynomial.

Lemma 3.5. *Let* $0 \le j_i \le k-1$, $i = 1, 2$ *and* $0 \le j_1 + j_2 \le k-1$; *the* (j_1, j_2)*th partial derivative of bivariate polynomial* P *on hyperplane* $\Gamma_0(\delta)$ *where vector* $\delta' = (\delta_1, \delta_2)$ *with* $\delta_2 \neq 0$ *is formulated as*

$$P_{j_1 j_2}(\boldsymbol{x}) = \sum_{0 \le c \le k-(j_1+j_2)} \left[\sum_{0 \le d \le c} \frac{(-1)^{c-d}(j_1+d)!\,(j_2+c-d)!}{\delta_2^{c-d} \quad d! \quad (c-d)!} \times \beta_{j_1+d\,j_2+c-d}\,\delta_1^{c-d} \right] x_1^c. \tag{3.10}$$

Let $L_{j_1j_2}(c)$ be the vector such that

$$L_{j_1j_2}(c)\cdot\boldsymbol{\beta} = \sum_{0\le d\le c} \frac{(-1)^{c-d}(j_1+d)!\,(j_2+c-d)!}{\delta_2^{c-d}\quad d!\quad (c-d)!} \times \beta_{j_1+d\,j_2+c-d}\,\delta_1^{c-d}. \tag{3.11}$$

Then

$$P_{j_1j_2}(\boldsymbol{x}) = \sum_{0\le c\le k-(j_1+j_2)} L_{j_1j_2}(c)\cdot\boldsymbol{\beta}\,x_1^c. \tag{3.12}$$

The relations between the restriction vectors, and the basis class are exactly the same as that of Theorem 2.4 with hyperplane $\Gamma_1(\delta_1,\delta_2)$, where the restriction basis is $\{L_{i0}(c)\colon 0\le c\le k-i,\ i=0,1,\dots,k-1\}$. However, unlike $\Gamma_1(\delta_1,\delta_2)$, the hyperplane $\Gamma_0(\delta)$ produces $L_{k-s0}(0)\cdot(\beta^r-\beta^{r-1})=0$, and hence $\beta^r_{k-s0}=\beta^{r-1}_{k-s0}$. We delete vectors $L_{k-s0}(0)$ for $s=0,\dots,k$ and set a partial restriction basis as the following matrix:

$$R^{**} = \begin{bmatrix} L(0)\\ L(1)\\ \vdots\\ L(k)\end{bmatrix},$$

where

$$L(s) = \begin{bmatrix} L_{k-s-1\,0}(1)\\ L_{k-s-2\,0}(2)\\ \vdots\\ L_{k-s-m\,0}(m)\\ \vdots\\ L_{0\,0}(k-s)\end{bmatrix},\quad s=0,1,\dots,k-1 \tag{3.13}$$

as follows:

$$\begin{array}{llllll}
\beta_{k-s0} & \beta_{k-s-1\,1} & \cdots\ \beta_{k-s-m\,m} & \cdots & \beta_{1\,k-s-1} & \beta_{0\,k-s}\\[4pt]
(k-s)! & -(k-s-1)!\dfrac{\delta_1}{\delta_2} & & & & \\
\vdots & & & & & \\
\dfrac{(k-s)!}{m!} & \dfrac{(k-s-1)!}{(m-1)!}\,\dfrac{\delta_1}{\delta_2} & \cdots\ (-1)^m(k-s-m)!\,\dfrac{\delta_1^m}{\delta_2^m} & & & \\
\vdots & & & & & \\
1 & \dfrac{-\delta_1}{\delta_2} & \cdots & & \dfrac{(-1)^{k-s-1}\delta_1^{k-s-1}}{\delta_2^{k-s-1}} & \dfrac{(-1)^{k-s}\delta_1^{k-s}}{\delta_2^{k-s}}
\end{array} \tag{3.14}$$

for $s=0,1,\dots,k-1$ and where $m=1,\dots,k-s$.

