SEMIPARAMETRIC PENALIZED SPLINE REGRESSION

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Abstract

In this paper, we propose a new semiparametric regression estimator by using a hybrid technique of a parametric approach and a nonparametric penalized spline method. The overall shape of the true regression function is captured by the parametric part, while its residual is consistently estimated by the nonparametric part. Asymptotic theory for the proposed semiparametric estimator is developed, showing that its behavior is dependent on the asymptotics for the nonparametric penalized spline estimator as well as on the discrepancy between the true regression function and the parametric part. As a naturally associated application of asymptotics, some criteria for the selection of parametric models are addressed. Numerical experiments show that the proposed estimator performs better than the existing kernel-based semiparametric estimator and the fully nonparametric estimator, and that the proposed criteria work well for choosing a reasonable parametric model.

Key Words and Phrases: Asymptotic theory, Bias reduction, *B*-spline, Parametric model, Penalized spline, Semiparametric regression

1. Introduction

There have been several nonparametric smoothing techniques used in regression problems, such as lowess (locally weighted scatter plot smoothing), kernel smoothing, spline smoothing, wavelet, the series method, and so on. The nonparametric estimators generally have consistency, which is an advantage of this approach. Hence, if the nonparametric estimator is used, we can expect that the true regression can be captured as the sample size increases. However, because the form of a nonparametric estimator is sometimes complicated, the interpretation of the estimated structure might not be clear.

On the other hand, in a parametric regression problem with the true regression function controlled by a finite-dimensional parameter vector, the estimated structure is easy to understand, however, the estimator does not always have consistency. Therefore, there are advantages and disadvantages associated with each of these approaches. This motivates us to consider a hybrid of parametric and nonparametric methods for the regression problem and we, in fact, introduce a semiparametric regression method so that the estimator has the advantages of both approaches.

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The semiparametric method in this paper consists of two steps. In the first step, we utilize an appropriate parametric estimator. In the second step, we apply a certain nonparametric smoother to the residual data associated with the parametric estimator in the first step. The parametric estimator in the first step and the nonparametric smoother in the second step are combined into the proposed semiparametric estimator.

Similar semiparametric approaches for smoothing have been developed by many authors. Hjort and Glad (1995) and Naito (2004) discussed similar methods in density estimation literature. Glad (1998) and Naito (2002) addressed the semiparametric regression method. Martins et al. (2008) introduced general decomposition, including additive and multiplicative corrections in regression. Recently, Fan et al. (2009) discussed the semiparametric approach in the framework of a generalized linear model. Note that the aforementioned works all used kernel smoothing in the second step estimation.

Our proposal is to utilize the penalized spline method for residual smoothing in the second step. This is a typical technique used in nonparametric regression problems with sufficient fitness and appropriate smoothness, which was developed by O'Sullivan (1986) and Eilers and Marx (1996). Many of its applications are summarized in Ruppert, et al (2003). Throughout this paper, the fully nonparametric penalized spline estimator is designated by NPSE, while the semiparametric penalized spline estimator, including the two-step manipulations mentioned above, is denoted by SPSE. In this paper, the advantages of using the penalized spline method instead of the kernel method are described both theoretically and numerically. In particular, we found that the SPSE has better behavior than the semiparametric local linear estimator (SLLE) in simulation.

This paper is organized as follows. We elaborate on the proposed SPSE in Section 2. Section 3 discusses the asymptotic properties of the SPSE, which can be obtained using a combination of the asymptotic results for the parametric estimator and for the NPSE developed by Claeskens et al. (2009). The asymptotic bias of the SPSE depends on the initial parametric model utilized in the first step. The form of the asymptotic bias suggests a method of choosing the parametric model for the first step. A theoretical comparison of SPSE with SLLE is also given in the context of asymptotic bias, which reveals that the use of the penalized spline rather than a kernel smoother in the second step is valid. In Section 4, some criteria for parametric model selection will be clarified. If a parametric model chosen by the criteria discussed in Section 4 is used as the parametric part of the SPSE, its asymptotic bias will become smaller than that of the NPSE. The results of a simulation are reported in Section 5. The simulation studies include checking the accuracy of the SPSE and comparing it with the NPSE and the SLLE as regression estimators. The performance of the parametric model selection discussed in Section 4 is also investigated. Related discussion and issues for future research are provided in Section 6. Proofs for the theoretical results are given in the Appendix.

2. Semiparametric penalized spline estimator

Consider the relationship of the dataset $\{(x_i, y_i) : i = 1, \cdots, n\}$ as the regression model

$$y_i = f(x_i) + \varepsilon_i, \ \ i = 1, \cdots, n,$$

where the explanatory $\{x_i\}_{1 \le i \le n}$ are generated from density $m(x)$ with its support on $[0, 1]$, $f(x) = E[Y|X = x]$ is an unknown regression function, and the errors $\{\varepsilon_i\}_{1 \le i \le n}$ are assumed to be uncorrelated with $E[\varepsilon_i|X_i = x_i] = 0$ and $V[\varepsilon_i|X_i = x_i] = \sigma^2(x_i) < \infty$.

Let $f(x|\boldsymbol{\beta}), \boldsymbol{\beta} \in B \subseteq \mathbb{R}^M$ be a parametric model. We now construct the semiparametric estimator of $f(x)$. First we obtain an appropriate estimator $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ via a suitable method of estimation. Then $f(x)$ can be written as

$$f(x) = f(x|\hat{\boldsymbol{\beta}}) + f(x|\hat{\boldsymbol{\beta}})^\gamma r_\gamma(x, \hat{\boldsymbol{\beta}}), \tag{1}$$

where $r_\gamma(x, \boldsymbol{\beta}) = \{f(x) - f(x|\boldsymbol{\beta})\}/f(x|\boldsymbol{\beta})^\gamma$ for some $\gamma \in \{0, 1\}$. When $\gamma = 0$, this decomposition becomes $f(x) = f(x|\hat{\boldsymbol{\beta}}) + \{f(x) - f(x|\hat{\boldsymbol{\beta}})\}$, which is called an additive correction. When $\gamma = 1$, on the other hand, we have a multiplicative correction $f(x) = f(x|\hat{\boldsymbol{\beta}})\{f(x)/f(x|\hat{\boldsymbol{\beta}})\}$. By using the parameter γ, we can treat additive and multiplicative corrections systematically (see, Fan et al. (2009)). In the second step, $r_\gamma(x, \hat{\boldsymbol{\beta}})$ is estimated by applying a nonparametric technique to $\{(x_i, \{y_i - f(x_i|\hat{\boldsymbol{\beta}})\}/f(x_i|\hat{\boldsymbol{\beta}})^\gamma) : i = 1, \cdots, n\}$. The SPSE is obtained as

$$\hat{f}(x, \gamma) = f(x|\hat{\boldsymbol{\beta}}) + f(x|\hat{\boldsymbol{\beta}})^\gamma \hat{r}_\gamma(x, \hat{\boldsymbol{\beta}}), \tag{2}$$

where $\hat{r}_\gamma(x, \hat{\boldsymbol{\beta}})$ is a nonparametric estimator of $r_\gamma(x, \hat{\boldsymbol{\beta}})$.

We adopt the penalized spline to estimate $r_\gamma(x, \hat{\boldsymbol{\beta}})$. Let $\{B_{-p+1}^{[p]}(x), \cdots, B_{K_n}^{[p]}(x)\}$ be the B-spline basis of degree p with equally spaced knots $\kappa_k = k/K_n (k = -p + 1, \cdots, K_n + p)$. Then we consider the B-spline model

$$s(x) = \sum_{k=-p+1}^{K_n} B_k^{[p]}(x) b_k$$

as an approximation to $r_\gamma(x, \hat{\boldsymbol{\beta}})$, where b_k's are unknown parameters. The definition and fundamental properties of the B-spline basis are detailed in de Boor (2001). Let $\boldsymbol{R}_\gamma$ be the n-vector with ith element $\{y_i - f(x_i|\hat{\boldsymbol{\beta}})\}/f(x_i|\hat{\boldsymbol{\beta}})^\gamma$ and let $Z = (B_{-p+j}^{[p]}(x_i))_{ij}$ and $\boldsymbol{b} = (b_{-p+1} \cdots b_{K_n})'$. The penalized spline estimator $\hat{\boldsymbol{b}} = (\hat{b}_{-p+1} \cdots \hat{b}_{K_n})'$ of $\boldsymbol{b}$ is defined as the minimizer of

$$(\boldsymbol{R}_\gamma - Z\boldsymbol{b})'(\boldsymbol{R}_\gamma - Z\boldsymbol{b}) + \lambda_n \boldsymbol{b}' D_q' D_q \boldsymbol{b}, \tag{3}$$

where λ_n is the smoothing parameter and $(K_n + p - q) \times (K_n + p)$th matrix D_q is the qth difference matrix. The estimator of $r_\gamma(x, \hat{\boldsymbol{\beta}})$ is defined as

$$\hat{r}_\gamma(x, \hat{\boldsymbol{\beta}}) = \sum_{k=-p+1}^{K_n} B_k^{[p]}(x) \hat{b}_k = \boldsymbol{B}(x)'(Z'Z + \lambda_n D_q' D_q)^{-1} Z' \boldsymbol{R}_\gamma, \tag{4}$$

where $\boldsymbol{B}(x) = (B_{-p+1}^{[p]}(x) \cdots B_{K_n}^{[p]}(x))'$.

In Figure 1, an example of the SPSE is drawn. In the left panel, the true function $f(x) = \exp[-x^2]\sin(2\pi x)$ and the least square estimator $f(x|\hat{\boldsymbol{\beta}})$ of $f(x|\boldsymbol{\beta}) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$ are shown. In the middle panel, the residuals of $f(x|\hat{\boldsymbol{\beta}})$ and the penalized spline estimator of $r_0(x, \hat{\boldsymbol{\beta}})$ are drawn. In the right panel, the true function and the SPSE as given in (2) are drawn. As the interpretation of $\hat{f}(x)$ for this example, the parametric part captures the overall shape of $f(x)$ and the nonparametric part explains details which could not be captured by the $f(x|\hat{\boldsymbol{\beta}})$. Similarly, we can construct an SPSE with multiplicative correction.
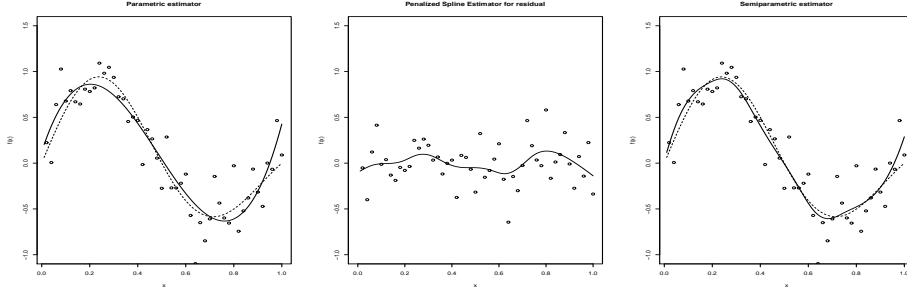
Figure 1: Plots for one random sample of true $f(x)$ (dashed) and the parametric estimator $f(x|\hat{\boldsymbol{\beta}})$ (solid) in the left panel, the residuals and the penalized spline estimator of $\hat{r}_0(x,\hat{\boldsymbol{\beta}})$ (solid) in the middle panel, and the true $f(x)$ (dashed) and the SPSE $\hat{f}(x,0)$ (solid) in the right panel.

