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Abstract

Nonlinear regression modeling based on basis expansions has been widely used to explore data with complex structure. A crucial issue in nonlinear regression model is the choice of adjusted parameters including hyper-parameters for prior distribution and the number of basis functions. The selection of these parameters can be viewed as a model selection and evaluation problem. We derive an information criterion for the Bayesian predictive distribution in the case of both of regression coefficient and variance are unknown. Our proposed method make a selection of the appropriate value of hyper-parameters and the number of basis functions. Real data and simulation data analysis show that our proposed modeling strategy performs well in various situations.

Key Words: Basis expansion, the Bayesian predictive distribution, Predictive information criterion, Model selection, Nonlinear regression model

1 Introduction

Nonlinear regression models based on basis expansions provide a useful tool to analyze data with complex structure. The essential idea for basis expansions is to express a regression function as a linear combination of prescribed function, called basis functions (Hastie *et al.* (2001), Konishi and Kitagawa (2008)).

Since maximum likelihood methods yield unstable parameter estimates, the adopted model is usually estimated by those such as the method of maximum penalised likelihood (Good and Gaskins (1971), Green and Silverman (1994)), the method of regularisation or the Bayes approach and so on.

As one of the Bayesian approach, there are several studies on the Bayesian predictive distribution. Therefore choosing an appropriate prior distribution, the Bayesian predictive distribution can be configured better than plug-in predictive distribution (Komaki (1996)). Bishop (2006) introduced the Bayesian predictive distribution in the framework of regression models and showed a relationship between Maximum A Posteriori (MAP) estimator and Ridge estimator (Hoerl and Kennard (1970)).

One of the critical issue with Bayesian modeling is how to evaluate the goodness of the Bayesian predictive distributions. The goodness of Bayesian predictive distribution can be evaluated by the Kullback-Leibler information (Kullback and Leibler (1951)) between the true distribution and the Bayesian predictive distribution.

Kitagawa (1997) discussed the Bayesian predictive distribution and its evaluation method. Kitagawa (1997) consider the multivariate linear Gaussian model with an unknown mean and a known covariance matrix. Moreover, in this framework, he showed that the Bayesian predictive distribution is Gaussian distribution, and he derived PIC (Predictive Information Criterion) for evaluation of the Bayesian predictive distribution. Here, a significant difference from the case of maximum likelihood estimation is that the covariance matrix is assumed to be known.

In this paper, we derived the new model selection criteria based on Kitagawa (1997) to evaluate the Bayesian predictive distribution in framework of nonlinear regression model. The aim of this paper is to introduce procedures for choosing the values of hyper-parameters in the prior distribution and the number of basis functions simultaneously. Moreover, we use prior distribution introduced by Denison *et al.* (2002) and the Bayesian predictive distribution which can be obtained when both regression coefficient and variance are assumed to be unknown (Bishop (2006)).

The paper is organized as follow. In section 2, we describe a framework of nonlinear regression model based on basis expansions. In section 3, we derive the Bayesian predictive distribution for the nonlinear regression model when both of regression coefficients and regression variance are unknown. In section 4, we propose new model selection criterion for evaluating goodness of the Bayesian predictive distribution based on Kitagawa (1997). In section 5, we investigate the performance of the proposed model selection criterion by real data analysis and Monte Carlo simulations. Some concluding remarks are described in Section 6.

2 Nonlinear regression model based on basis expansion method

Suppose that $\{(y_i, \boldsymbol{x}_i); i = 1, ..., n\}$ be n sets of data obtained in terms of the response variable y and p-dimensional explanatory variables $\boldsymbol{x} = (x_1, ..., x_p)^T$. In order to draw information from the data, we consider the Gaussian nonlinear regression model

$$y_i = u(\boldsymbol{x}_i) + \varepsilon_i, \quad i = 1, 2, ..., n, \tag{1}$$

where $u(\cdot)$ is true smooth function and errors ε_i are sets of independent zero-mean normal samples with variance σ^2. Here, we consider basis expansions approximation. That is, the problem is to estimate the function $u(\cdot)$ from the observed data, and we use the basis functions. In the basis expansion approach (Eilers and Marx, 1996), the unknown $u(\boldsymbol{x}_i)$ is approximated by a linear combination of basis functions

$$u(\boldsymbol{x}_i) = w_0 + \sum_{j=1}^{m} w_j \phi_j(\boldsymbol{x}_i) = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i), \tag{2}$$

where $\boldsymbol{\phi}(\boldsymbol{x}) = (1, \phi_1(\boldsymbol{x}), ..., \phi_m(\boldsymbol{x}))^T$ is a vector of basis functions and $\boldsymbol{w} = (w_0, w_1, ..., w_m)^T$ is an unknown coefficient parameter vector.

