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Bayesian semiparametric Regression Using Spline

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Abstract

In this paper, we consider semiparametric regression model where the mean function of this model has two part, the parametric (first part) is assumed to be linear function of p-dimensional covariates and nonparametric (second part) is assumed to be a smooth penalized spline. By using a convenient connection between penalized splines and mixed models, we can representation semiparametric regression model as mixed model. Bayesian approach is employed to making inferences on the resulting mixed model coefficients, and we prove some theorems about posterior.

Keywords

Mixed models, Semiparametric regression, Penalized spline, Bayesian inference, Prior density, Posterior density, Bayes factor.

1. Introduction

Consider the model:

$$y_i = \sum_{j=0}^{p} \beta_j x_{ji} + m(x_{p+1,i}) + \epsilon_i \qquad ,i = 1,2,\dots,n \qquad (1)$$

Where $y_1 ,\dots, y_n$ response variables and the unobserved errors are $\epsilon_1 ,\dots, \epsilon_n$ are known to be i.i.d. normal with mean 0 and covariance $\sigma_\epsilon^2 I$ with σ_ϵ^2 known.

The mean function of the regression model in (1) has two parts. The parametric (first part) is assumed to be linear function of p-dimensional covariates x_{ji} and nonparametric (second part) $m(x_{p+1,i})$ is function defined on some index set $T \subset R^1$. Inferences a bout model (1) such as its estimation as well as model checking are of interest.

A Bayesian approach to (fully) semiparametric regression problems typically requires specifying prior distributions on function spaces which is rather difficult to handle. The extent of the complexity of this approach can be gauged from sources such as Angers and Delampady (see [1]), and Lenk (see[7]), and so on.

In this paper, a simple Bayesian approach to semiparametric regression, so that with the help of a reference prior they can be transformed to prior density functions. By using penalized spline for the nonparametric function (second part) of the model (1) we can representation semiparametric regression model (1) as mixed model and Bayesian approach is employed to making inferences on the resulting mixed model coefficients, and we prove some theorems about posterior.

2. Mixed Models

The general form of a linear mixed model for the ith subject (i = 1,…, n) is given as follows (see [9,12,13]),

$$Y_i = X_i\beta + \sum_{j=1}^{r} Z_{ij}u_{ij} + \epsilon_i \quad , \quad u_{ij} \sim N(0, G_j),\ \epsilon_i \sim N(0, R_i), \qquad (2)$$

where the vector Y_i has length m_i, X_i and Z_{ij} are, respectively, a $m_i \times p$ design matrix and a $m_i \times q_i$ design matrix of fixed and random effects. β is a p-vector of fixed effects and u_{ij} are the q_i-vectors of random effects. The variance matrix G_j is a $q_i \times q_i$ matrix and R_i is a $m_i \times m_i$ matrix.

We assume that the random effects $\{u_{ij}\,; i = 1, \dots, n\,; j = 1, \dots, r\}$ and the set of error terms $\{\epsilon_1, \dots, \epsilon_n\}$ are independent. In matrix notation,

$$Y = X\beta + Zu + \epsilon \qquad (3)$$

Here $Y = (Y_1, \dots, Y_n)^T$ has length $N = \sum_{i=1}^{n} m_i$, $X = (X_1^T, \dots, X_n^T)^T$ is a $N \times p$ design matrix of fixed effects, Z is a $N \times q$ block diagonal design matrix of random effects, $q = \sum_{j=1}^{r} q_j$, $u = (u_1^T, \dots, u_r^T)^T$ is a q-vector of random effects, $R = diag(R_1, \dots, R_n)$ is a $N \times N$ matrix and $G = diag(G_1, \dots, G_r)$ is a $q \times q$ block diagonal matrix.

3. Spline Semiparametric regression and Prior

The model (1) can be expressed as a smooth penalized spline with q degree, then it's become as (see [12]):

$$y_i = \sum_{j=0}^{p} \beta_j x_{ji} + \sum_{j=1}^{q} \beta_{p+j} x_{p+1,i}^{j} + \sum_{k=1}^{K} \{u_k (x_{p+1,i} - k_k)_+^q + \epsilon_i\,, \qquad (4)$$

where $k_1, \dots, k_K$ are inner knots $a < k_1 <,,,< k_K < b$.

By using a convenient connection between penalized splines and mixed models. Model (4) is rewritten as follows (see [9,12,13])

$$Y = X\beta + Zu + \epsilon \qquad (5)$$

where

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_p \\ \beta_{p+1} \\ \vdots \\ \beta_{p+q} \end{bmatrix}, \quad u = \begin{bmatrix} u_1 \\ \vdots \\ u_K \end{bmatrix}, Z = \begin{bmatrix} (x_{p+1,1} - k_1)_+^q & \cdots & (x_{p+1,1} - k_K)_+^q \\ \vdots & \ddots & \vdots \\ (x_{p+1,n} - k_1)_+^q & \cdots & (x_{p+1,n} - k_K)_+^q \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & x_{11} & \dots & x_{p1} & x_{p+1,1} & \dots & x_{p+1,1}^q \\ 1 & x_{12} & \dots & x_{p2} & x_{p+1,2} & \dots & x_{p+1,2}^q \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1n} & \dots & x_{pn} & x_{p+1,n} & \dots & x_{p+1,n}^q \end{bmatrix}$$