3. Asymptotic Result

Asymptotics for the NPSE were developed by Claeskens et al. (2009). By using their results, we show the asymptotic bias and variance, and asymptotic distribution of the SPSE. We now give some assumptions regarding the asymptotics of the SPSE.

Assumptions

1. There exists $a > 0$ such that $a < f(x|\boldsymbol{\beta})$ for all $x \in [0,1]$, $\boldsymbol{\beta} \in B$.

2. $\sup_{z \in [0,1]} \{m(z)\} < \infty$.

3. $|\partial f(x|\boldsymbol{\beta})/\partial \beta_i| < \infty$, for $x \in [0,1]$, $\boldsymbol{\beta} \in B$, $i = 1, \cdots, m$.

4. $|\partial^2 f(x|\boldsymbol{\beta})/\partial \beta_i \partial \beta_j| < \infty$, for $x \in [0,1]$, $\boldsymbol{\beta} \in B$, $i, j = 1, \cdots, m$.

5. $|d^i f(x)/dx^i| < \infty$, for $x \in [0,1]$, $i = 1, \cdots, p+1$.

6. $K_n = o(n^{1/2})$.

7. λ_n^{-1} is larger than the maximum eigenvalue of $(Z'Z)^{-1/2}D_q'D_q(Z'Z)^{-1/2}$.

Define the $(K_n + p) \times (K_n + p)$ matrix $G = (g_{ij})_{ij}$, where

$$g_{ij} = \int_0^1 B_{-p+i}^{[p]}(u)B_{-p+j}^{[p]}(u)m(u)du$$

and the $(K_n + p) \times (K_n + p)$ matrix $G(\sigma, \beta, \gamma) = (g_{\sigma,ij})_{ij}$, where

$$g_{\sigma,ij} = \int_0^1 B_{-p+i}^{[p]}(u)B_{-p+j}^{[p]}(u)\frac{\sigma^2(u)m(u)}{f(u|\boldsymbol{\beta})^{2\gamma}}du.$$

In the sequel, we define $\Gamma(\lambda_n) = G + (\lambda_n/n)D_q'D_q$. Let $\boldsymbol{b}^*(\boldsymbol{\beta}, \gamma)$ be a best L_∞ approximation to $(f(x) - f(x|\boldsymbol{\beta}))/f(x|\boldsymbol{\beta})^\gamma$. This means that $\boldsymbol{b}^*(\boldsymbol{\beta}, \gamma)$ satisfies

$$\sup_{x \in (0,1)} \left| \frac{f(x) - f(x|\boldsymbol{\beta})}{f(x|\boldsymbol{\beta})^\gamma} + b_{a1}(x|\boldsymbol{\beta}, \gamma) - \boldsymbol{B}(x)'\boldsymbol{b}^*(\boldsymbol{\beta}, \gamma) \right| = o(K_n^{-(p+1)}),$$

where

$$b_{a1}(x|\boldsymbol{\beta},\gamma) = -\left(\frac{f(x) - f(x|\boldsymbol{\beta})}{f(x|\boldsymbol{\beta})^\gamma}\right)^{(p+1)} \frac{K_n^{-(p+1)}}{(p+1)!} \sum_{j=1}^{K_n} I(\kappa_{j-1} \le x < \kappa_j) B_{p+1}\left(\frac{x - \kappa_{j-1}}{K_n^{-1}}\right),$$

$I(a < x < b)$ is the indicator function of the interval (a,b) and $B_p(x)$ is the pth Bernoulli polynomial.

We now discuss a condition of the parametric estimator. Let F be the true distribution of (X,Y) and let F_n be the corresponding empirical distribution. The estimator $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ is defined as the functional form $\hat{\boldsymbol{\beta}} = T(F_n)$, where $T(\cdot)$ is a real valued function defined on the set of all distributions. We can then see that $\lim_{n\to\infty} \hat{\boldsymbol{\beta}} \to \boldsymbol{\beta}_0$, where $\boldsymbol{\beta}_0 = T(F)$ is defined as the optimizer of some distance measure ρ. We assume that $f(x|\boldsymbol{\beta}_0)$ is the best approximation of $f(x)$. By the definition of $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0$ can be expressed as

$$\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0 = \frac{1}{n}\sum_{i=1}^n I(X_i, Y_i) + \frac{d}{n} + \delta_n, \tag{5}$$

where $I(X_i, Y_i)$ is the influence function defined as

$$I(X, Y) = \lim_{\varepsilon\to 0}\left\{\frac{T((1-\varepsilon)F + \varepsilon\delta(X,Y)) - T(F)}{\varepsilon}\right\}$$

with $E[I(X_i, Y_i)] = 0$ and finite covariance matrix, the delta function $\delta(X,Y)$ has probability 1 at a point (X,Y), and d is the bias of $\hat{\boldsymbol{\beta}}$. The remaining term δ_n has mean $O(n^{-2})$ for each component.

We investigate the asymptotic property of $\hat{f}(x,\gamma)$ by a two-step procedure for clarity. First we derive the asymptotic expectation and variance of $\hat{f}_0(x,\gamma) = f(x|\boldsymbol{\beta}_0) + f(x|\boldsymbol{\beta}_0)^\gamma \hat{r}_\gamma(x, \boldsymbol{\beta}_0)$. Here, $\hat{r}_\gamma(x, \boldsymbol{\beta}_0)$ is the penalized spline smoother of $r_\gamma(x, \boldsymbol{\beta}_0)$. Second, we show that the difference between $\hat{f}(x,\gamma)$ and $\hat{f}_0(x,\gamma)$ vanishes asymptotically. Since $\boldsymbol{\beta}_0$ is no longer stochastic, the asymptotic property of $\hat{f}_0(x,\gamma)$ is dependent only on the nonparametric penalized spline estimator of $r_\gamma(x, \boldsymbol{\beta}_0)$. Hence we obtain

$$\begin{aligned} E[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n] &= f(x|\boldsymbol{\beta}_0) + f(x|\boldsymbol{\beta}_0)^\gamma E[\hat{r}_\gamma(x, \boldsymbol{\beta}_0)|\boldsymbol{X}_n], \\ V[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n] &= f(x|\boldsymbol{\beta}_0)^{2\gamma} V[\hat{r}_\gamma(x, \boldsymbol{\beta}_0)|\boldsymbol{X}_n]. \end{aligned}$$

Here for a random variable U_n, $E[U_n|\boldsymbol{X}_n]$ and $V[U_n|\boldsymbol{X}_n]$ are the conditional expectation and variance of U_n given $(X_1, \cdots, X_n) = (x_1, \cdots, x_n)$.

To obtain the asymptotic property of $\hat{r}_\gamma(x, \boldsymbol{\beta}_0)$, we can exploit the result developed by Claeskens et al.(2009), in which the behavior of NPSE obtained via

$$(\boldsymbol{y} - Z\boldsymbol{b})'(\boldsymbol{y} - Z\boldsymbol{b}) + \mu_n \int_0^1 \{s^{(q)}(x)\}^2 dx, \tag{6}$$

was investigated, where $\boldsymbol{y} = (y_1 \ \cdots \ y_n)'$ and μ_n is the smoothing parameter. For this penalty term, there exists $(K_n + p - q) \times (K_n + p)$th matrix Δ_q such that $\int_0^1\{s^{(q)}(x)\}^2 dx = \boldsymbol{b}'\Delta_q' R\Delta_q \boldsymbol{b}$, where R is the square matrix having its (i,j)-component

$$\int_0^1 B_{-p+q+i}^{[p-q]}(x)B_{-p+q+j}^{[p-q]}(x)dx$$

which can be shown to be $O(K_n^{-1})$. Especially in case of the equidistant knots, it holds that $\Delta_q = K_n^q D_q$. By combining above equalities altogether, the penalty term $\lambda_n \boldsymbol{b}' D_q' D_q \boldsymbol{b}$ in (3) can be seen as a special case of $\mu_n \boldsymbol{b}' \Delta_q' R \Delta_q \boldsymbol{b}$ with replacing R to $K_n^{-1} I$ and $\lambda_n = \mu_n K_n^{2q-1}$. Further replacement of $\boldsymbol{y}$ to $\boldsymbol{R}_\gamma$ in (6) shows that asymptotics for $\hat{r}_\gamma(x, \boldsymbol{\beta}_0)$ closely relates to that for the NPSE. Claeskens et al. (2009) developed asymptotics for the NPSE under two scenarios: (a) K_q, the maximum eigenvalue of $\mu_n (Z'Z)^{-1/2} \Delta_q' R \Delta_q (Z'Z)^{-1/2}$, is less than 1, or (b) $K_q \geq 1$. Our focus goes to the case (a) since it involves the regression spline estimator ($\lambda_n = 0$), and hence we need Assumption 7 which guarantees $K_q < 1$. Therefore the following Proposition can be obtained by using Theorem 2 (a) of Claeskens et al. (2009).