For several times, splines (Green and Silverman (1994)), B-splines (de Boor (2001), Imoto and Konishi (2003)) and radial basis functions (Bishop (1995), Ripley (1996)) are used here for basis functions.

From equation (1) and (2), for n independent observations, the nonlinear regression model based on basis functions $\phi_j(\boldsymbol{x})$ $(j = 1, ..., m)$ is expressed as

$$y_i = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) + \varepsilon_i, \quad i = 1, ..., n. \tag{3}$$

Since the nonlinear regression model (3) has a probability density function

$$f(y_i|\boldsymbol{x}_i; \boldsymbol{w}, \sigma^2) = \frac{1}{\sqrt{(2\pi\sigma^2)}} \exp\left[-\frac{\left\{y_i - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)\right\}^2}{2\sigma^2}\right], \quad i = 1, ..., n. \tag{4}$$

The unknown parameters in the model are the set of coefficients, $\boldsymbol{w} = (w_0, w_1, \cdots, w_m)^T$ and the regression variance σ^2.

3 Estimation

For n independent observations $\{(y_i, \boldsymbol{x}_i); i = 1, ..., n\}$, the nonlinear regression model based on basis expansions given in section 2 is expressed as

$$y_i = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) + \varepsilon_i, \quad i = 1, ..., n. \tag{5}$$

where $\boldsymbol{\phi}(\boldsymbol{x}_i) = (1, \phi_1(\boldsymbol{x}_i), ..., \phi_m(\boldsymbol{x}_i))^T$, $\boldsymbol{w} = (w_0, w_1, ..., w_m)^T$ and ε_i are error terms.

Then the maximum likelihood estimates of the coefficient vector $\boldsymbol{w}$ and σ^2 are respectively given by

$$\hat{\boldsymbol{w}}_{\text{MLE}} = (\Phi^T\Phi)^{-1}\Phi^T\boldsymbol{y}, \quad \hat{\sigma}^2_{\text{MLE}} = \frac{1}{n}(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_{\text{MLE}})^T(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_{\text{MLE}}), \tag{6}$$

where $\mathbf{1} = (1, 1, ..., 1)^T$, $\Phi = (\mathbf{1}, \boldsymbol{\phi}(\boldsymbol{x}_1), \boldsymbol{\phi}(\boldsymbol{x}_2), \cdots, \boldsymbol{\phi}(\boldsymbol{x}_n))^T$ and $\boldsymbol{y} = (y_1, ..., y_n)^T$. However, when fitting a nonlinear regression model to data with a complex structure, the maximum likelihood method often yields unstable estimation and leads to overfitting. We therefore estimate $\boldsymbol{w}$, σ^2 by maximizing the posterior distribution,

$$\pi(\boldsymbol{w}, \sigma^2 \ |\boldsymbol{y}) = \frac{f(\boldsymbol{y}|\boldsymbol{w}, \sigma^2)\pi(\boldsymbol{w}, \sigma^2)}{\int\int f(\boldsymbol{y}|\boldsymbol{w}, \sigma^2)\pi(\boldsymbol{w}, \sigma^2)d\boldsymbol{w}d\sigma^2} \tag{7}$$

where, $\pi(\boldsymbol{w}, \sigma^2)$ is a prior distribuion. Moreover, we consider the parametric model given by equation (5), and make assume for the known variance. One of the typical forms for the conjugate prior distribution is given by a Gaussian distribution of the form,

$$\boldsymbol{w} \sim N(\mathbf{0}, (n\lambda)^{-1}I_m). \tag{8}$$

Then, the posterior distribution $\pi(\boldsymbol{w}|\boldsymbol{y})$ is still Gaussian distribution of mean vector $\boldsymbol{\xi}$ and variance-covariance matrix V,

$$\boldsymbol{\xi} = (\Phi^T\Phi + n\lambda\sigma^2 I_m)^{-1}\Phi^T\boldsymbol{y}, \quad V = \sigma^2(\Phi^T\Phi + n\lambda\sigma^2 I_m)^{-1}, \tag{9}$$

where λ is a hyperparameter. Then, we use the MAP estimator which is well-known as ridge estimator (Hoerl and Kennard (1970)),

$$\hat{\boldsymbol{w}} = (\Phi^T\Phi + n\lambda\sigma^2 I_m)^{-1}\Phi^T\boldsymbol{y}. \tag{10}$$