We assume that the function g is:

$$g = X\beta + Zu \qquad (6)$$

And its prior guess g^o can be written as:

$$g^o = X\beta \qquad (7)$$

Further, some of the a priori information penalized spline coefficients can be translated into:

$$E(\epsilon) = 0; \qquad var(\epsilon) = \sigma_\epsilon^2 I$$
$$E(\beta) = 0; \qquad var(\beta) = \sigma_\beta^2 I \qquad (8)$$
$$E(u) = 0; \qquad var(u) = \sigma_u^2 I$$

The term $X\beta$ in (5) is the pure polynomial component of the spline, and Zu is the component with spline truncated functions with covariance $\sigma_u^2\, Q$, where $Q = ZZ^T$. Letting $(\beta, u, \sigma_u^2, \sigma_\epsilon^2)$ be the parameter vector, the mixed model specifies a $N(0, \sigma_u^2 I)$ prior on u as well as the likelihood, $f(Y|\beta, u, \sigma_u^2, \sigma_\epsilon^2)$. To specify a complete Bayesian model, we also need a prior distribution on $(\beta, \sigma_u^2, \sigma_\epsilon^2)$. Assuming that little is known about β, it makes sense to put an improper uniform prior on β. Or, if a proper prior is desired, one could use a $N(0, \sigma_\beta^2 I)$ prior with σ_β^2 so large that, for all intents and purposes, the normal distribution is uniform on the range of β. Therefore, we will use $\pi_0(\beta) \equiv 1$. We will assume that the prior on σ_ϵ^2 is inverse gamma with parameters A_ϵ and B_ϵ – denoted $IG(A_\epsilon, B_\epsilon)$ – so that its density is

$$\pi_0(\sigma_\epsilon^2) = \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} (\sigma_\epsilon^2)^{-(A_\epsilon+1)} \exp\left(-\frac{B_\epsilon}{\sigma_\epsilon^2}\right) \qquad (9)$$

Also, we assume that:
$\sigma_u^2 \sim IG(A_u, B_u)$

Here $A_\epsilon, B_\epsilon, A_u$ and B_u are "hyperparameters" that determine the priors and must be chosen by the statistician. These hyperparameters must be strictly positive in order for the priors to be proper. If A_ϵ and B_u were zero, then $\pi_0(\sigma_\epsilon^2)$ would be proportional to the improper prior $\frac{1}{\sigma_\epsilon^2}$, which is equivalent to log(σ_ϵ) having an improper uniform prior. Therefore, choosing A_ϵ and B_ϵ both close to zero (say, both equal to 0.1) gives an essentially noninformative, but proper, prior. The same reasoning applies to A_u and B_u. The model we have constructed is a hierarchical Bayes model, where the random variables are arranged in a hierarchy such that distributions at each level are determined by the random variables in the previous levels. At the bottom of the hierarchy are the known hyperparameters. At the next level are the fixed effects parameters and variance components whose distributions are determined by the hyperparameters. At the level above this are the random effects, u and ϵ, whose distributions are determined by the variance components. The top level contains the data y. (see [13])

4. Posterior calculations

We have the model

$$Y|F, \sigma_u^2, \sigma_\epsilon^2 \sim N(CF, \sigma_\epsilon^2 I_n + \sigma_u^2 Q). \qquad (10)$$

where $C = [X \;\; Z]$.

Unless F has a normal prior distribution or a hierarchical prior with a conditionally normal prior distribution, analytical simplifications in the computation of posterior quantities are not expected. For such cases, we have the joint posterior density of the penalized spline coefficients F and the error variances σ_ϵ^2 and σ_u^2 given by the expression.

$\pi(F, \sigma_u^2, \sigma_\epsilon^2|Y) \propto f(Y|F, \sigma_u^2, \sigma_\epsilon^2)\ \pi_0(F, \sigma_u^2, \sigma_\epsilon^2)$

Where f is the likelihood. From (14), f can be expressed as

$f(Y|F, \sigma_u^2, \sigma_\epsilon^2) \propto |\sigma_\epsilon^2 I_n + \sigma_u^2 Q|^{-1/2} exp\{\frac{-1}{2}(Y - CF)^T (\sigma_\epsilon^2 I_n + \sigma_u^2 Q)^{-1}(Y - CF)\}$

Proceeding further, suppose π_0 of the form

$$\pi_0(F, \sigma_u^2, \sigma_\epsilon^2) = \pi_1(\sigma_u^2, \sigma_\epsilon^2) \qquad (11)$$

which is constant in F, is chosen.

Markov Chain Monte Carlo (MCMC) based approaches to posterior computations are now readily available. For example, Gibbs sampling is straightforward (see [1,13]).

Note that $Q = CDC^T = ZZ^T$

where $D = \begin{bmatrix} 0_{p+q+1} & 0 \\ 0 & I_{n-(p+q+1)} \end{bmatrix}$

and $\sigma_u^2 D = \begin{bmatrix} 0_{p+q+1} & 0 \\ 0 & \sigma_u^2 I_{n-(p+q+1)} \end{bmatrix}$

we see

$$Y|F, \sigma_u^2, \sigma_\epsilon^2 \sim N(CF, \sigma_\epsilon^2 I_n + \sigma_u^2 Q) \qquad (12)$$

However, the prior of F given σ_u^2 specified that $F|\sigma_u^2 \sim N(0, \sigma_u^2 D)$

Therefore, it follows that

$$Y|\sigma_u^2, \sigma_\epsilon^2 \sim N(0, \sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T) \qquad (13)$$

where $\sigma_u^2 Q = C\sigma_u^2 DC^T$

$$F|Y, \sigma_u^2, \sigma_\epsilon^2 \sim N(A_1 Y, A_2) \qquad (14)$$

where

$$A_1 = \sigma_u^2 D\, C^T (\sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T)^{-1} \qquad (15)$$

$$A_2 = \sigma_u^2 D - \sigma_u^4 D\, C^T (\sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T)^{-1} CD \qquad (16)$$