PROPOSITION 3.1. *Let* $f \in C^{p+1}, f(\cdot|\boldsymbol{\beta}) \in C^{p+1}$. *Then, under the Assumptions, for a fixed* $x \in (0,1)$,

$$E[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n] = f(x) + b_a(x|\boldsymbol{\beta}_0,\gamma) + b_\lambda(x|\boldsymbol{\beta}_0,\gamma) + o_P(K_n^{-(p+1)}) + o_P(\lambda_n n^{-1} K_n^{1-q}),$$

$$V[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n] = \frac{f(x|\boldsymbol{\beta}_0)^{2\gamma}}{n} \boldsymbol{B}(x)' \Gamma(\lambda_n)^{-1} G(\sigma, \beta_0, \gamma) \Gamma(\lambda_n)^{-1} \boldsymbol{B}(x) + o_P(K_n n^{-1}),$$

where

$$b_a(x|\boldsymbol{\beta}_0,\gamma) = -\frac{f(x|\boldsymbol{\beta}_0) r_\gamma^{(p+1)}(x|\boldsymbol{\beta}_0)}{K_n^{p+1}(p+1)!} \sum_{j=1}^{K_n} I(\kappa_{j-1} \leq x < \kappa_j) B_{p+1}\left(\frac{x - \kappa_{j-1}}{K_n^{-1}}\right),$$

$$b_\lambda(x|\boldsymbol{\beta}_0,\gamma) = -\frac{\lambda_n}{n} f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)' \Gamma(\lambda_n)^{-1} D_q' D_q \boldsymbol{b}^*(\boldsymbol{\beta}_0,\gamma).$$

We now give the asymptotic result for $\hat{f}(x,\gamma)$. By using (5), $f(x|\hat{\boldsymbol{\beta}})$ and $\hat{r}_\gamma(x, \hat{\boldsymbol{\beta}})$ are expanded about $f(x|\boldsymbol{\beta}_0)$ and $\hat{r}_\gamma(x, \boldsymbol{\beta}_0)$, respectively. From the details of the proof in the Appendix, we find that the asymptotic expectation and variance of $\hat{f}(x,\gamma)$ are dominated by those of $\hat{f}_0(x,\gamma)$ and we obtain the following theorem.

THEOREM 3.2. *Let* $f \in C^{p+1}, f(\cdot|\boldsymbol{\beta}_0) \in C^{p+1}$. *Then under the Assumptions, for a fixed* $x \in (0,1)$,

$$\begin{aligned} E[\hat{f}(x,\gamma)|\boldsymbol{X}_n] &= f(x) + b_a(x|\boldsymbol{\beta}_0,\gamma) + b_\lambda(x|\boldsymbol{\beta}_0,\gamma) \\ &\quad + O_P(n^{-1}) + o_P(K_n^{-(p+1)}) + o_P(\lambda_n n^{-1} K_n^{1-q}), \\ V[\hat{f}(x,\gamma)|\boldsymbol{X}_n] &= \frac{f(x|\boldsymbol{\beta}_0)^{2\gamma}}{n} \boldsymbol{B}(x)' \Gamma(\lambda_n)^{-1} G(\sigma, \beta_0, \gamma) \Gamma(\lambda_n)^{-1} \boldsymbol{B}(x) + o_P(K_n n^{-1}), \end{aligned}$$

where $b_a(x|\boldsymbol{\beta}_0,\gamma)$ *and* $b_\lambda(x|\boldsymbol{\beta}_0,\gamma)$ *are those given in Proposition 3.1.*

Theorem 3.2 and Lyapunov's theorem yield the asymptotic distribution of the SPSE.

THEOREM 3.3. *Suppose that* $E[|\varepsilon_i|^{2+\delta}|X_i = x_i] < \infty$ *for some* $\delta \geq 2$ *and the Assumptions are satisfied. Then, using* $K_n = O(n^{1/(2p+3)})$ *and* $\lambda_n = O(n^{(p+q+1)/(2p+3)})$,

$$\frac{\hat{f}(x,\gamma) - f(x) - b_a(x|\boldsymbol{\beta}_0,\gamma) - b_\lambda(x|\boldsymbol{\beta}_0,\gamma)}{\sqrt{V[\hat{f}(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{D} N(0,1),$$

where $b_a(x|\boldsymbol{\beta}_0,\gamma)$ *and* $b_\lambda(x|\boldsymbol{\beta}_0,\gamma)$ *are those given in Proposition 3.1.*

From Lemma 6.3 of Zhou et al. (1998), we see that $\lambda_n = O(n^{(p+q+1)/(2p+3)})$ can be achieved by Assumption 7. If $\lambda_n = 0$, we obtain the semiparametric regression spline estimator from (2). Thus, it is clear that the asymptotic result of the semiparametric regression spline is contained in Theorems 3.2 and 3.3. These are obtained from one parametric model. If we choose a polynomial model as $f(x|\boldsymbol{\beta})$, we obtain the following Corollary.

COROLLARY 3.4. *Let $f_q(x|\boldsymbol{\beta}_q)(q \leq p)$ be the qth polynomial model. Then, under $\lambda_n = 0$ and $\gamma = 0$, or $\lambda_n > 0$ and $\gamma = 0$, using $p = 1$, $D_2'D_2$ and equidistant knots, the SPSE is the same as the NPSE.*

Remark 1   From Theorem 3.3, as the advanced analysis, we can construct the asymptotic pointwise confidence interval of $f(x)$ by estimating the variance of the error.

Remark 2   Theorems 3.2 and 3.3 can be applied for $\gamma \in \{0, 1\}$. When $\gamma = 0$, the results become those for additive correction. When $\gamma = 1$, $b_a(x|\boldsymbol{\beta}_0, 1)$ and the variance agrees with those of the estimator for multiplicative correction. In $b_\lambda(x|\boldsymbol{\beta}_0, 1)$, it is understood that $\boldsymbol{b}^*(\boldsymbol{\beta}_0, 1)$ is a best L_∞ approximation of $f(x)/f(x|\boldsymbol{\beta}_0) - 1$. Therefore, $\boldsymbol{b}^*(\boldsymbol{\beta}_0, 1)$ can be written as $\boldsymbol{b}^*(\boldsymbol{\beta}_0, 1) = \boldsymbol{b}^* - \boldsymbol{1}$, where $\boldsymbol{b}^*$ is a best L_∞ approximation of $f(x)/f(x|\boldsymbol{\beta}_0)$ and $\boldsymbol{1}$ is a $(K_n + p)$ vector with all components equal to 1. In conclusion, $b_\lambda(x|\boldsymbol{\beta}_0, 1)$ can be written as

$$b_\lambda(x|\boldsymbol{\beta}_0, 1) = -\frac{\lambda_n}{n} f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)' \Gamma(\lambda_n)^{-1} D_q' D_q \boldsymbol{b}^*$$

because all components of $D_q' D_q \boldsymbol{1}$ have vanished.

Remark 3   When $f(x) = f(x|\boldsymbol{\beta}_0)$ is assumed, $b_a(x|\boldsymbol{\beta}_0, \gamma) = 0$ and $b_\lambda(x|\boldsymbol{\beta}_0, \gamma) = 0$ are obtained by choosing $\boldsymbol{b}^*(\gamma, \boldsymbol{\beta}_0) = \boldsymbol{0}$ as a best L_∞ approximation of 0. For $\gamma = 1$, in particular, $b_a(x|\boldsymbol{\beta}_0, 1) = 0$ and $b_\lambda(x|\boldsymbol{\beta}_0, 1) = 0$ both hold even in cases where $f(x) = cf(x|\boldsymbol{\beta}_0)$ with any constant $c \neq 0$.

Remark 4   If we use the local pth polynomial technique in the second step estimation, we obtain the asymptotic bias $b_\ell(x|\boldsymbol{\beta}_0)$ as

$$b_\ell(x|\boldsymbol{\beta}_0, \gamma) = \begin{cases} \dfrac{-f(x|\boldsymbol{\beta}_0) r_\gamma^{(p+1)}(x|\boldsymbol{\beta}_0)}{h_n^{-(p+1)}(p+1)!} \displaystyle\int_{\mathbb{R}} z^{p+1} H_p(z) dz, & p \; : \; \text{odd}, \\[4mm] \dfrac{-f(x|\boldsymbol{\beta}_0)}{h_n^{-(p+2)}} \left\{ \dfrac{r_\gamma^{(p+2)}(x|\boldsymbol{\beta}_0)}{(p+2)!} + \dfrac{r_\gamma^{(p+1)}(x|\boldsymbol{\beta}_0) m'(x)}{(p+1)! m(x)} \right\} \displaystyle\int_{\mathbb{R}} z^{p+2} H_p(z) dz, & p \; : \; \text{even}, \end{cases}$$

where h_n is bandwidth and $H_p(z)$ is the pth order kernel function. If K_n^{-1} and h_n are equal and p is odd, the difference between $b_a(x|\boldsymbol{\beta}_0)$ and $b_\ell(x|\boldsymbol{\beta}_0)$ is only that of

$$\sum_{j=1}^{K_n} I(\kappa_{j-1} \leq x < \kappa_j) B_{p+1}\left(\frac{x - \kappa_{j-1}}{K_n^{-1}}\right) \quad \text{and} \quad \int_{\mathbb{R}} z^{p+1} H_p(z) dz. \tag{7}$$

If we can calculate (7), we would be able to compare the bias of the SPSE with that of the semiparametric local polynomial kernel estimator. As an example, when $p = 1$, it is easy to show that $B_2(x) = x^2 - x + 1/6 < 1/5$ for $x \in [0, 1]$, while we have $\int_{\mathbb{R}} z^2 H_G(z) dz = 1$

for the Gaussian kernel $H_G(z)$ and $\int_{\mathbb{R}} z^2 H_E(z) dz = 1/5$ for the Epanechnikov kernel $H_E(z)$. Therefore $b_a(x|\boldsymbol{\beta}_0)$ is smaller than $b_\ell(x|\boldsymbol{\beta}_0)$ in this situation, which reveals that the semiparametric regression spline estimator ($\lambda_n = 0$) is superior than the SLLE.