In many cases, we use the plug-in type model $f(\boldsymbol{y}|\hat{\boldsymbol{w}}, \hat{\sigma}^2)$ as a statistical model which is a nonlinear regression model based on basis expansion method. However, in this paper, we consider the Bayesian predictive distribution (Bishop (2006)) defined as

$$f(\boldsymbol{z}|\boldsymbol{y}) = \int\int f(\boldsymbol{z}|\boldsymbol{w}, \sigma^2)\pi(\boldsymbol{w}, \sigma^2 \ |\boldsymbol{y})d\boldsymbol{w}d\sigma^2. \tag{11}$$

where $\boldsymbol{z} = (z_1, z_2, ..., z_n)^T$ is a n-dimensional future data vector generated independently by the observed $\boldsymbol{y} = (y_1, y_2, ..., y_n)^T$.

Moreover, if regression variance σ^2 is known and we use the assumption of equation (3) and (8), as a result, the Bayesian predictive distribution is given by Gaussian distribution of mean vector $\boldsymbol{\mu}$ and variance-covariance matrix Σ analythically,

$$\boldsymbol{\mu} = \Phi\hat{\boldsymbol{w}}_n, \quad \Sigma = \sigma^2(2\Phi\Phi^T + n\lambda\sigma^2 I_n)(\Phi\Phi^T + n\lambda\sigma^2 I_n)^{-1}. \tag{12}$$

We consider another type of conjugate prior distribution, when both $\boldsymbol{w}$ and σ^2 are unknown, and one of correspondingly the conjugate prior distribution $\pi(\boldsymbol{w}, \sigma^2)$ which gives a Gaussian-inverse gamma distribution (Denison *et. al.* (2002)).

Now, we assume that the prior on the regression coefficients given the regression variance is a Gaussian distribution, and the prior on the regression variance is inverse-gamma distribution, by its specified following parameters.

$$\boldsymbol{w}|\sigma^2 \sim N(\mathbf{0}, \sigma^2(n\lambda I_m)^{-1}), \quad \sigma^2 \sim IG\left(\nu_0/2, \eta_0/2\right). \tag{13}$$

As a consequence of our assumptions, posterior distribution on the regression coefficients giving the regression variance is given by a Gaussian distribution, and the posterior distribution on the regression variance is an inverse-gamma distribution respectively as

$$\boldsymbol{w}|\sigma^2, \boldsymbol{y} \sim N(\hat{\boldsymbol{w}}_n, \sigma^2 \hat{A}_n), \quad \sigma^2|\boldsymbol{y} \sim IG\left(\hat{\nu}_n/2, \hat{\eta}_n/2\right), \tag{14}$$

where

$$\begin{aligned}
\hat{\eta}_n &= \eta_0 + (\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_{\text{MLE}})^T(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_{\text{MLE}}) + \hat{\boldsymbol{w}}_{\text{MLE}}^T \left\{n\lambda I_m + (\Phi^T\Phi)^{-1}\right\}^{-1} \hat{\boldsymbol{w}}_{\text{MLE}}, \\
\hat{\boldsymbol{w}}_n &= (\Phi^T\Phi + (n\lambda)^{-1}I_m)^{-1}\Phi^T\Phi\hat{\boldsymbol{w}}_{\text{MLE}} \\
\hat{A}_n &= (\Phi^T\Phi + n\lambda I_m)^{-1}, \quad \hat{\nu}_n = n + \nu_0, \ .
\end{aligned} \tag{15}$$

In this case, according to Bishop (2006), the predictive distribution was given by student t-distribution. The Bayesian predictive distribution is Student t-distribution with $\hat{\nu}_n$ degrees of freedom ,

$$\boldsymbol{z}|\boldsymbol{y} \sim St(\hat{\boldsymbol{\mu}}, \hat{\Sigma}^*, \hat{\nu}_n) \tag{16}$$

where, $\hat{\boldsymbol{\mu}}$ and $\hat{\Sigma}^*$ are given by

$$\hat{\boldsymbol{\mu}} = \Phi\hat{\boldsymbol{w}}_n, \quad \hat{\Sigma}^* = \frac{\hat{\lambda}_n}{\hat{\nu}_n}(\Phi\hat{A}_n\Phi^T + I_n), \tag{17}$$

respectively. The Student t-distribution is well known to have more probability in its tails than a normal distribution with the same location and scale parameters.