We can rewrite covariance of Y given F, σ_u^2 and σ_ϵ^2 as

$$\sigma_\epsilon^2 I_n + \sigma_u^2 Q = \sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T = C\sigma_\epsilon^2 \left(C^{-1} I_n C^{T^{-1}} + \frac{\sigma_u^2}{\sigma_\epsilon^2} D\right) C^T$$

$$= C\sigma_\epsilon^2 \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D\right)^{-1} C^T, \text{ where } D^{-1} = D.$$

Result 1:

$$F|Y, \sigma_u^2, \sigma_\epsilon^2 \sim N\left\{\left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D\right)^{-1} C^T Y, \sigma_\epsilon^2 \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D\right)^{-1}\right\} \qquad (17)$$

Proof:

Since $E(F|Y) = A_1 Y$

$$= \sigma_u^2 D\, C^T (\sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T)^{-1}$$

$$= \sigma_u^2 D\, C^T \left(C\sigma_\epsilon^2 \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D\right)^{-1} C^T\right)^{-1} Y$$

$$= \sigma_u^2 D\, C^T \left(C^{T^{-1}} \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D\right) \frac{C^{-1}}{\sigma_\epsilon^2}\right) Y$$

$$= \frac{\sigma_u^2}{\sigma_\epsilon^2} D \left(C^T C^{T^{-1}} C^T C C^{-1} + C^T C^{T^{-1}} \frac{\sigma_\epsilon^2}{\sigma_u^2} D C^{-1}\right) C^{T^{-1}} C^T Y$$

$$= \frac{\sigma_u^2}{\sigma_\epsilon^2} D \left(C^T C^{T^{-1}} + \frac{\sigma_\epsilon^2}{\sigma_u^2} D C^{-1} C^{T^{-1}}\right) C^{T^{-1}} C^T Y$$

$$= \frac{\sigma_u^2}{\sigma_\epsilon^2} D \left(I_n + \frac{\sigma_\epsilon^2}{\sigma_u^2} D C^{-1} C^{T^{-1}} \right) C^T Y$$

$$= \frac{\sigma_u^2}{\sigma_\epsilon^2} D \left(\frac{\sigma_\epsilon^2}{\sigma_u^2} D C^{-1} C^{T^{-1}} + I_n \right) C^T Y$$

$$= \left(C^{-1} C^{T^{-1}} + \frac{\sigma_u^2}{\sigma_\epsilon^2} D \right) C^T Y$$

$$= \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D \right)^{-1} C^T Y$$

By same way we can prove the covariance is $\sigma_\epsilon^2 \left(C^T C + \frac{\sigma_\epsilon^2}{\sigma_u^2} D \right)^{-1}$.

Now proceeding as in [3], we employ spectral decomposition to obtain $CDC^T = BHB^T$, where $H = diag(h_1, \dots, h_n)$ is the matrix of eigenvalues and B is the orthogonal matrix of eigenvectors. Thus,

$$\sigma_\epsilon^2 I_n + [C\sigma_u^2 DC^T] = \sigma_\epsilon^2 I_n + B\sigma_u^2 HB^T = B\sigma_\epsilon^2 I_n B^T + B\sigma_u^2 HB^T = B\sigma_\epsilon^2 \left(I_n + \frac{\sigma_u^2}{\sigma_\epsilon^2} H \right) B^T$$

$$= \sigma_\epsilon^2 B(I_n + \delta H) B^T$$

where $\delta = \sigma_u^2/\sigma_\epsilon^2$. Then, the first stage (conditional) marginal density of Y given σ_ϵ^2 and δ can be written as

$$m(Y|\sigma_\epsilon^2, \delta) = \frac{1}{(2\pi\sigma_\epsilon^2)^{n/2}} \frac{1}{\det[I_n + \delta H]^{1/2}} \exp\{ -\frac{1}{2\sigma_\epsilon^2} Y^T B(I_n + \delta H) B^T Y$$

$$= \frac{1}{(2\pi\sigma_\epsilon^2)^{n/2}} \frac{1}{[\prod_{i=1}^n [1+\delta h_i]]^{1/2}} \exp\{ -\frac{1}{2\sigma_\epsilon^2} (\sum_{i=1}^n \frac{s_i^2}{1+\delta h_i})\}, \quad (18)$$

where $s = (s_1, \dots, s_n)^T = B^T Y$. We choose the prior on σ_ϵ^2, $\delta = \sigma_u^2/\sigma_\epsilon^2$, qualitatively similar to the used in [1]. Specifically, we take $\pi_1(\sigma_\epsilon^2, \delta)$ to be proportional to the product of an inverse gamma density $\{B_\epsilon^{A_\epsilon}/\Gamma(A_\epsilon)\} exp(-B_\epsilon/\sigma_\epsilon^2)(\sigma_\epsilon^2)^{-(A_\epsilon+1)}$ for σ_ϵ^2 and the density of a $F(b,a)$ distribution for δ (for suitable choice of B_ϵ, A_ϵ, b and a). Conditions apply on a and b such that (see [1]):

The prior covariance of $\delta (= \frac{2b^2(a+b-2)}{a(b-4)(b-2)^2})$ is infinite.

The fisher information number $= (\frac{a^2(b+2)(b+6)}{2(a-4)(a+b+2)})$ is minimum.

The prior mode $= (\frac{b(a-2)}{a(b+2)})$ is greater than 0.