4. Parametric model selection

In this section, we describe how to choose a parametric model. From Remark 3, if the true regression function satisfies $f \in \{f(\cdot|\boldsymbol{\beta})|\boldsymbol{\beta} \in B \subseteq \mathbb{R}^M\}$, the bias of the SPSE is reduced. Hence we determine the initial parametric model in a bias reduction context. Specifically, our purpose is to choose a parametric model such that the asymptotic bias of the SPSE becomes smaller than that of the NPSE:

$$|b_a(x|\boldsymbol{\beta}_0, \gamma)| < |b_a(x)| \quad \text{and} \quad |b_\lambda(x|\boldsymbol{\beta}_0, \gamma)| < |b_\lambda(x)|, \text{ for all } x \in (0, 1), \tag{8}$$

where $b_a(x)$ and $b_\lambda(x)$ are the asymptotic biases of the NPSE. If $f(x|\boldsymbol{\beta})$ is constant, $b_a(x|\boldsymbol{\beta}_0, \gamma)$ and $b_\lambda(x|\boldsymbol{\beta}_0, \gamma)$ are equivalent to $b_a(x)$ and $b_\lambda(x)$, respectively. When the same K_n and λ_n are used in both the SPSE and the NPSE, (8) can be rewritten as $L_a(x, \gamma) > 0$ and $L_\lambda(x, \gamma) > 0$ for all $x \in (0, 1)$, where

$$L_a(x, \gamma) = |f^{(p+1)}(x)| - \left| f(x|\boldsymbol{\beta}_0)^\gamma \left(\frac{f(x) - f(x|\boldsymbol{\beta}_0)}{f(x|\boldsymbol{\beta}_0)^\gamma} \right)^{(p+1)} \right|$$

and

$$L_\lambda(x, \gamma) = |\boldsymbol{B}(x)'\Gamma(\lambda_n)^{-1} D_q' D_q \boldsymbol{b}_f^*| - |f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)'\Gamma(\lambda_n)^{-1} D_q' D_q \boldsymbol{b}^*(\boldsymbol{\beta}_0, \gamma)|,$$

where $\boldsymbol{b}_f^*$ is a best L_∞ approximation to $f(x)$. As a pilot estimator of f and its $(p+1)$th derivative, we can use the local polynomial estimator $\hat{f}$ with degree $p + 2$. Then the estimator of $L_a(x, \gamma)$ and $L_\lambda(x, \gamma)$ can be obtained as

$$\hat{L}_a(x, \gamma) = |\hat{f}^{(p+1)}(x)| - \left| f(x|\hat{\boldsymbol{\beta}})^\gamma \left(\frac{\hat{f}(x) - f(x|\hat{\boldsymbol{\beta}})}{f(x|\hat{\boldsymbol{\beta}})^\gamma} \right)^{(p+1)} \right|$$

and by using empirical form,

$$\hat{L}_\lambda(x, \gamma) = |\boldsymbol{B}(x)'\Lambda^{-1} D_q' D_q (Z'Z)^{-1} Z' \hat{\boldsymbol{f}}| - |f(x|\hat{\boldsymbol{\beta}})^\gamma \boldsymbol{B}(x)'\Lambda^{-1} D_q' D_q (Z'Z)^{-1} Z' \hat{\boldsymbol{r}}_\gamma|,$$

where $\Lambda = Z'Z + \lambda_n D_q' D_q$, $\hat{\boldsymbol{f}} = (\hat{f}(x_1) \cdots \hat{f}(x_n))'$ and $\hat{\boldsymbol{r}}_\gamma$ is an n-vector with ith component $\{\hat{f}(x_i) - f(x_i|\hat{\boldsymbol{\beta}})\}/f(x_i|\hat{\boldsymbol{\beta}})^\gamma$. Here, we use the fact that

$$\lambda_n f(x|\hat{\boldsymbol{\beta}})^\gamma \boldsymbol{B}(x)'\Lambda^{-1} D_q' D_q (Z'Z)^{-1} Z' \hat{\boldsymbol{r}}_\gamma = b_\lambda(x|\boldsymbol{\beta}_0, \gamma) + o_P(\lambda_n K_n n^{-1}),$$

which is detailed in the proof of Theorem 2 (a) of Claeskens et al. (2009). We choose one parametric model by relative evaluation. Let

$$C_{a \cap \lambda}(f(\cdot|\boldsymbol{\beta})) = \# \left\{ z_j \in (0, 1) \Big| \hat{L}_a(z_j, \gamma) > 0, \hat{L}_\lambda(z_j, \gamma) > 0, j = 1, \cdots, J \right\},$$

for a given parametric model $f(\cdot|\boldsymbol{\beta})$ and some finite grid points $\{z_j\}_1^J$ on $(0, 1)$. Here, $\#A$ denotes the cardinality of A. After preparing a class of candidate parametric models $\{f_k = f_k(\cdot|\boldsymbol{\beta}_k); k = 1, \cdots, K\}$, we choose a parametric model satisfying

$$f(x|\boldsymbol{\beta}) = \operatorname*{argmax}_{f_k} \{C_{a \cap \lambda}(f(\cdot|\boldsymbol{\beta}_k))\}. \tag{9}$$

In summary, for each parametric model f_k, we calculate $\hat{L}_a$, $\hat{L}_\lambda$ and $C_{a\cap\lambda}(f(\cdot|\boldsymbol{\beta}_k))$. By using the parametric model which satisfies (9), we construct the SPSE. If we can choose a good parametric model and a good $\hat{\boldsymbol{\beta}}$, the SPSE will have better behavior than the NPSE.

Remark 5 When we construct the semiparametric regression spline estimator (SPSE with $\lambda_n = 0$), we obtain $b_\lambda(x|\boldsymbol{\beta}_0, \gamma) \equiv 0$. Therefore, $C_{a\cap\lambda}$ depends only on $L_a(x, \gamma)$.

Remark 6 We see that the bias term $b_a(x|\boldsymbol{\beta}_0, \gamma)$ appears due to the use of the B-spline model. On the other hand, $b_\lambda(x|\boldsymbol{\beta}_0, \gamma)$ arises from the penalty component. If we use the regression spline, $b_\lambda(x|\boldsymbol{\beta}_0, \gamma)$ vanishes and the bias of the estimator becomes less than that of the penalized spline estimator. However, the regression spline often provides overfitting. Thus, we use the penalized method for obtaining a smooth curve. If $\lambda_n > 0$, a certain amount of smoothness in the estimator is assured. However, $b_\lambda(x|\boldsymbol{\beta}_0, \gamma)$ may grow too large because of the influence of the parametric model. Therefore under $\lambda_n > 0$, we suggest choosing $f(x|\boldsymbol{\beta})$ such that $b_\lambda(x|\boldsymbol{\beta}_0, \gamma)$ becomes less than $b_\lambda(x)$. Hence, together with $L_a(x, \gamma)$, the parametric model chosen by $C_{a\cap\lambda}$ appears to bring fitness and smoothness to the SPSE.

5. Simulation

In this section, we examine the results of a numerical study to confirm the effects of the SPSE on a finite sample. We choose a parametric model by the criteria discussed in Section 4. We also compare the performance of the SPSE to those of the NPSE, the SLLE and the fully nonparametric local linear estimator (NLLE). In all situations, we utilize the linear ($p = 1$) and cubic ($p = 3$) splines and the second difference penalty ($q = 2$) for the second step nonparametric estimation. The SPSEs with linear and cubic splines are designated as SPSE1 and SPSE3, respectively. NPSE1 and NPSE3 are labeled similarly. The number of knots and the smoothing parameter are determined by GCV. The design points $\{x_i\}_1^n$ are drawn from a uniform density on $[0,1]$ and the errors $\{\varepsilon_i\}_1^n$ are generated from the normal with mean 0 and variance $\sigma^2(x_i)$. Let

$$C_a = C_a(f(\cdot|\boldsymbol{\beta})) = \# \left\{ z_j \in (0,1) \Big| \hat{L}_a(z_j, \gamma) > 0, j = 1\cdots, J \right\},$$

$$C_\lambda = C_\lambda(f(\cdot|\boldsymbol{\beta})) = \# \left\{ z_j \in (0,1) \Big| \hat{L}_\lambda(z_j, \gamma) > 0, j = 1, \cdots, J \right\},$$

$$C_{a\cap\lambda} = C_{a\cap\lambda}(f(\cdot|\boldsymbol{\beta})) = \# \left\{ z_j \in (0,1) \Big| \hat{L}_a(z_j, \gamma) > 0, \hat{L}_\lambda(z_j, \gamma) > 0, j = 1, \cdots, J \right\},$$

where $z_j = j/J, J = 100$. We prepare a class of candidate parametric models $\{f_k = f_k(\cdot|\boldsymbol{\beta}_k)|k = 1, \cdots, K\}$. For each f_k, we calculate C_a, C_λ and $C_{a\cap\lambda}$. We use a number of repetitions $R = 1000$. For each iteration, we pick up f_k from candidate models which maximize C_a. The same manipulation is implemented for C_λ and $C_{a\cap\lambda}$. Finally we count the number of times that f_k is picked up during the iterations. For comparison, we also show the model selection by using the AIC and the Takeuchi information criterion (TIC) detailed in Konishi and Kitagawa (2008).

Let

$$B_j = \frac{1}{R}\sum_{r=1}^{R} \hat{f}_r(z_j) - f(z_j), \quad V_j = \frac{1}{R}\sum_{r=1}^{R} \left\{ \hat{f}_r(z_j) - \frac{1}{R}\sum_{r=1}^{R} \hat{f}_r(z_j) \right\}^2,$$

Table 1: The results of parametric model selection in Example 1.

$n = 25$		SPSE1			SPSE3			IC	
method	model	C_a	C_λ	$C_{a \cap \lambda}$	C_a	C_λ	$C_{a \cap \lambda}$	AIC	TIC
	sin	1000	901	1000	1000	1000	1000	850	938
$\gamma = 0$	$poly1$	0	0	0	0	0	0	0	0
	$poly3$	0	99	0	0	0	0	150	62
	sin	997	917	974	997	837	953	850	938
$\gamma = 1$	$poly1$	0	34	3	0	77	4	0	0
	$poly3$	1	33	20	3	86	43	150	62

where $\hat{f}_r(z_j)$ is the estimator for the rth repetition. Let ISB $= 100^{-1} \sum_{j=1}^{100} B_j^2$, V $= 100^{-1} \sum_{j=1}^{100} V_j$ and MISE $=$ ISB $+$ V be the estimates of integrated squared bias, integrated variance and mean integrated squared error of $\hat{f}$, respectively. For comparison, the ISB, V and MISE of the SLLE and the NLLE were also calculated. In the SLLE and the NLLE, we used the Gaussian kernel and its bandwidth h_n was obtained by the direct plug-in approach (Ruppert et al. (1995)).

Example 1   The true function is $f(x) = 2 + \sin(2\pi x)$. We use three different specified parametric models:

$$f(x|\boldsymbol{\beta}) = \left\{ \begin{array}{ll} \beta_0 + \beta_1 \sin(2\pi x), & f_1 = sin, \\ \beta_0 + \beta_1 x, & f_2 = poly1, \\ \beta_0 + \beta_1 x + \beta_2^2 + \beta_3 x^3, & f_3 = poly3. \end{array} \right.$$

The true curve can be approximated by sin. The curve $poly1$ is a rough model and $poly3$ is close to the true f. The variance of the error is $\sigma^2(x) = (0.5)^2$ and the sample size is $n = 25$. The coefficients of the covariate are estimated by the maximum likelihood method for each model. This set-up is similar to that used by Glad (1998).