4. A Bayesian approach for estimating bivariate knot

In this section, we address the knot estimation based on a Bayesian method that extends a Bayesian technique by Chin Choy and Broemeling (1980) for switching linear regression model to the restricted linear regression model. For simplicity, we consider only the 4-piece rectangle regression spline with a vertical hyperplane and a horizontal hyperplane. Let $\binom{x_{11}}{x_{21}}, \ldots, \binom{x_{1n}}{x_{2n}}$ be the observed values of $\boldsymbol{x} = \binom{x_1}{x_2}$. For each (u, v), $1 \leq u,\ v \leq n$, the vector $\delta' \equiv (\delta_1, \delta_2) = (x_{1u}, x_{2v})$ determines a knot vector that slice the space $\mathbb{R}^2$ into 4 rectangle pieces. The maximum number of pairwise distinct pairs (x_{1u}, x_{2v}) is n^2. For setting (x_{1u}, x_{2v}) as a knot, we require that the number of observations $\boldsymbol{x}_i$ in each rectangle is large enough so that unique restricted least-squares estimate can be obtained. Denote by J the index set of (u, v) that makes the restricted least-squares estimate uniquely determined. For (u, v) in J, let $(\boldsymbol{y}, \boldsymbol{X})$ be set under the line in Section 2 with knot spaces $\Gamma_1(\binom{x_{1u}}{0})$ and $\Gamma_2(\binom{0}{x_{2v}})$. To determine the knot point $\delta = \binom{x_{1u}}{x_{2v}}$ is now equivalent to determine the index $\binom{u}{v}$ in J. We further denote by $\boldsymbol{R}\binom{u}{v}$ the restriction matrix with knot vector $\binom{x_{1u}}{x_{2v}}$. Now, we set an assumption set.

Assumption A. (a_1) The knot index is uniformly distributed over the set J.

(a_2) The spline parameter, β is assigned the improper prior

$$\pi(\beta) \propto \text{constant}.$$

(a_3) The error variable ε has normal distribution with mean zero and variance σ^2, when σ^2 has the well-known noninformative prior distribution

$$\pi_\sigma(\sigma^2) = 1/\sigma^2 \quad \text{for } 0 < \sigma^2 < \infty.$$

The following theorem provides a posterior joint probability density function of the knot index and the regression parameters.

Theorem 4.1. *Under Assumption A, the posterior probability density function of β and knot index $\binom{u}{v}$ is*

$$\pi(\tbinom{u}{v}, \beta \mid \boldsymbol{y}) \propto [(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)]^{-(n+2)/2}$$

subject to $\boldsymbol{R}\binom{u}{v}\boldsymbol{\beta} = 0$.

To obtain the estimate of the knot index, one way with this posterior density is by solving

$$\arg\inf_J (\boldsymbol{y} - \boldsymbol{X}\hat{\beta}_{\text{rls}})'(\boldsymbol{y} - \boldsymbol{X}\hat{\beta}_{\text{rls}}),$$

where $\hat{\beta}_{\text{rls}}$ is the restricted least-squares estimate with restriction matrix $\boldsymbol{R}\binom{u}{v}$.

Acknowledgements

The author is grateful to the referees for their helpful comments.

Appendix

Proof of Lemma 2.2. The (j_1, j_2)th partial derivative of bivariate polynomial P in $\boldsymbol{P}$ is

$$P_{j_1 j_2}(\boldsymbol{x}) = \sum_{l=0}^{k-(j_1+j_2)} \sum_{b_1+b_2=l} \frac{(j_1+b_1)!(j_2+b_2)!}{b_1!b_2!} \beta_{j_1+b_1 j_2+b_2} x_1^{b_1} x_2^{b_2}. \tag{A.1}$$

As we assume that $\delta_2 \neq 0$, the hyperplane $\Gamma_1(\delta)$ is then

$$\Gamma_1(\delta) = \left\{ \left(x_1, \frac{1-\delta_1 x_1}{\delta_2} \right) : x_1 \in \mathbb{R} \right\}, \tag{A.2}$$

where we replace x_2 by $((1-\delta_1 x_1)/\delta_2)$.

Denote the subpolynomial with degree l of $P_{j_1 j_2}$ on $\Gamma_1(\delta)$ by P_l. Then

$$p_l(x_1) = \sum_{b_1+b_2=l} \sum_{0 \le n \le b_2} (-1)^n \frac{1}{\delta_2^{b_2}} \frac{(j_1+b_1)!}{b_1!} \frac{(j_2+b_2)!}{b_2!} \binom{b_2}{n} \delta_1^n \times \beta_{j_1+b_1 j_2+b_2} x_1^{b_1+n}. \tag{A.3}$$

We claim that $p_l(x_1)$ is a one-variable polynomial of degree l. By rearrangement of p_l, we have

$$p_l(x_1) = \sum_{0 \le c \le l} \sum_{0 \le n \le c} \frac{(-1)^n}{\delta_2^{l-(c-n)}} \frac{(j_1+c-n)!}{(c-n)!} \frac{(j_2+(l-c+n))!}{(l-c+n)!} \binom{l-c+n}{n} \times \beta_{j_1+c-n\, l-c+n} \delta_1^n x_1^c. \tag{A.4}$$