This can be done by choosing $2 < b \le 4$ and $a = 8(b+2)/(b-2)$

Once $\pi_1(\sigma_\epsilon^2, \delta)$ is chosen as above, we obtain the posterior density of δ given Y, the posterior mean and covariance matrix of F as in the following theorems.

Theorem1: the posterior density of δ given Y is:

$$\pi_{22}(\delta|Y) \propto \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} (\prod_{i=1}^n (1+\delta h_i))^{-1/2} \left(2\mathrm{B}_\epsilon + \sum_{i=1}^n \frac{s_i^2}{1+\delta h_i} \right)^{-(n+2A_\epsilon+2)/2} \quad (19)$$

Proof:

$$\pi_{22}(\delta|Y) = \int m(Y|\sigma_\epsilon^2, \delta)\, f(\delta, b, a)\, f(\sigma_\epsilon^2, A_\epsilon, B_\epsilon) d\sigma_\epsilon^2$$

$$= \int \frac{1}{(2\pi\sigma_\epsilon^2)^{n/2}} (\prod_{i=1}^n (1+\delta h_i))^{-1/2} \frac{b^{b/2} a^{a/2}}{B(b,a)} \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}}$$

$$\exp\left\{ -\frac{1}{2\sigma_\epsilon^2} \left(\sum_{i=1}^n \frac{s_i^2}{1+\delta h_i} \right) \right\} \frac{\mathrm{B}_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} (\sigma_\epsilon^2)^{-(A_\epsilon+1)} \exp\left(-\frac{\mathrm{B}_\epsilon}{\sigma_\epsilon^2} \right) d\sigma_\epsilon^2$$

$$= \frac{(2\pi)^{-n/2}}{\Gamma(A_\epsilon)} \frac{b^{b/2}a^{a/2}}{B(b,a)} \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} \int \left(\prod_{i=1}^{n}(1+\delta h_i)\right)^{-1/2} \exp\left\{-\frac{1}{2\sigma_\epsilon^2}\left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)\right\} (\sigma_\epsilon^2)^{-(n+2A_\epsilon+2)/2} d\sigma_\epsilon^2$$

$$= \frac{(2\pi)^{-n/2}}{\Gamma(A_\epsilon)} \frac{b^{b/2}a^{a/2}}{B(b,a)} \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} (2)^{(n+2A_\epsilon+2)/2} \int \left(\prod_{i=1}^{n}(1+\delta h_i)\right)^{-1/2} \exp\left\{-\frac{1}{2\sigma_\epsilon^2}\left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)\right\} \left(\frac{2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}}{2\sigma_\epsilon^2}\right)^{(n+2A_\epsilon+2)/2} \left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+hd_i}\right)^{-(n+2A_\epsilon+2)/2} d\sigma_\epsilon^2$$

$$\propto \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} \int \left(\prod_{i=1}^{n}(1+\delta h_i)\right)^{-1/2} \exp\left\{-\frac{1}{2\sigma_\epsilon^2}\left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)\right\} \left(\frac{2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}}{2\sigma_\epsilon^2}\right)^{[(n+2A_\epsilon+4)/2]-1} \left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)^{-(n+2A_\epsilon+2)/2} d\sigma_\epsilon^2$$

$$\propto \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} \Gamma((n+2A_\epsilon+4)/2) \left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)^{-(n+2A_\epsilon+2)/2} \left(\prod_{i=1}^{n}(1+\delta h_i)\right)^{-1/2}$$

$$\propto \frac{\delta^{(b/2)-1}}{(a+b\delta)^{-(a+b)/2}} \left(\prod_{i=1}^{n}(1+\delta h_i)\right)^{-1/2} \left(2B_\epsilon + \sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)^{-(n+2A_\epsilon+2)/2}$$

Theorem2: The posterior mean and covariance matrix of F are:

$$E(F|Y) = DC^T BE\{(I_n + \delta H)^{-1} \mid Y\}s \quad (20)$$

And

$$var(F|Y) = \frac{1}{n+2A_\epsilon+2} E\left[\left(2B_\epsilon + \left(\sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)\right) |Y\right] D - \frac{1}{n+2A_\epsilon+2} HC^T BE\left[\left(2B_\epsilon + \left(\sum_{i=1}^{n}\frac{s_i^2}{1+\delta h_i}\right)\right) [I_n + \delta H]^{-1} |Y\right] B^T CD + E[R(\delta)R(\delta)^T|Y],$$

(21)

where $R(\delta) = DC^T B(I_n + \delta H)^{-1}s$

Proof:

From (14):

$$\begin{aligned} E(F|Y) &= A_1 Y \\ &= \sigma_u^2 D\, C^T\, (\sigma_\epsilon^2 I_n + C\sigma_u^2 DC^T)^{-1} Y \\ &= \sigma_u^2 DC^T\, \{\sigma_\epsilon^2 B(I_n + \delta H)B^T\}^{-1} Y \\ &= \frac{\sigma_u^2}{\sigma_\epsilon^2} DC^T B^{T^{-1}} (I_n + \delta H)^{-1} B^{-1} Y \end{aligned}$$

Since B is the orthogonal matrix of eigenvectors, then $B^{-1} = B^T$ and $B^{T^{-1}} = B$.

Therefore

$E(F|Y) = DC^T B\, \delta\, (I_n + \delta H)^{-1} B^T Y$

$\quad = DC^T B\, E((I_n + \delta H)^{-1}|Y) s$

where the expectation $E((I_n + \delta H)^{-1}|Y)$ is taken with respect to $\pi_{22}(\delta|Y)$ (see theorem 1 above). And by the same way we can prove the variance of F given Y.