Table 1 includes the number of times that each parametric model f_k was chosen based on each criterion. In C_a, C_λ and $C_{a \cap \lambda}$, sin was selected in almost all iterations. This result is desirable because sin coincides with the true function f. We also observe that the AIC and the TIC often choose sin. When the number of times sin is chosen is taken into consideration, it seems that $C_{a \cap \lambda}$ is a better selector than the AIC and the TIC.

Results for ISB, V and MISE of the SPSE and the NPSE are given in Table 2. The SPSE with sin succeeds in regards to bias reduction even with a small sample size, and variance and MISE of the SPSE are also smaller than those of the NPSE. In additive correction, the result of SPSE1 with $poly1$ is exactly the same as that of the NPSE (see Corollary 1). If we use $poly3$, MISE of the SPSE is smaller than that of the NPSE, although the squared bias is somewhat larger in multiplicative correction. In both ISB, V and MISE, the values of the SPSE are smaller than those of the SLLE. We implemented the same method of analysis for the case $n = 200$. The ISB, V and MISE of the SPSE and those of the NPSE were almost the same, although these are not shown in this paper.

Table 2: Results of integrated squared bias, variance and mean integrated squared bias of Example 1. All entries for ISB,V and MISE are 10^3 times their actual values.

$n = 25$		SPSE1			SPSE3			SLLE		
method	model	ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
	sin	0.009	8.308	8.318	0.009	7.907	7.917	0.029	9.032	9.061
$\gamma = 0$	*poly1*	1.450	12.111	13.562	1.110	10.056	11.166	2.370	14.105	16.476
	poly3	1.250	10.949	12.199	0.873	9.636	10.510	2.071	15.825	17.898
	sin	0.011	8.394	8.405	0.010	8.292	8.302	0.026	10.708	10.734
$\gamma = 1$	*poly1*	1.571	12.322	13.893	1.565	12.212	13.777	2.357	13.860	16.217
	poly3	2.016	11.198	13.215	1.016	10.198	11.215	2.942	12.472	15.415
$n = 25$		NPSE1			NPSE3			NLLE		
Fully nonparametric		ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
method		1.450	12.111	13.562	1.108	11.030	12.138	2.370	14.105	16.476

Table 3: The results of parametric model selection in Example 2.

$n = 25$		SPSE1			SPSE3			IC	
method	model	C_a	C_λ	$C_{a\cap\lambda}$	C_a	C_λ	$C_{a\cap\lambda}$	AIC	TIC
	poly1	0	0	0	0	0	0	0	0
	poly2	0	49	30	0	8	0	0	0
$\gamma = 0$	*poly3*	956	472	511	0	939	0	415	693
	poly4	6	43	6	5	2	15	116	8
	poly5	6	356	312	967	37	982	306	298
	poly6	0	3	85	20	1	3	163	1
	poly1	2	43	37	2	35	49	0	0
	poly2	13	4	6	173	44	46	0	0
$\gamma = 1$	*poly3*	755	376	410	756	606	514	415	693
	poly4	0	15	71	0	0	1	116	8
	poly5	169	366	246	10	166	213	306	298
	poly6	3	119	135	1	35	49	163	1

Example 2 The same true function f used in Example 1 is adopted and the sample size is $n = 25$. A class of initial parametric models is chosen, consisting of qth degree polynomials ranging from $q = 1$ to 6 and designated as *poly1*, ..., *poly6*, respectively, and $\sigma^2 = 1$. This parametric model clearly does not contain the true f and the estimator becomes unstable because the variance of error is relatively large.

In Table 3, we tabulate the number of times out of a 1000 repetitions that each polynomial model is selected based on bias reduction and information criteria. In multiplicative correction, *poly3* was selected by C_a, C_λ and $C_{a\cap\lambda}$ most often. In additive correction of SPSE1, *poly3* was selected by C_a most often. On the other hand, in SPSE3, C_a and $C_{a\cap\lambda}$ selected *poly5*. Finally, AIC and TIC most often selected *poly3* and *poly5*. It appears that our criteria and the information criteria tend to choose the same model.

The ISB, V and MISE of the estimators are shown in Table 4. In additive correction, *poly5* has the smallest ISB. We note that $C_{a\cap\lambda}$ chooses *poly5* in SPSE3. In both corrections, *poly3* has the smallest V and MISE in all models. On the whole, the SPSE

Table 4: Results of integrated squared bias, variance and mean integrated squared error for Example 2. All entries for ISB,V and MISE are 10^3 times their actual values.

$n = 25$		SPSE1			SPSE3			SLLE		
method	model	ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
	poly1	1.213	232.429	233.643	1.417	256.275	257.692	1.991	246.245	248.236
	poly2	0.846	226.256	227.103	0.695	239.949	240.645	2.836	236.124	238.960
$\gamma = 0$	*poly3*	0.776	225.508	226.285	0.729	210.204	210.933	1.157	243.466	244.623
	poly4	1.322	251.572	252.894	1.476	236.314	237.791	2.626	229.014	231.640
	poly5	0.161	251.777	251.938	0.122	238.596	238.717	0.128	277.704	277.832
	poly6	0.162	236.066	236.227	0.134	233.793	233.927	0.119	235.824	235.943
	poly1	1.665	230.226	231.891	1.746	253.074	254.820	2.109	254.547	256.657
	poly2	0.534	268.503	269.037	0.321	225.818	226.138	2.871	256.551	259.421
$\gamma = 1$	*poly3*	0.323	213.758	214.081	0.519	214.566	215.086	1.545	237.094	238.638
	poly4	0.924	233.528	234.452	0.735	245.211	245.956	2.858	259.805	262.662
	poly5	0.390	218.850	219.240	0.624	221.162	221.786	0.733	243.170	243.903
	poly6	0.356	241.451	241.807	0.678	241.242	241.920	0.895	240.767	241.662
$n = 25$		NPSE1			NPSE3			NLLE		
Fully nonparametric		ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
method		1.213	232.429	233.643	1.629	249.219	250.848	1.991	246.245	248.236

displays better behavior than the SLLE although there are some exceptions.

Example 3   The set-up of the true function and parametric models are the same as in Example 2, but the sample size is set to $n = 75$. We utilize the error variance defined as $\sigma^2(x) = (x - 0.5)^2 + 0.1$. However the parametric estimator is composed by the ordinary least squares method.

In Table 5, the results of the parametric model selection are shown. In additive correction of SPSE1, $C_{a \cap \lambda}$ indicates that the best model is *poly5* although C_a selects *poly3* every time. In multiplicative correction, *poly3* is selected by C_a many times while C_λ and $C_{a \cap \lambda}$ select *poly5*. From the definition of $C_{a \cap \lambda}$, it is understood that *poly5* is selected in a fitness and smoothness context. On the other hand, AIC and TIC choose *poly3* and *poly5*, respectively. We note that the use of AIC might not be appropriate in this situation since the prepared model does not include the true f and, hence, we place more confidence in TIC. On the other hand, when we select the parametric model only by the maximum of the log-likelihood, *poly5* was chosen 1000 times. Therefore, it seems that the bias correction in AIC is too strong in this situation.

In Table 6, the ISB, V and MISE of the SPSE are tabulated. In both corrections, the SPSE with *poly5* and *poly6* have overwhelmingly small ISBs compared with those of *poly1-poly4*. As C_a and C_λ focus on bias reduction, it appears that $C_{a \cap \lambda}$ chooses *poly5* because it often has a small bias. On the other hand, *poly3* has good V and MISE, while *poly5* does not. For ISB, V and MISE, the values of the SPSE is smaller than those of the SLLE, respectively.

Example 4   The true model is $f(x) = 4 + e^{-x}\{\sin(7\pi x) + 2\cos(3\pi x)\}$ and the error

Table 5: The results of parametric model selection in Example 3.

$n = 75$		SPSE1			SPSE3			IC	
method	model	C_a	C_λ	$C_{a\cap\lambda}$	C_a	C_λ	$C_{a\cap\lambda}$	AIC	TIC
	poly1	0	0	0	0	0	0	0	0
	poly2	0	5	0	0	65	0	0	0
$\gamma = 0$	*poly3*	1000	47	8	0	142	0	457	0
	poly4	0	2	172	0	12	21	94	2
	poly5	0	604	630	945	624	872	296	950
	poly6	0	277	113	17	66	68	153	48
	poly1	8	2	8	8	51	62	0	0
	poly2	64	222	168	62	150	118	0	0
$\gamma = 1$	*poly3*	894	17	86	890	101	104	457	0
	poly4	0	72	104	0	20	31	94	2
	poly5	0	363	398	5	295	333	296	950
	poly6	0	182	85	3	253	214	153	48

Table 6: Results of integrated squared bias, variance and mean integrated squared bias of Example 3. All entries for ISB, V and MISE are 10^3 times their actual values.

$n = 75$		SPSE1			SPSE3			SLLE		
method	model	ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
	poly1	0.061	1.330	1.390	0.065	1.237	1.302	0.645	6.529	7.175
	poly2	0.017	1.326	1.343	0.007	1.231	1.238	0.734	6.298	7.032
$\gamma = 0$	*poly3*	0.017	1.325	1.343	0.007	1.230	1.237	0.249	6.292	6.541
	poly4	0.062	1.343	1.405	0.066	1.251	1.317	0.608	6.732	7.340
	poly5	0.003	1.377	1.380	0.002	1.285	1.287	0.017	4.863	4.880
	poly6	0.004	1.435	1.440	0.002	1.350	1.354	0.019	5.552	5.571
	poly1	0.062	1.337	1.399	0.068	1.246	1.314	1.084	6.167	7.251
	poly2	0.024	1.328	1.352	0.021	1.235	1.256	0.997	6.186	7.183
$\gamma = 1$	*poly3*	0.030	1.325	1.342	0.014	1.233	1.248	0.314	6.279	6.593
	poly4	0.072	1.348	1.419	0.078	1.258	1.336	0.420	6.476	6.896
	poly5	0.003	1.380	1.383	0.002	1.290	1.292	0.023	4.925	4.949
	poly6	0.003	1.438	1.441	0.002	1.353	1.355	0.025	5.528	5.553
$n = 75$		NPSE1			NPSE3			NLLE		
Fully nonparametric		ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
method		0.061	1.330	1.390	0.065	1.237	1.302	0.645	6.529	7.175

Table 7: The results of parametric model selection in Example 4.