Futhermore, by the assumption of equation (3) and (13), the Bayesian predictive distribution for nonlinear regression model based on basis expansion, $h(\boldsymbol{z}|\boldsymbol{y}; \lambda, \eta, \nu)$ is given by

$$\begin{aligned}
h(\boldsymbol{z}|\boldsymbol{y}; \lambda, \eta, \nu) = &\left\{\Gamma\left((n + \hat{\nu}_n)/2\right)/\Gamma\left(\hat{\nu}_n/2\right)\left(\pi\hat{\nu}_n\right)^{\frac{n}{2}}\right\} \left|(\hat{\lambda}_n/\hat{\nu}_n)(\Phi\hat{A}_n\Phi^T + I_n)\right|^{-\frac{1}{2}} \\
&\times \left[1 + (1/\hat{\nu}_n)(\boldsymbol{z} - \Phi\hat{\boldsymbol{w}}_n)^T \left\{(\hat{\lambda}_n/\hat{\nu}_n)(\Phi\hat{A}_n\Phi^T + I_n)\right\}^{-1} (\boldsymbol{z} - \Phi\hat{\boldsymbol{w}}_n)\right]^{-\left(\frac{n+\hat{\nu}_n}{2}\right)}
\end{aligned} \tag{18}$$

4 Model selection criterion

In the Bayesian nonlinear regression model, we have crucial problems to solve, such as the choices of a hyper-parameter λ for the prior distribution, and the number of basis functions m. Kitagawa (1997) proposed the predictive information criterion (PIC) for evaluating goodness of the Bayesian predictive distribution in framework of multivariate Gaussian linear model, under the assumption of unknown regression coefficient and known variance. According to Kitagawa (1997), PIC is given by

$$\mathrm{PIC} = -2 \log h(\boldsymbol{y}|\boldsymbol{y}, \lambda) + 2B_p \tag{19}$$

where B_p is bias term of the expected log-likelihood estimated by the log-likelihood.

In the case of the Bayesian predictive distribution (12) in section 3, according to Kitagawa (1997), PIC is derived as

$$\mathrm{PIC} = n \log(2\pi) + \log|\Sigma| + (\boldsymbol{y} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y} - \boldsymbol{\mu}) + 2\mathrm{tr}\left\{(2\Phi\Phi^T + n\lambda\sigma^2 I)^{-1}\Phi\Phi^T\right\}$$

where,

$$\boldsymbol{\mu} = \Phi(\Phi^T\Phi + n\lambda\sigma^2 I)^{-1}\Phi^T\boldsymbol{y}, \quad \Sigma = \sigma^2(2\Phi\Phi^T + n\lambda\sigma^2 I)(\Phi\Phi^T + n\lambda\sigma^2 I)^{-1}. \tag{20}$$

In this paper, we derive the information criterion for the Bayesian predictive distribution in framework of nonlinear regression model where both of the regression coefficient and variance are unknown.

Since the Bayesian predictive distribution (18) which is derived in section 3, we consider applying the Laplace approximation method.

We use the Laplace's approximation method (Tierney and Kadane (1986), Davison (1986)) which has been extensively investigated as a useful tool for approximation the Bayesian predictive distributions. It aims to find a Gaussian approximation to a probability density defined over a set of continuous variables.

According to Konishi and Kitagawa (2008), if we regard $\hat{\boldsymbol{w}}_\star$ and $\hat{\sigma}^2_\star$ as the model of $n^{-1}\{\log f(\boldsymbol{y}|\boldsymbol{w}, \sigma^2) + \log \pi(\boldsymbol{w}, \sigma^2)\}$, the Laplace approximation method yields the Bayesian predictive distribution in framework of nonlinear regression model, in the form $h(\boldsymbol{z}|\boldsymbol{y}) = f(\boldsymbol{z}|\hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star)(1 + O_p(n^{-1}))$. Moreover, in this framework, we can analytically calculate mode of (14),

$$\hat{\boldsymbol{w}}_\star = (\Phi^T\Phi + n\lambda I_m)^{-1}\Phi^T\boldsymbol{y}, \ \hat{\sigma}^2_\star = C\left\{(\boldsymbol{y} - \Phi\boldsymbol{w}_\star)^T(\boldsymbol{y} - \Phi\boldsymbol{w}_\star) + n\lambda\boldsymbol{w}_\star^T\boldsymbol{w}_\star + \nu_0\right\}.$$

where $C = 1/(n + m + \nu_0 + 2)$.