5. Model checking and Bayes factors

An important and useful model checking problem in the present setup is checking the two models

$H_o : g = X\beta = g^o$ versus $H_1 : g = X\beta + Zu \neq g^o$.

Under H_1, ($g = g(F), \sigma_u^2, \sigma_\epsilon^2$) is given the prior $\pi_0(F, \sigma_u^2, \sigma_\epsilon^2) I(g \neq g^o)$, whereas under H_o, $\pi_0(\sigma_\epsilon^2)$ induced by $\pi_0(F, \sigma_u^2, \sigma_\epsilon^2)$ is the only part needed. In order to conduct the model checking, we compute the Bayes factor, B_{01}, of H_o relative to H_1:

$$B_{01}(Y) = \frac{m(Y|H_o)}{m(Y|H_1)} \qquad (22)$$

where $m(Y|H_i)$ is the predictive (marginal) density of Y under model $H_i, i = 0,1$. We have

$$m(Y|H_o) = \int f(Y|g^o, \sigma_\epsilon^2) \pi_0(\sigma_\epsilon^2)\, d\sigma_\epsilon^2$$

and

$$m(Y|H_1) = \int f(Y|F, \sigma_u^2, \sigma_\epsilon^2) \pi_0(F, \sigma_u^2, \sigma_\epsilon^2)\, dF d\sigma_u^2 d\sigma_\epsilon^2$$

As in the previous section $\pi_0(\sigma_u^2, \sigma_\epsilon^2)$ will be constant in F, while σ_ϵ^2 is inverse gamma and is independent of $v_1 = \sigma_\epsilon^2 / \sigma_u^2$ which is given the $F_{a,b}$ prior distribution. (Equivalently, $\delta = \sigma_u^2/\sigma_\epsilon^2$ is given the $F_{b,a}$, Specifically, $\pi_0(\sigma_\epsilon^2) = \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} (\sigma_\epsilon^2)^{-(A_\epsilon+1)} exp\left(-\frac{B_\epsilon}{\sigma_\epsilon^2}\right)$, where A_ϵ and B_ϵ (small) are suitably chosen. Therefore,

$$m(Y|H_o) = \int f(Y|g^o, \sigma_\epsilon^2) \pi_0(\sigma_\epsilon^2)\, d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \int (\sigma_\epsilon^2)^{-n/2} \exp\left(-\frac{B_\epsilon}{\sigma_\epsilon^2}\right) (\sigma_\epsilon^2)^{-(A_\epsilon+1)} \exp\left(-\frac{(Y - g^o(x))^2}{2\sigma_\epsilon^2}\right) d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \int (\sigma_\epsilon^2)^{-(n/2 + A_\epsilon + 1)} \exp\left(-\frac{B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2}{\sigma_\epsilon^2}\right) d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \int (\sigma_\epsilon^2)^{-(\frac{n}{2} + A_\epsilon + 1)} (B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2)^{\frac{n}{2} + A_\epsilon + 1} (B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2)^{-(\frac{n}{2} + A_\epsilon + 1)} \exp\left(-\frac{B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2}{\sigma_\epsilon^2}\right) d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \int \frac{(B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2)^{\frac{n}{2} + A_\epsilon + 1}}{(\sigma_\epsilon^2)^{(\frac{n}{2} + A_\epsilon + 1)}} \exp\left(-\frac{B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2}{\sigma_\epsilon^2}\right) (B_\epsilon + \frac{1}{2}(y_i - g^o(x_i))^2)^{-(\frac{n}{2} + A_\epsilon + 1)} d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \int \left(\frac{B_\epsilon+\frac{1}{2}(y_i-g^o(x_i))^2}{\sigma_\epsilon^2}\right)^{(\frac{n}{2}+A_\epsilon+2)-1} \exp\left(-\frac{B_\epsilon+\frac{1}{2}(y_i-g^o(x_i))^2}{\sigma_\epsilon^2}\right)(B_\epsilon+\frac{1}{2}(y_i - g^o(x_i))^2)^{-(\frac{n}{2}+A_\epsilon+1)}\, d\sigma_\epsilon^2$$

$$= (2\pi)^{-n/2} \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)} \Gamma(\tfrac{n}{2}+A_\epsilon+1)(B_\epsilon+\tfrac{1}{2}(y_i-g^o(x_i))^2)^{-(\frac{n}{2}+A_\epsilon+1)}\, d\sigma_\epsilon^2 \qquad (23)$$

Further, using (13) it follows that:

$$m(Y|H_1,\sigma_\epsilon^2,\delta) = (2\pi\sigma_\epsilon^2)^{-\frac{n}{2}} \left(\prod_{i=1}^n(1+\delta h_i)\right)^{-1/2} \exp\left\{-\frac{1}{2\sigma_\epsilon^2}\left(\sum_{i=1}^n \frac{s_i^2}{1+\delta h_i}\right)\right\} \qquad (24)$$