For convenience, let $d = c - n$; we further have

$$p_l(x_1) = \sum_{0 \le c \le l} \sum_{0 \le d \le c} \frac{(-1)^{c-d}}{\delta_2^{l-d}} \frac{(j_1+d)!}{d!} \frac{(j_2+l-d)!}{(l-d)!} \binom{l-d}{c-d} \times \beta_{j_1+d\, l-d} \delta_1^{c-d} x_1^c. \tag{A.5}$$

Then (A.1) and (A.5) further imply Lemma 2.2. □

The proofs of Lemmas 3.1 and 3.5 are analogous to the above and are neglected.

Proof of Theorem 2.4. Eq. (2.5) gives

$$L_{r-j\,j}(b)\cdot\boldsymbol{\beta} = \sum_{l=b}^{k-r}\sum_{0\le d_1\le b}\frac{(-1)^{b-d_1}}{\delta_2^{l-d_1}}\frac{(r-j+d_1)!(j+l-d_1)!}{d_1!(l-d_1)!}\binom{l-d_1}{b-d_1}\delta_1^{b-d_1} \times \beta_{r-j+d_1\,j+(l-d_1)}, \tag{A.6}$$

$$L_{r-j\,j-1}(b+1)\cdot\boldsymbol{\beta} = \sum_{l=b}^{k-r}\sum_{0\le d_1\le b+1}\frac{(-1)^{b+1-d_1}}{\delta_2^{l+1-d_1}}\frac{(r-j+d_1)!(j+l-d_1)!}{d_1!(l+1-d_1)!} \times\binom{l+1-d_1}{b+1-d_1}\delta_1^{b+1-d_1}\beta_{r-j+d_1\,j+l-d_1}, \tag{A.7}$$

and

$$L_{r-j+1\,j-1}(b)\cdot\boldsymbol{\beta} = \sum_{l=b}^{k-r}\sum_{d_1=1}^{b+1}\frac{(-1)^{b-d_1+1}}{\delta_2^{l-d_1+1}}\frac{(r-j+d_1)!(j+l-d_1)!}{(d_1-1)!(l-d_1+1)!} \times\binom{l-d_1+1}{b-d_1+1}\times\delta_1^{b-d_1+1}\beta_{r-j+d_1\,j+l-d_1}. \tag{A.8}$$

Then

$$\frac{(b+1-d_1)}{(l-d_1+1)!}\binom{l-d_1+1}{b-d_1+1} = \frac{1}{(l-d_1)}\binom{l-d_1}{b-d_1}$$

and with simplification we have

$$-(b+1)\times L_{r-j\,j-1}(b+1)\cdot\boldsymbol{\beta} + L_{r-j+1\,j-1}(b)\cdot\boldsymbol{\beta} = \frac{\delta_1}{\delta_2}L_{r-j\,j}(b)\cdot\boldsymbol{\beta}.$$

$$f_{j_1 0}(x_1) = \sum_{c=0}^{k-j_1}(L_{j_1 0}(c)\cdot\boldsymbol{\beta})x_1^c,$$

where

$$L_{j_1 0}(c)\cdot\boldsymbol{\beta} = \sum_{l=c}^{k-j_1}\sum_{d_1=0}^{c}\frac{(-1)^{c-d_1}(j_1+d_1)}{\delta_2^{l-d_1}\ \ d_1!}\binom{l-d_1}{c-d_1}\delta_1^{c-d_1}\beta_{j_1+d_1\,l-d_1}.$$

Let $L^{(0)}, L^{(1)}, \ldots, L^{(k)}$ be defined as in (2.22). It is easy to see that $L^{(0)}$ is the matrix stated in (2.23) and obviously vectors of $L^{(0)}$ are linearly independent.