By using the nonlinear regression model based on basis expansion methods, our proposed model selection criterion is given as

$$\mathrm{PIC} = n\log(2\pi) + n\log(\hat{\sigma}_\star^2) + \frac{1}{\hat{\sigma}_\star^2}(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)^T(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)$$
$$+2\left(\frac{\sigma^{2*}}{\hat{\sigma}_\star^2}\right)\mathrm{tr}\left[\Phi(\Phi^T\Phi + n\lambda I_m)^{-1}\Phi^T\right]. \qquad (21)$$

However, our proposed model selection criterion contains the unknown true regression variance σ^{2*}. Then, we use two types of (21), actually. We first consider the true variance, substituting the maximum likelihood estimator of the variance estimated from the data. As a consequence, PIC results can be expressed as following:

$$\mathrm{PIC}_{\mathrm{MLE}} = n\log(2\pi) + n\log(\hat{\sigma}_\star^2) + \frac{1}{\hat{\sigma}_\star^2}(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)^T(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)$$
$$+2\left(\frac{\hat{\sigma}_{\mathrm{MLE}}^2}{\hat{\sigma}_\star^2}\right)\mathrm{tr}\left[\Phi(\Phi^T\Phi + n\lambda I_m)^{-1}\Phi^T\right]. (22)$$

We next consider that the true variance substituting the mode of the posterior distribution.

$$\mathrm{PIC}_{\mathrm{Mode}} = n\log(2\pi) + n\log(\hat{\sigma}_\star^2) + \frac{1}{\hat{\sigma}_\star^2}(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)^T(\boldsymbol{y} - \Phi\hat{\boldsymbol{w}}_\star)$$
$$+2\mathrm{tr}\left[\Phi(\Phi^T\Phi + n\lambda I_m)^{-1}\Phi^T\right]. (23)$$

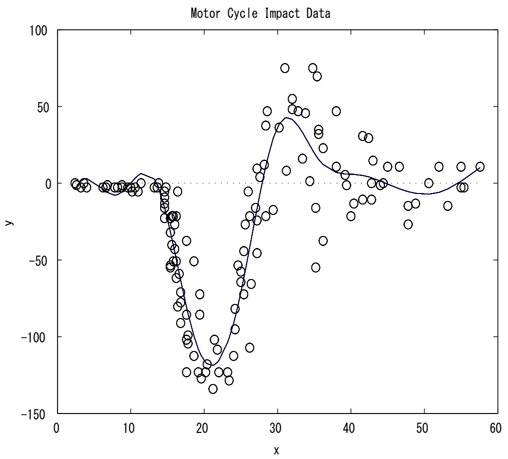
We select the optimal values of the number of basis functions and a hyper-parameter that minimize PIC.

5 numerical example

5.1 analysis of real data

We illustrate the proposed procedure to choose the smoothing parameter and the number of basis functions through the analysis of the motorcycle impact data (Silverman (1985), Härdle (1990), Eilers and Marx (1996)). The motorcycle impact data were simulated to investigate the efficacy of crash helmets and it comprised a series of measurements of head acceleration in units of gravity and times in milliseconds after impact.

We fit the Bayesian predictive distribution based on B-spline regression model with Gaussian noise (1) to the motorcycle impact data. Then we choose the number of basis functions m and the smoothing parameter λ that minimize the information criterion for the Bayesian predictive distribution $\mathrm{PIC}_{\mathrm{MLE}}$ and $\mathrm{PIC}_{\mathrm{Mode}}$ given by equation (22), (23). For the analysis of the motorcycle impact data, we set the candidate values of m and λ to $\{4, ..., 15\}$ and $\left\{10^{10(i-100)/99}; i = 1, ..., 100\right\}$, respectively. The criterion $\mathrm{PIC}_{\mathrm{MLE}}$ selected $m = 13$ and $\lambda = 1.62 \times 10^{-9}$, while $\mathrm{PIC}_{\mathrm{Mode}}$ selected $m = 13$ and $\lambda = 2.59 \times 10^{-9}$. The corresponding fitted curve is shown in Fig. 2 (solid curve).