Therefore,

$$m(Y|H_1) = \int m(Y|M_1,\sigma_\epsilon^2,\delta)\,\pi_0(\sigma_\epsilon^2,\delta)\, d\sigma_\epsilon^2\, d\delta$$

$$= \int \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)}(\sigma_\epsilon^2)^{-(A_\epsilon+1)} \exp\left(-\frac{B_\epsilon}{\sigma_\epsilon^2}\right)(2\pi\sigma_\epsilon^2)^{-n/2}\left(\prod_{i=1}^n(1+\delta h_i)\right)^{-1/2}$$

$$\exp\left\{-\frac{1}{2\sigma_\epsilon^2}\left(\sum_{i=1}^n \frac{s_i^2}{1+hd_i}\right)\right\}\pi_0(\delta)\, d\sigma_\epsilon^2\, d\delta$$

$$= \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)}(2\pi)^{-n/2}\int \left(\prod_{i=1}^n(1+\delta h_i)\right)^{-1/2}\pi_0(\delta)$$

$$\left\{\int \exp\left\{-\frac{1}{\sigma_\epsilon^2}\left(B_\epsilon+\frac{1}{2}\sum_{i=1}^n\frac{s_i^2}{1+\delta h_i}\right)\right\} d\sigma_\epsilon^2\right\}\, d\delta$$

$$= \frac{B_\epsilon^{A_\epsilon}}{\Gamma(A_\epsilon)}(2\pi)^{-n/2}\Gamma(n/2+A_\epsilon)\int \left(\prod_{i=1}^n(1+\delta h_i)\right)^{-1/2}$$

$$\pi_0(\delta)\ \left(B_\epsilon+\frac{1}{2}\sum_{i=1}^n\frac{s_i^2}{1+\delta h_i}\right)^{-(n/2+c-1)}\ d\delta \qquad (25)$$

6.1. Prior robustness of Bayes factors

For any constant c also contributes the same prior information about F. Therefore, a study of the robustness of the Bayes factor. Here we consider a sensitivity study using the density ratio class defined as follows. Since the prior π that we use has the form

$\pi(F,\sigma_u^2,\sigma_\epsilon^2) \propto \pi_0(F,\sigma_u^2,\sigma_\epsilon^2)$,

we consider the class of priors

$C = \{\pi : c_1\pi_0(F,\sigma_u^2,\sigma_\epsilon^2) \le \alpha\pi(F,\sigma_u^2,\sigma_\epsilon^2) \le c_2\pi_0(F,\sigma_u^2,\sigma_\epsilon^2), \quad \alpha > 0\}$

For specified $0 < c_1 < c_2$. We would like to investigate how the Bayes factor (22) behaves as the prior π varies in C. We note that for any $\pi \in C$, the Bayes factor B_{01} has the form

$$B_{01} = \frac{\int f(Y|g^o,\sigma_\epsilon^2)\,\pi(F,\sigma_u^2,\sigma_\epsilon^2)\, dF\, d\sigma_u^2\, d\sigma_\epsilon^2}{\int f(Y|F,\sigma_u^2,\sigma_\epsilon^2)\,\pi(F,\sigma_u^2,\sigma_\epsilon^2)\, dF\, d\sigma_u^2\, d\sigma_\epsilon^2}$$

Even though the integration in the numerator above need not involve F, σ_u^2, we do so to apply the following result (see [1,2,3,7,9]).

Consider the density-ratio class

$\Gamma_{DR} = \{\pi :\ L(\eta) \le \alpha\pi(\eta) \le U(\eta)\ for\ some\ \alpha > 0\}$

, for specified non-negative functions L and U. Further, let $q \equiv q^+ + q^-$ be the usual decomposition of q into its positive and negative parts, i.e., $q^+(u) = max\{q(u),0\}$ and $q^-(u) = -max\{-q(u),0\}$. Then we have the following theorem.

Theorem 3: For functions q_1 and q_2 such that $\int q_i(\eta)|U(\eta)\, d\eta < \infty$, for i = 1, 2, and with q_2 positive a.s. with respect to all $\pi \in \Gamma_{DR}$,

$$\inf_{\pi\in\Gamma_{DR}} \frac{\int q_1(\eta)\, \pi(\eta)\, d\eta}{\int q_2(\eta)\, \pi(\eta)\, d\eta}$$

is the unique solution ϑ of

$$\int(q_1(\eta) - \vartheta q_2(\eta))^{-} U(\eta) d\eta + \int(q_1(\eta) - \vartheta q_2(\eta))^{+} L(\eta) d\eta = 0 \qquad (26)$$

$$\sup_{\pi\in\Gamma_{DR}} \frac{\int q_1(\eta)\, \pi(\eta)\, d\eta}{\int q_2(\eta)\, \pi(\eta)\, d\eta}$$

is the unique solution ϑ of

$$\int(q_1(\eta) - \vartheta q_2(\eta))^{+} U(\eta) d\eta + \int(q_1(\eta) - \vartheta q_2(\eta))^{-} L(\eta) d\eta = 0 \qquad (27)$$

Proof:

To prove first part

$$\int q_1(\eta)^{-}\, U(\eta) d\eta \; + \int q_1(\eta)^{+}\, L(\eta) d\eta \; - \vartheta \int q_2(\eta)^{-}\, U(\eta) d\eta \; - \vartheta \int q_2(\eta)^{+}\, L(\eta) d\eta \; = 0$$

$$\Rightarrow \int (q_1(\eta)^{-}\, U(\eta) + q_1(\eta)^{+}\, L(\eta)) d\eta \; - \vartheta \int (q_2(\eta)^{-}\, U(\eta) + q_2(\eta)^{+}\, L(\eta)) d\eta \; = 0$$

$$\Rightarrow \vartheta = \frac{\int (q_1(\eta)^{-}\, U(\eta) + q_1(\eta)^{+}\, L(\eta)) d\eta}{\int (q_2(\eta)^{-}\, U(\eta) + q_2(\eta)^{+}\, L(\eta)) d\eta}$$

By theorem 4.1. in DeRobertis and Hartigan (1981) (see [6]).