$n = 50$		SPSE1			SPSE3			IC	
method	model	C_a	C_λ	$C_{a \cap \lambda}$	C_a	C_λ	$C_{a \cap \lambda}$	AIC	TIC
	sin	997	998	992	987	996	972	1	0
$\gamma = 0$	cos	3	2	0	7	4	17	602	11
	$poly1$	0	0	0	1	0	0	0	0
	$poly4$	0	0	2	0	0	0	397	902
	$poly8$	0	0	3	0	0	0	0	87
	sin	887	823	686	887	821	791	1	0
$\gamma = 1$	cos	77	17	1	77	114	43	602	11
	$poly1$	0	11	37	0	0	0	0	0
	$poly4$	0	56	109	0	23	93	397	902
	$poly8$	0	47	88	0	14	28	0	87

variance is $\sigma^2(x) = 0.5$. The parametric model is

$$f(x|\boldsymbol{\beta}) = \begin{cases} \beta_0 + e^{-x}\{\beta_1 + \beta_2 \sin(7\pi x) + \beta_3 \cos(3\pi x)\}, & f_1 = sincos, \\ \beta_0 + e^{-x}\{\beta_1 + \beta_2 \sin(7\pi x)\}, & f_2 = sin, \\ \beta_0 + e^{-x}\{\beta_1 + \beta_2 \cos(3\pi x)\}, & f_3 = cos, \\ \beta_0 + e^{-x}\{\beta_1 + \beta_2 x\}, & f_4 = poly1, \\ \beta_0 + e^{-x}\{\beta_1 + \beta_2 x + \cdots + \beta_5 x^4\}, & f_5 = poly4, \\ \beta_0 + e^{-x}\{\beta_1 + \beta_2 x + \cdots + \beta_9 x^8\}, & f_6 = poly8 \end{cases}$$

The function $sincos$ corresponds to the true function.

In Table 7, the results of the parametric model selection are tabulated. The $sincos$, corresponding to the true f, was not included in the model selection since it should be chosen frequently. In both corrections, $\gamma = 0, 1$, sin was chosen by C_a, C_λ and $C_{a \cap \lambda}$ most often. On the other hand, TIC selected $poly4$, and AIC selected cos and $poly4$ quite often.

In Table 8, the ISB, V and MISE of the estimators are shown. In both corrections, $\gamma = 0, 1$, the behavior of the SPSE with sin is superior than that of the SPSE with any other model except $sincos$. We observe that the SPSE with the initial parametric model selected by $C_{a \cap \lambda}$ shows better behavior than that with the model selected by information criteria.

Furthermore it can be seen that ISB, V and MISE of the SLLE with $sincos$ are significantly smaller than those of the SPSE with any parametric model. On the other hand, if we use incorrect models (other than $sincos$) in the SLLE, then the ISB, V and MISE of the SLLE are larger than those of the SPSE.

Remark 7   In all examples, we also compared the behavior of the SPSE and the SLLE under the conditions that K_n is equal to the ceiling of h_n^{-1} and that $\lambda_n = n^p/n^{2p+3}$. From these results, we have confirmed that the ISB of the SPSE is smaller than that of the SLLE for each parametric model. In contrast, the V and MISE of the SPSE are larger than those of the SLLE. Thus, it seems that the SPSE produces overfitting.

Table 8: Results of integrated squared bias, variance and mean integrated squared error for Example 4. All entries for ISB,V and MISE are 10^3 times their actual values.

$n = 50$		SPSE1			SPSE3			SLLE		
method	model	ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
	sincos	0.051	87.361	87.412	0.041	81.564	81.605	0.025	64.752	64.777
	sin	2.689	86.891	89.580	3.270	81.053	84.323	15.416	85.149	100.566
$\gamma = 0$	*cos*	17.206	87.095	104.302	13.195	86.217	99.411	21.039	92.615	113.654
	poly1	19.095	89.314	108.409	13.950	88.674	102.624	25.920	104.183	130.103
	poly4	15.990	91.930	107.920	11.733	90.234	101.967	25.716	106.923	132.639
	poly8	16.492	94.013	110.505	11.896	92.078	103.975	22.992	108.436	131.428
	sincos	0.051	88.492	88.543	0.040	82.978	83.018	0.025	63.735	63.761
	sin	4.968	87.858	92.825	6.245	82.485	88.730	18.049	83.225	101.274
$\gamma = 1$	*cos*	17.269	89.904	107.174	12.525	89.165	101.690	20.751	92.491	113.242
	poly1	18.981	90.991	109.972	13.360	90.053	103.413	28.430	94.194	122.624
	poly4	15.451	94.073	109.524	11.155	92.079	103.233	24.959	106.714	131.673
	poly8	15.534	95.991	111.525	10.936	93.630	104.566	26.838	106.554	133.392
$n = 50$		NPSE1			NPSE3			NLLE		
Fully nonparametric		ISB	V	MISE	ISB	V	MISE	ISB	V	MISE
method		18.884	88.770	107.653	13.878	88.201	102.079	26.859	93.344	120.204

6. Discussion

We have discussed the SPSE using a parametric model. We see that the SPSE has better behavior than the NPSE, provided we can choose a good $f(x|\boldsymbol{\beta})$ in the first parametric step. A similar conclusion can be drawn for the semiparametric regression spline estimator by letting $\lambda_n = 0$. Though the asymptotic results in this paper have been developed under the scenario $K_q < 1$ in Claeskens et al.(2009), it would be also possible to investigate asymptotic properties of the SPSE under the scenario $K_q \geq 1$.

In the field of kernel smoothing, Fan et al. (2009) noted that the semiparametric local polynomial estimator can also be constructed in the additive model (Hastie and Tibshirani (1990)). The reason for this is the asymptotic result of nonparametric kernel regression in the additive model, which has previously been developed by Ruppert and Opsomer (1997) and Opsomer (2000). On the other hand, it appears that the asymptotic results for the penalized spline estimator have still not been sufficiently investigated in comparison to kernel smoothing. While it is beyond the scope of this paper, this semiparametric approach with a penalized spline can be also extended to the generalized linear model. In this sense, there are still many topics that should be examined in theoretical studies of the penalized spline method.

Appendix

For a matrix $A_n = (a_{ij,n})_{ij}$, if $\max_{i,j}\{n^\alpha|a_{ij,n}|\} = O_P(1)(o_P(1))$, then it is written as $a_n = O_P(n^{-\alpha}\mathbf{1}\mathbf{1}')(o_P(n^{-\alpha}\mathbf{1}\mathbf{1}'))$. When A_n is vector, define $A_n = O_P(n^{-\alpha}\mathbf{1})(o_P(n^{-\alpha}\mathbf{1}))$ like a matrix case. This notation will be used for matrices with fixed sizes and sizes depending on n. For the proofs of Proposition 1, Theorems 1-2 and Corollary 1, we define $\Lambda_n = n^{-1}\Lambda$. We need additional lemmas as follows.

Lemma 1 *Let $A = (a_{ij})_{ij}$ be $(K_n + p)$ matrix. Assume that $K_n \to \infty$ as $n \to \infty$, $A = O_P(K_n^\alpha \mathbf{1}\mathbf{1}')$. Then $A\Lambda_n^{-1} = O(K_n^{1+\alpha}\mathbf{1}\mathbf{1}')$*

Lemma 2 *Let $g : \mathbb{R} \to \mathbb{R}$ be any function with $\sup\limits_{x \in \mathbb{R}}\{g(x)\} < \infty$. Then, $\int_0^1 B_i(u)g(u)du = O(K_n^{-1})$ and $\int_0^1 B_i(u)B_j(u)g(u)du = O(K_n^{-1})$.*

Lemmas 1 and 2 are shown by fundamental properties of B-spline(see, Claeskens et al. (2009) and Zhou et al. (1998)).

PROOF OF PROPOSITION 3.1. First we calculate the asymptotic expectation of $\hat{r}_\gamma(x, \boldsymbol{\beta}_0)$:

$$E[\hat{r}_\gamma(x, \boldsymbol{\beta}_0)|\boldsymbol{X}_n] = f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)'\Lambda^{-1}Z'E[\boldsymbol{r}_\gamma|\boldsymbol{X}_n],$$

where

$$E[\boldsymbol{r}_\gamma|\boldsymbol{X}_n] = \left(\frac{f(x_1) - f(x_1|\boldsymbol{\beta}_0)}{f(x_1|\boldsymbol{\beta}_0)^\gamma} \quad \cdots \quad \frac{f(x_n) - f(x_n|\boldsymbol{\beta}_0)}{f(x_n|\boldsymbol{\beta}_0)^\gamma}\right)'$$

By using Theorem 2 (a) of Claeskens et al. (2009), if $\{f(x) - f(x|\boldsymbol{\beta}_0)\}/f(x|\boldsymbol{\beta}_0)^\gamma$ is regarded as regression function, we have

$$
\begin{aligned}
E[\hat{r}_\gamma(x, \boldsymbol{\beta}_0)|\boldsymbol{X}_n] &= \frac{f(x) - f(x|\boldsymbol{\beta}_0)}{f(x|\boldsymbol{\beta}_0)^\gamma} + b_{a1}(x|\boldsymbol{\beta}_0, \gamma) + b_{\lambda 1}(x|\boldsymbol{\beta}_0, \gamma) \\
&\quad + o_P(K_n^{-(p+1)}) + o_P(\lambda_n n^{-1} K_n^{1-q}),
\end{aligned}
$$

where $b_{\lambda 1}(x|\boldsymbol{\beta}_0, \gamma) = -(\lambda_n/n)\boldsymbol{B}(x)'\Gamma(\lambda_n)^{-1}D_q'D_q\boldsymbol{b}^*(\boldsymbol{\beta}_0, \gamma)$. Therefore, the expectation of $\hat{f}_0(x, \gamma)$ can be written as

$$
\begin{aligned}
E[\hat{f}_0(x, \gamma)|\boldsymbol{X}_n] &= f(x|\boldsymbol{\beta}_0) + f(x|\boldsymbol{\beta}_0)^\gamma E[\hat{r}_\gamma(x, \boldsymbol{\beta}_0)|\boldsymbol{X}_n] \\
&= f(x) + f(x|\boldsymbol{\beta}_0)^\gamma \{b_{a1}(x|\boldsymbol{\beta}_0, \gamma) + b_{\lambda 1}(x|\boldsymbol{\beta}_0, \gamma)\} \\
&\quad + o_P(K_n^{-(p+1)}) + o_P(\lambda_n n^{-1} K_n^{1-q}) \\
&= f(x) + b_a(x|\boldsymbol{\beta}, \gamma) + b_\lambda(x|\boldsymbol{\beta}, \gamma) + o_P(K_n^{-(p+1)}) + o_P(\lambda_n n^{-1} K_n^{1-q}).
\end{aligned}
$$