We derive the general form of matrix $L^{(s)}$. The ith row of $L^{(s)}$ is $L_{k-s-i}(i)$, $i = 0, 1, \ldots, k-s$. $L_{k-s-i}(i)\cdot\boldsymbol{\beta}$ is

$$\sum_{l=i}^{s+i} h_{s+i-m}\cdot\boldsymbol{\beta}^m, \tag{A.9}$$

where, w.l.o.g, we let

$$h_{s+i-m}\cdot\boldsymbol{\beta}^m = \sum_{d_1=0}^{i}\frac{(-1)^{i-d_1}(k-s-i+d_1)!}{\delta_2^{l-d_1}\ \ d_1!}\binom{l-d_1}{i-d_1}\delta_1^{i-d_1}\beta_{k-s-i+d_1+l-d_1},$$

$m = 0, 1, \ldots, s$, and $\beta^{m'} = (\beta_{k-s\,s-m}\,\beta_{k-s-1\,s-m+1}, \ldots, \beta_{k-s-i+1}\,\beta_{k-s-i\,s+i-m})$. $L_{k-s-i}(i)$ is the horizontal joining of $\{h_{s+i-m}$: $m = 0, 1, \ldots, s\}$. By setting

$$M_{(s)}^{(m)} = \begin{bmatrix} h_{s-m} \\ h_{s+1-m} \\ \vdots \\ h_{s+i-m} \end{bmatrix},$$

we have $L^{(s)} = [M_{(s)}^{(0)}, M_{(s)}^{(1)}, \ldots, M_{(s)}^{(s)}]$. From (A.10), for $m = 0, 1, \ldots, s$, $M_{(s)}^{(m)}$ is the matrix stated in (2.24). The last nonzero elements of $L^{(s)}$ corresponding to the last nonzero elements of submatrix $M_{(s)}^{(s)}$ are $\{\beta_{k-s0}, \beta_{k-s-11}, \ldots, \beta_{0k-s}\}$, respectively. Hence, row vectors of $L^{(s)}$ are linearly independent. Then vectors of matrix $\boldsymbol{R}$ are linearly independent and vectors of $\boldsymbol{R}$ are a $\Gamma_1(\delta_1, \delta_2)$-based restriction basis. □

Proof of Theorem 3.3. Part (a) follows easily from (3.4).

Fix(j, j'), $0 \le j, j' \le k-1$ where j, j' can be equal. We have, from (3.4),

$$f_{0j}(x_1) = \sum_{c_1}^{k-j} \left(\sum_{l=c_1}^{k-j} \frac{(j+l-c_1)!}{\delta_2^{l-c_1}(l-c_1)!} \beta_{c_1\,j+l-c_1} \right) x_1^{c_1}$$

and

$$f_{0j'}(x_1) = \sum_{c_2}^{k-j'} \left(\sum_{l=c_2}^{k-j'} \frac{(j'+l-c_2)!}{\delta_2^{l-c_2}(l-c_2)!} \beta_{c_2\,j'+l-c_2} \right) x_1^{c_2}.$$

Consider (c_1, c_2) where $0 \le c_1 \le k-j$, $0 \le c_2 \le k-j'$ and $c_1 \ne c_2$. Then

$$L_{0j}(c_1)\cdot\boldsymbol{\beta} = \sum_{l=c}^{k-j} \frac{(j+l-c_1)!}{\delta_2^{l-c_1}\ (l-c_1)!} \beta_{c_1\,j+l-c_1}$$

and

$$L_{0j'}(c_2)\cdot\boldsymbol{\beta} = \sum_{l=c_2}^{k-j'} \frac{(j'+l-c_2)!}{\delta_2^{l-c_2}\ (l-c_2)!} \beta_{c_2\,j'+l-c_2}.$$

$L_{0j}(c_1)\cdot L_{0j'}(c_2) = 0$ if $c_1 \ne c_2$, which holds for arbitrary (j, j'). If $c_1 \ne c_2$, the sets $\{L_{0j}(c_1)$: $j = 0, 1, \ldots, k-c_1\}$ and $\{L_{0j'}(c_2)$: $j = 0, 1, \ldots, k-c_2\}$ are then linearly independent. We will need to show that, for each c, $0 \le c \le k$, the set $\{L_{0j}(c)$: $0 \le j \le k-c\}$ is a set of linearly independent vectors. Let c, $0 \le c \le k$; then there are only j for which $j \le k-c$ correspond to restriction vector $L_{0j}(c)$. The matrix of linear restriction vectors is formed as a vertical joining of set $\{L_{0j}(c)$: $0 \le j \le k-c$, $0 \le c \le k\}$ as of (3.8) and (3.9).

The fact of linear independence follows from the fact that R_c is a diagonal matrix; hence vectors of R^* of (3.8) are a $\Gamma_1(0, \delta_2)$-based restriction basis.

Proof of Theorem 4.1. This is done by integrating the joint probability density function of $\binom{u}{v}$, $\boldsymbol{\beta}, \boldsymbol{y}$, and σ^2 with the transformation variable $(\boldsymbol{y} - \boldsymbol{X\beta})'(\boldsymbol{y} - \boldsymbol{X\beta})/\sigma^2$.

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