$\left(q_1(\eta)^{-}\, U(\eta) + q_1(\eta)^{+}\, L(\eta)\right) = inf_{\pi\in\Gamma_{DR}} Kq_1(\eta)$, where $K \in I(L, U)$,

$$\Rightarrow \vartheta = \frac{\int \inf_{\pi\in\Gamma_{DR}} Kq_1(\eta)\, d\eta}{\int \inf_{\pi\in\Gamma_{DR}} Kq_2(\eta)\, d\eta}$$

and let $K = a\pi(\eta)$ then

$$\Rightarrow \vartheta = \inf_{\pi\in\Gamma_{DR}} \frac{\int a\, q_1(\eta)\, \pi(\eta)\, d\eta}{\int a\, q_2(\eta)\, \pi(\eta)\, d\eta}$$

$$\Rightarrow \vartheta = \inf_{\pi\in\Gamma_{DR}} \frac{\int q_1(\eta)\, \pi(\eta)\, d\eta}{\int q_2(\eta)\, \pi(\eta)\, d\eta}$$

Then the $inf_{\pi\in\Gamma_{DR}} \frac{\int q_1(\eta)\, \pi(\eta)\, d\eta}{\int q_2(\eta)\, \pi(\eta)\, d\eta}$ is the solution of ϑ, now to prove unique solution suppose $\vartheta_0 = \inf_{\pi\in\Gamma_{DR}} \frac{\int q_1(\eta)\, \pi(\eta)\, d\eta}{\int q_2(\eta)\, \pi(\eta)\, d\eta}$, $c_1 = \inf_{\pi\in\Gamma_{DR}} \int q_2(\eta)\, \pi(\eta)\, d\eta$ and $c_2 = \sup_{\pi\in\Gamma_{DR}} \int q_2(\eta)\, \pi(\eta)\, d\eta$. Then $0 < c_1 < c_2 < \infty$ and $|\vartheta_0| < \infty$ it follows that $\vartheta_0 \geq \vartheta$ if and only if $\int(q_1(\eta) - \vartheta q_2(\eta))^{-} U(\eta) d\eta + \int(q_1(\eta) - \vartheta q_2(\eta))^{+} L(\eta) d\eta \geq 0$.Moreover, for any $\epsilon \geq 0$, $\vartheta + \epsilon/c_1 \leq \vartheta_0$ implies $\int(q_1(\eta) - \vartheta q_2(\eta))^{-} U(\eta) d\eta + \int(q_1(\eta) - \vartheta q_2(\eta))^{+} L(\eta) d\eta \geq \epsilon$ which in turn implies $\vartheta + \epsilon/c_2 \leq \vartheta_0$; thus ; $\vartheta_0 > \vartheta$ if and only if $\int(q_1(\eta) - \vartheta q_2(\eta))^{-} U(\eta) d\eta + \int(q_1(\eta) - \vartheta q_2(\eta))^{+} L(\eta) d\eta > 0$. Hence, then ϑ is the unique solution.

Now to prove second part

$$\int q_1(\eta)^{+}\, U(\eta) d\eta \; + \int q_1(\eta)^{-}\, L(\eta) d\eta \; - \vartheta \int q_2(\eta)^{+}\, U(\eta) d\eta \; - \vartheta \int q_2(\eta)^{-}\, L(\eta) d\eta \; = 0$$

$$\Rightarrow \int (q_1(\eta)^+ \, U(\eta) + q_1(\eta)^- \, L(\eta))d\eta \;-\; \vartheta \int (q_2(\eta)^+ \, U(\eta) + q_2(\eta)^- \, L(\eta))d\eta \;= 0$$

$$\Rightarrow \vartheta = \frac{\int (q_1(\eta)^+ \, U(\eta) + q_1(\eta)^- \, L(\eta))d\eta}{\int (q_2(\eta)^+ \, U(\eta) + q_2(\eta)^- \, L(\eta))d\eta}$$

Also by theorem 4.1. in DeRobertis and Hartigan (1981) (see [6]),

$(q_1(\eta)^+ \, U(\eta) + q_1(\eta)^- \, L(\eta)) = sup_{\pi \in \Gamma_{DR}} K q_1(\eta)$,where $K \in I(L, U)$,

$$\Rightarrow \vartheta = \frac{\int \sup_{\pi \in \Gamma_{DR}} K q_1(\eta) \; d\eta}{\int \sup_{\pi \in \Gamma_{DR}} K q_2(\eta) \; d\eta}$$

$$\Rightarrow \vartheta = \frac{\int \sup_{\pi \in \Gamma_{DR}} a q_1(\eta) \, \pi(\eta) \, d\eta}{\int \sup_{\pi \in \Gamma_{DR}} a q_2(\eta) \pi(\eta) \; d\eta}$$

$$\Rightarrow \vartheta = \sup_{\pi \in \Gamma_{DR}} \frac{\int q_1(\eta) \, \pi(\eta) \, d\eta}{\int q_2(\eta) \, \pi(\eta) \, d\eta}$$

By same way of proof the unique of first part above (the proof complete) .