Next we show the asymptotic variance of $\hat{f}_0(x, \gamma)$. It is easy to see that

$$
\begin{aligned}
&V[\hat{f}_0(x, \gamma)|\boldsymbol{X}_n] \\
&= f(x|\boldsymbol{\beta})^{2\gamma}\boldsymbol{B}(x)'\Lambda^{-1}Z'V[\boldsymbol{r}_\gamma|\boldsymbol{X}_n]Z\Lambda^{-1}\boldsymbol{B}(x) \\
&= \frac{f(x|\boldsymbol{\beta})^{2\gamma}}{n^2}\boldsymbol{B}(x)'\Lambda_n^{-1}Z'\left(\text{diag}\left[\frac{\sigma^2(x_1)}{f(x_1|\boldsymbol{\beta})^{2\gamma}}, \cdots, \frac{\sigma^2(x_n)}{f(x_n|\boldsymbol{\beta})^{2\gamma}}\right]\right)Z\Lambda_n^{-1}\boldsymbol{B}(x).
\end{aligned}
$$

The (i, j)-component of $n^{-1}Z'V[\boldsymbol{r}_\gamma|\boldsymbol{X}_n]Z$ can be calculated as

$$
\begin{aligned}
&\left(\frac{1}{n}Z'\left(\text{diag}\left[\frac{\sigma^2(x_1)}{f(x_1|\boldsymbol{\beta})^2}, \cdots, \frac{\sigma^2(x_n)}{f(x_n|\boldsymbol{\beta})^2}\right]\right)Z\right)_{ij} \\
&= \frac{1}{n}\sum_{k=1}^n B_{-p+i}^{[p]}(x_k)B_{-p+j}^{[p]}(x_k)\frac{\sigma^2(x_k)}{f(x_k|\boldsymbol{\beta})^2} \\
&= \int_0^1 B_{-p+i}^{[p]}(u)B_{-p+j}^{[p]}(u)\frac{\sigma^2(u)m(u)}{f(u|\boldsymbol{\beta})^2}du(1 + o_P(1)).
\end{aligned}
$$

Hence, we obtain

$$V[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n] = \frac{f(x|\boldsymbol{\beta})^{2\gamma}}{n}\boldsymbol{B}(x)'\Gamma(\lambda_n)^{-1}G(\sigma,\beta,\gamma)\Gamma(\lambda_n)^{-1}\boldsymbol{B}(x) + o_P(K_n n^{-1}).$$

Before proof of Theorem 3.2, we define some symbols. For any function $g(\cdot|\boldsymbol{\beta})$ which is smooth for $\boldsymbol{\beta}$,

$$g^{(1)}(\cdot|\boldsymbol{\beta}_0) = \frac{\partial g(\cdot|\boldsymbol{\beta})}{\partial\boldsymbol{\beta}}\Big|_{\boldsymbol{\beta}=\boldsymbol{\beta}_0}, \quad g^{(2)}(\cdot|\boldsymbol{\beta}_0) = \frac{\partial^2 g(\cdot|\boldsymbol{\beta})}{\partial\boldsymbol{\beta}\partial\boldsymbol{\beta}'}\Big|_{\boldsymbol{\beta}=\boldsymbol{\beta}_0}.$$

We use Taylor expansion of $g(\cdot|\hat{\boldsymbol{\beta}})$ around $\boldsymbol{\beta}_0$, giving

$$g(\cdot|\hat{\boldsymbol{\beta}}) = g(\cdot|\boldsymbol{\beta}_0) + g^{(1)}(\cdot|\boldsymbol{\beta}_0)'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) + \frac{1}{2}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)'g^{(2)}(\cdot|\boldsymbol{\beta}_0)(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) + o_P(n^{-1}). \quad (10)$$

PROOF OF THEOREM 3.2. We first note from (2) that the SPSE is expressed as

$$\hat{f}(x,\gamma) = f(x|\hat{\boldsymbol{\beta}}) + \boldsymbol{B}(x)'\Lambda^{-1}Z'\boldsymbol{r}_\gamma(\hat{\boldsymbol{\beta}}),$$

where

$$\boldsymbol{r}_\gamma(\hat{\boldsymbol{\beta}}) \quad = \quad (r_\gamma(y_1|\hat{\boldsymbol{\beta}}) \ \cdots \ r_\gamma(y_n|\hat{\boldsymbol{\beta}}))'$$

and $r_\gamma(y_i|\hat{\boldsymbol{\beta}}) = f(x|\hat{\boldsymbol{\beta}})^\gamma\{y_i - f(x_i|\hat{\boldsymbol{\beta}})\}/f(x_i|\hat{\boldsymbol{\beta}})^\gamma$.

Taylor expansion yields that

$$\hat{f}(x,\gamma) = \hat{f}_0(x,\gamma) + \hat{f}^{(1)}(x,\gamma)'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) + \frac{1}{2}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)'\hat{f}^{(2)}(x,\gamma)(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) + o_P(n^{-1}), \quad (11)$$

where

$$\hat{f}^{(1)}(x,\gamma) = f^{(1)}(x|\boldsymbol{\beta}_0) + \sum_{j=1}^{n}\left\{\boldsymbol{B}(x_j)'\Lambda^{-1}\boldsymbol{B}(x)\right\}r_\gamma^{(1)}(y_j|\boldsymbol{\beta}_0)$$

and

$$\hat{f}^{(2)}(x,\gamma) = f^{(2)}(x|\boldsymbol{\beta}_0) + \sum_{j=1}^{n}\left\{\boldsymbol{B}(x_j)'\Lambda^{-1}\boldsymbol{B}(x)\right\}r_\gamma^{(2)}(y_j|\boldsymbol{\beta}_0).$$

First we derive the asymptotic expectation of $\hat{f}(x,\gamma)$. The term $E[\hat{f}_0(x,\gamma)|\boldsymbol{X}_n]$ has been already derived in Proposition 1. Direct calculations with repeated use of (5) and Lemmas 1 and 2 yield that

$$\frac{1}{n}\sum_{\alpha=1}^{n}E\left[f^{(1)}(x|\boldsymbol{\beta}_0)'\left\{I(x_\alpha,Y_\alpha) + \frac{d}{n} + \delta_n\right\}\Big|\boldsymbol{X}_n\right] = \frac{1}{n}E[f^{(1)}(x|\boldsymbol{\beta}_0)'d|\boldsymbol{X}_n] + O(n^{-2})$$

$$= O(n^{-1})$$

and

$$\frac{1}{n}\sum_{\alpha=1}^{n}\sum_{j=1}^{n}\left\{\boldsymbol{B}(x_j)'\Lambda^{-1}\boldsymbol{B}(x)\right\}E\left[r_\gamma^{(1)}(Y_j|\boldsymbol{\beta}_0)'\left\{I(x_\alpha,Y_\alpha) + \frac{d}{n} + \delta_n\right\}\Big|\boldsymbol{X}_n\right]$$

$$= \frac{1}{n}\sum_{j=1}^{n}\left\{\boldsymbol{B}(x_j)'\Lambda^{-1}\boldsymbol{B}(x)\right\}E\left[r_\gamma^{(1)}(Y_j|\boldsymbol{\beta}_0)'\left\{I(x_j,Y_j) + \frac{d}{n}\right\}\Big|\boldsymbol{X}_n\right] + O_P(n^{-2})$$

$$= O_P(n^{-1}).$$

Hence we obtain

$$E[\hat{f}^{(1)}(x,\gamma)'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)|\boldsymbol{X}_n] = O_P(n^{-1}). \tag{12}$$

Analogously,

$$E[(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)'\hat{f}^{(2)}(x,\gamma)(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)|\boldsymbol{X}_n] = O_P(n^{-1}) \tag{13}$$

can be also shown. (12) and (13) are smaller order than the bias terms of $\hat{f}_0(x,\gamma)$. Therefore the bias of $\hat{f}(x,\gamma)$ is essentially dominated by the bias of $\hat{f}_0(x,\gamma)$.

Next we turn to the variance of $\hat{f}(x,\gamma)$. It follows from direct evaluation using (5) that

$$V[\hat{f}^{(1)}(x,\gamma)'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)|\boldsymbol{X}_n] = O_P(n^{-1}).$$

And simple but tedious calculations finally yield

$$V[(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)'\hat{f}^{(2)}(x,\gamma)(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)|\boldsymbol{X}_n] = O_P(n^{-2}).$$

All terms of relating to covariance appeared from the right hand side of (11) can be shown to be negligible order by Cauchy-Schwarz inequality. Hence the variance of $\hat{f}(x,\gamma)$ is dominated by that of $\hat{f}_0(x,\gamma)$.

PROOF OF THEOREM 3.3. Let $\hat{r}(x,\gamma) = \boldsymbol{B}(x)'\Lambda^{-1}Z'\boldsymbol{r}_\gamma(\hat{\boldsymbol{\beta}})$. Then the semiparametric estimator can be written as $\hat{f}(x,\gamma) = f(x|\hat{\boldsymbol{\beta}}) + \hat{r}(x,\gamma)$. We now prove

$$\frac{\hat{f}(x,\gamma) - E[\hat{f}(x,\gamma)|\boldsymbol{X}_n]}{\sqrt{V[\hat{f}(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{D} N(0,1) \tag{14}$$

by using Lyapunov theorem. First, from $\sqrt{n}(f(x|\hat{\boldsymbol{\beta}}) - E[f(x|\hat{\boldsymbol{\beta}})|\boldsymbol{X}_n]) = O_P(1)$ and $V[\hat{f}(x,\gamma)|\boldsymbol{X}_n] = O(K_n n^{-1})$, we have

$$\frac{f(x|\hat{\boldsymbol{\beta}}) - E[f(x|\hat{\boldsymbol{\beta}})|\boldsymbol{X}_n]}{\sqrt{V[\hat{f}(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{P} 0.$$