Now we shall discuss this result for the Gaussian membership function only. Then, since the prior π that we use has the form $\pi_0(F, \sigma_u^2, \sigma_\epsilon^2) \propto \pi_0(\sigma_u^2, \sigma_\epsilon^2)$, and we don't intend to vary $\pi_0(\sigma_u^2, \sigma_\epsilon^2)$ in our analysis, we redefine C_A as

$C \;= \{ \pi(F) : \; c_1 \pi_0(F) \leq \; \alpha \pi(F) \; \leq \; c_2 \pi_0(F), \qquad \alpha > 0 \}$

For specified $0 < c_1 < c_2$. Now, were express B_{01} as

$$B_{01} \;= \frac{\int \{ \int f(Y|g^o, \sigma_\epsilon^2) \; \pi_0(\sigma_\epsilon^2) \, d\sigma_\epsilon^2 \} \pi(F) dF}{\int \{ \int f(Y|F, \sigma_u^2, \sigma_\epsilon^2) \; \pi_0(\sigma_u^2, \sigma_\epsilon^2) d\sigma_u^2 d\sigma_\epsilon^2 \} \pi(F) dF} = \frac{\int q_1(F) \; \pi(F) \; dF}{\int q_2(F) \; \pi(F) \; dF}$$

where

$$q_1(F) = \int f(Y|g^o, \sigma_\epsilon^2) \, \pi_0(\sigma_\epsilon^2) \, d\sigma_\epsilon^2$$

$$q_2(F) = \int f(Y|F, \sigma_u^2, \sigma_\epsilon^2) \; \pi_0(\sigma_u^2, \sigma_\epsilon^2) d\sigma_u^2 d\sigma_\epsilon^2$$

Then by theorem 3 is readily applicable, and we obtain the following theorem:

Theorem 4:

$\inf_{\pi \in C_A} B_{01}(\pi)$ is the unique solution ϑ of

$$c_2 \int (q_1(F) - \vartheta q_2(F))^- dF + c_1 \int (q_1(F) - \vartheta q_2(F))^+ dF = 0 \qquad (28)$$

and $\sup_{\pi \in C_A} B_{01} \, (\pi)$ is the unique solution ϑ of

$$c_2 \int (q_1(F) - \vartheta q_2(F))^+ dF + c_1 \int (q_1(F) - \vartheta q_2(F))^- dF = 0 \qquad (29)$$

Proof:

To prove part one

$$c_2 \int q_1(F)^- U(F) dF + c_1 \int q_1(F)^+ L(F) dF - \vartheta c_2 \int q_2(F)^- U(F) dF - \vartheta c_1 \int q_2(F)^+ L(F) dF \;= 0$$

$$\Rightarrow \int (c_2 q_1(F)^- U(F) + c_1 q_1(F)^+ L(F)) dF \;\; - \; \vartheta \int (c_2 q_2(F)^- U(F) + c_1 q_2(F)^+ L(F)) dF = 0$$

$$\Rightarrow \vartheta = \frac{\int (c_2 q_1(F)^- \, U(F) + c_1 q_1(F)^+ \, L(F))dF}{\int (c_2 q_2(F)^- \, U(F) + c_1 q_2(F)^+ \, L(F))dF}$$

Then,

$(c_2 q_1(F)^- \, U(F) + c_1 q_1(F)^+ \, L(F)) = inf_{\pi \in \Gamma_{DR}} \, cKq_1(F)$ $, where \; K \in I(L,U), c \le c_1 + c_2$, then

$$\Rightarrow \vartheta = \frac{\int \inf_{\pi \in C_A} cKq_1(F) \; dF}{\int \inf_{\pi \in C_A} cKq_2(F) \; dF}$$

$$\Rightarrow \vartheta = \inf_{\pi \in C_A} \frac{\int q_1(F) \; dF}{\int q_2(F) \; dF}$$

$$\Rightarrow \vartheta = \inf_{\pi \in C_A} B_{01}(\pi)$$

To prove second part

$$c_2 \int q_1(F)^+ \, U(F)dF \; + \; c_1 \int q_1(F)^- \, L(F)dF \; - \; \vartheta c_2 \int q_2(F)^+ \, U(F)dF \; - \; \vartheta c_1 \int q_2(F)^- \, L(F)dF = 0$$

$$\Rightarrow \int (c_2 q_1(F)^+ \, U(F) + c_1 q_1(F)^- \, L(F))dF \; - \; \vartheta \int (c_2 q_2(F)^+ \, U(F) + c_1 q_2(F)^- \, L(F))dF \; = 0$$

$$\Rightarrow \vartheta = \frac{\int (c_2 q_1(F)^+ \, U(F) + c_1 q_1(F)^- \, L(F))dF}{\int (c_2 q_2(F)^+ \, U(F) + c_1 q_2(F)^- \, L(F))dF}$$

Then,

$(c_2 q_1(F)^+ \, U(F) + c_1 q_1(F)^- \, L(F) = sup_{\pi \in \Gamma_{DR}} \, cKq_1(F)$ $, where \; K \in I(L,U), c \le c_1 + c_2$, then

$$\Rightarrow \vartheta = \frac{\int \sup_{\pi \in \Gamma_{DR}} cKq_1(F) \; dF}{\int \sup_{\pi \in \Gamma_{DR}} cKq_2(F) \; dF}$$

$$\Rightarrow \vartheta = \sup_{\pi \in \Gamma_{DR}} \frac{\int q_1(F) \; dF}{\int q_2(F) \; dF}$$

$$\Rightarrow \vartheta = \sup_{\pi \in \Gamma_{DR}} B_{01}(\pi)$$

By same as the unique prove to first part in theorem 3.

5. Conclusions

In this paper we suggest approach to semiparametric regression by proposing an alternative to dealing with complicated analyses on function spaces. First the penalized spline is used for the model and by using a convenient connection between penalized splines and mixed models, we can representation semiparametric regression model as mixed model. The penalized spline assumed on g and pure polynomial on prior g°. Furthermore we obtain the posterior density of δ given Y, the posterior mean and covariance matrix of F (theorem 1, 2), and a Bayesian test is proposed to check whether the baseline function g° is compatible with the data or not and we proved the prior robustness of Bayes factors (theorem 3, 4).

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