Therefore, (14) can be obtained, provided that

$$\frac{\hat{r}(x,\gamma) - E[\hat{r}(x,\gamma)|\boldsymbol{X}_n]}{\sqrt{V[\hat{r}(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{D} N(0,1) \tag{15}$$

because $V[\hat{f}(x,\gamma)|\boldsymbol{X}_n]/V[\hat{r}(x,\gamma)|\boldsymbol{X}_n] \to 1 (n \to \infty)$. Furthermore, from the proof of Theorem 3.2, we obtain

$$\frac{\hat{r}(x,\gamma) - \hat{r}_0(x,\gamma)}{\sqrt{V[\hat{r}(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{P} 0, \quad \text{as} \quad n \to \infty$$

and $V[\hat{r}(x,\gamma)|\boldsymbol{X}_n]/V[\hat{r}_0(x,\gamma)|\boldsymbol{X}_n] \to 1 (n \to \infty)$, where

$$\hat{r}_0(x,\gamma) = \boldsymbol{B}(x)'\Lambda^{-1}Z'\boldsymbol{r}_\gamma(\boldsymbol{\beta}_0) = f(x|\boldsymbol{\beta}_0)^\gamma \sum_{i=1}^n \{\boldsymbol{B}(x_i)'\Lambda^{-1}\boldsymbol{B}(x)\} \frac{\{y_i - f(x_i|\boldsymbol{\beta}_0)\}}{f(x_i|\boldsymbol{\beta}_0)^\gamma}.$$

From now on, we try to show

$$\frac{\hat{r}_0(x,\gamma) - E[\hat{r}_0(x,\gamma)|\boldsymbol{X}_n]}{\sqrt{V[\hat{r}_0(x,\gamma)|\boldsymbol{X}_n]}} \xrightarrow{D} N(0,1) \qquad (16)$$

by applying the Lyapunov theorem. First we see that

$$\hat{r}_0(x,\gamma) - E[\hat{r}_0(x,\gamma)|\boldsymbol{X}_n] = f(x|\boldsymbol{\beta}_0)^\gamma \sum_{i=1}^{n} \{\boldsymbol{B}(x_i)'\Lambda^{-1}\boldsymbol{B}(x)\} \frac{\varepsilon_i}{f(x_i|\boldsymbol{\beta}_0)^\gamma}.$$

And it is easily confirmed that

$$f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)'\Lambda^{-1}\boldsymbol{B}(x_i) = O_P(K_n n^{-1}).$$

By above evaluations and the moment condition for ε_i, we have

$$E\left[\left|f(x|\boldsymbol{\beta}_0)^\gamma \{\boldsymbol{B}(x_i)'\Lambda^{-1}\boldsymbol{B}(x)\} \frac{\varepsilon_i}{f(x_i|\boldsymbol{\beta}_0)^\gamma}\right|^{2+\delta} \Big| \boldsymbol{X}_n\right]$$

$$= \frac{E[|f(x|\boldsymbol{\beta}_0)^\gamma \boldsymbol{B}(x)'\Lambda^{-1}\boldsymbol{B}(x_i)\varepsilon_i|^{2+\delta}|\boldsymbol{X}_n]}{|f(x_i|\boldsymbol{\beta}_0)|^{\gamma(2+\delta)}}$$

$$= O_P\left(\frac{K_n^{2+\delta}}{n^{2+\delta}}\right).$$

On the other hand, since $B_n^2 = V[\hat{r}_0(x,\gamma)|\boldsymbol{X}_n] = O_P(K_n n^{-1})$, we have

$$B_n^{2+\delta} = O_P\left(\left(\frac{K_n}{n}\right)^{(2+\delta)/2}\right).$$

Then it follows that

$$\frac{1}{B_n^{2+\delta}} \sum_{i=1}^{n} E\left[\left|f(x|\boldsymbol{\beta}_0)^\gamma \{\boldsymbol{B}(x_i)'\Lambda^{-1}\boldsymbol{B}(x)\} \frac{\varepsilon_i}{f(x_i|\boldsymbol{\beta}_0)^\gamma}\right|^{2+\delta} \Big| X_i\right]$$

$$= O_P\left(n\left(\frac{K_n}{n}\right)^{2+\delta}\right) O_P\left(\left(\frac{K_n}{n}\right)^{-(2+\delta)/2}\right)$$

$$= O_P\left(n\left(\frac{K_n}{n}\right)^{\frac{2+\delta}{2}}\right),$$

which tends to 0 in probability by $K_n = o(n^{1/2})$ and $\delta \geq 2$. This assures the Lyapunov condition, so that (16) holds. Note that $b_a(x|\boldsymbol{\beta}_0,\gamma) = O(K_n^{-(p+1)})$, $b_\lambda(x|\boldsymbol{\beta}_0,\gamma) = O(\lambda_n K_n n^{-1})$ and $V[\hat{f}(x,\gamma)|\boldsymbol{X}_n] = O(K_n n^{-1})$. It results from these evaluations and the assumptions for the order of K_n and λ_n that

$$\frac{E[\hat{f}(x,\gamma)|\boldsymbol{X}_n] - f(x) - b_a(x|\boldsymbol{\beta}_0,\gamma) - b_\lambda(x|\boldsymbol{\beta}_0,\gamma)}{\sqrt{V[\hat{f}(x,\gamma)|\boldsymbol{X}_n]}} \to 0,$$

which completes the proof.

Proof of Corollary 3.4. First, $f_q(x|\boldsymbol{\beta}_q)$ can be expressed as the linear combination of the pth B-spline basis. From the fundamental property of B-spline basis (see, p.95 of de Boor (2001)), actually, each x^j can be written as

$$x^{p-j} = \sum_{k=-p+1}^{K_n} \frac{(-1)^j(p-j)!}{p!} \phi_{k,p}^{(j)}(0) B_k^{[p]}(x), \quad j = p-q, \cdots, p,$$

where $\phi_{k,p}(z) = (\kappa_k - z)\cdots(\kappa_{k+p-1} - z)$ and we have

$$
\begin{aligned}
f_q(x|\boldsymbol{\beta}_q) &= \beta_0 + \beta_1 x + \cdots + \beta_q x^q \\
&= \sum_{j=p-q}^{p} \beta_{p-j} x^{p-j} \\
&= \sum_{k=-p+1}^{K_n} \left\{ \sum_{j=p-q}^{p} \beta_{p-j} \frac{(-1)^j(p-j)!}{p!} \phi_{k,p}^{(j)}(0) \right\} B_k^{[p]}(x). \quad (17)
\end{aligned}
$$

Note that (17) consist for any $\boldsymbol{\beta} \in B \subseteq \mathbb{R}^{q+1}$. The semiparametric penalized spline estimator is obtained by $\hat{f}(x,0) = f_q(x|\hat{\boldsymbol{\beta}}_q) + \hat{r}_0(x, \hat{\boldsymbol{\beta}}_q)$. Let $\hat{\boldsymbol{c}} = (\hat{c}_{-p+1} \cdots \hat{c}_{K_n})'$ be the $(K_n + p)$ vector defined as

$$\hat{c}_k = \sum_{j=p-q}^{p} \hat{\beta}_{p-j} \frac{(-1)^j(p-j)!}{p!} \phi_{k,p}^{(j)}(0), \quad k = -p+1, \cdots, K_n.$$

Then, we have $f_q(x|\hat{\boldsymbol{\beta}}_q) = \boldsymbol{B}(x)'\hat{\boldsymbol{c}}$ and

$$\hat{r}_0(x, \hat{\boldsymbol{\beta}}_q) = \boldsymbol{B}(x)'\hat{\boldsymbol{b}} = \boldsymbol{B}(x)'(Z'Z + \lambda_n D_q'D_q)^{-1}Z'(\boldsymbol{y} - Z\hat{\boldsymbol{c}}).$$

Therefore, we have

$$\hat{f}(x,0) = f_q(x|\hat{\boldsymbol{\beta}}_q) + \hat{r}_0(x, \hat{\boldsymbol{\beta}}_q) = \boldsymbol{B}(x)'\hat{\boldsymbol{c}} + \boldsymbol{B}(x)'(Z'Z + \lambda_n D_q'D_q)^{-1}Z'(\boldsymbol{y} - Z\hat{\boldsymbol{c}}). \quad (18)$$

When $\lambda_n = 0$, meaning that $\hat{r}_0(x, \hat{\boldsymbol{\beta}}_q)$ is regression spline, (18) can be written as

$$\hat{f}(x,0) = \boldsymbol{B}(x)'\hat{\boldsymbol{c}} + \boldsymbol{B}(x)'(Z'Z)^{-1}Z'(\boldsymbol{y} - Z\hat{\boldsymbol{c}}) = \boldsymbol{B}(x)'(Z'Z)^{-1}Z'\boldsymbol{y}$$

for all $p \geq 1$. So the semiparametric estimator and nonparametric estimator have the same form. If $\lambda_n > 0$, on the other hand,

$$
\begin{aligned}
\hat{f}(x,0) &= \boldsymbol{B}(x)'\hat{\boldsymbol{c}} - \boldsymbol{B}(x)'(Z'Z + \lambda_n D_m'D_m)^{-1}Z'Z\hat{\boldsymbol{c}} \\
&= \lambda_n \boldsymbol{B}(x)'(Z'Z + \lambda_n D_m'D_m)^{-1}D_q'D_q\hat{\boldsymbol{c}}
\end{aligned}
$$

does not become 0 unless $D_m'D_m\hat{\boldsymbol{c}} = \boldsymbol{0}$. However as far as we use $(p,m) = (1,2)$ and equidistant knots, we obtain $D_2'D_2\hat{\boldsymbol{c}} = \boldsymbol{0}$. The $(K_n + p - 2) \times (K_n + p)$ matrix D_2 has the form

$$D_2 = (d_{ij})_{ij} = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix}.$$

We way only prove $D_2\hat{c} = \mathbf{0}$. Because the kth component of $\hat{c}$ is

$$\sum_{j=0}^{p} \hat{\beta}_{p-j} \frac{(-1)^j (p-j)!}{p!} \phi_{k,p}^{(j)}(0),$$

we show that for $j = 0, 1$ and $p = 1$,

$$\sum_{k=-p+1}^{K_n} d_{ik} \phi_{k,1}^{(j)}(0) = 0, \quad i = 1, \cdots, K_n + p.$$

By the definition of d_{ik} and $\phi_{k,1}^{(j)}(z) = (\kappa_k - z)^{(j)}$, we have for $j = 0$,

$$\sum_{k=-p+1}^{K_n} d_{ik} \phi_{k,1}^{(0)}(0) = d_{i,i}\kappa_i + d_{i,i+1}\kappa_{i+1} + d_{i,i+2}\kappa_{i+2} = 0.$$

For $j = 1$, we obtain $\sum_{k=-p+1}^{K_n} d_{ik} \phi_{k,1}^{(1)}(0) = 0$. Therefore, $D_2\hat{c} = \mathbf{0}$ has been proven.

Acknowledgement

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