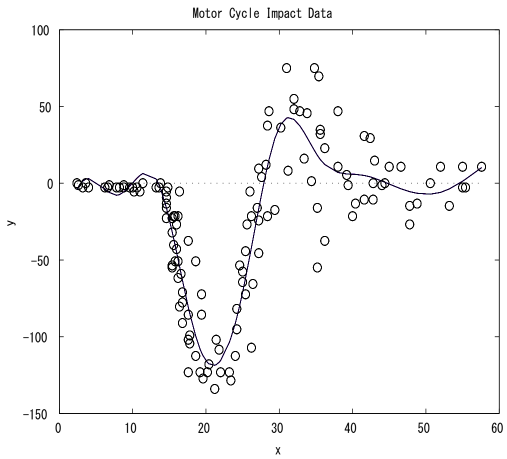


Figure 1: Real data examples: The motorcycle impact data: The left solid curved is the estimated curve based on $\mathrm{PIC}_{\mathrm{MLE}}$, The right solid curve is the estimated curve based on $\mathrm{PIC}_{\mathrm{Mode}}$.

5.2 curve fitting

For the second study, repeated random samples $\{(x_i, y_i); i = 1, ..., n\}$ with $n = 50,\ 100,\ 300$, were generated from a true regression model $y_i = u(x_i) + \varepsilon_i$. The design point x_i are uniformly distributed in $[0, 1]$ and the errors ε_i are independently, normally distributed with mean 0 and variance τ^2, where the standard deviation is taken as $\tau = 0.15R_y$ or $0.3R_y$ with R_y being the range of $u(x)$ over $x \in [0, 1]$. For the analysis of the Simulated data, we divide $[10^{-8}, 10^0]$ to 100 equal subintervals by points $\lambda_i (i = 0, ..., 100)$. We considered the following two cases for the true regression model:

$$u(x) = 1 - 48x + 218x^2 - 315x^3 + 145x^4, \tag{24}$$

$$u(x) = \sin(2\pi x^3). \tag{25}$$

We performed 300 repetitions, and then calculated average squared errors (ASE) defined by ASE $= \sum_{i=1}^{n} \{u(x_i) - \hat{y}_i\}^2 / n$ and predictive average squared errors (PASE) defined by PASE$=\sum_{i=1}^{n} \{z_i - \hat{y}_i\}^2 / n$ and deviations to assess the goodness of fit, respectively.

Where, z is the future observation data that generated from true regression model. Table 1 displays simulation results with ASE, PASE, the number of basis function m and hyper parameter λ.

Simulation results may be summarized as follows: Our proposed information criterion, $\mathrm{PIC}_{\mathrm{MLE}}$ and $\mathrm{PIC}_{\mathrm{Mode}}$, generally give good estimates in the sense of ASE and PASE, and yields stable hyper parameter estimates.

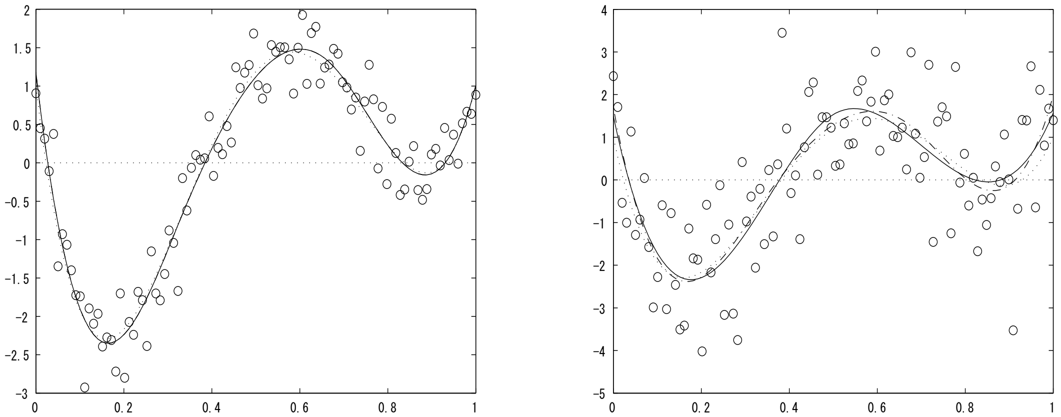


Figure 2: Examples of simulated data ($n = 100$; left: $\tau = 0.15R_y$; right: $\tau = 0.3R_y$): The dashed curve is the true regression curve $u(x) = 1 - 48x + 218x^2 - 315x^3 + 145x^4$, while the solid curved and dot-dashed curvethe are estimated curve based on $\mathrm{PIC}_{\mathrm{MLE}}$ and $\mathrm{PIC}_{\mathrm{Mode}}$, respectively.

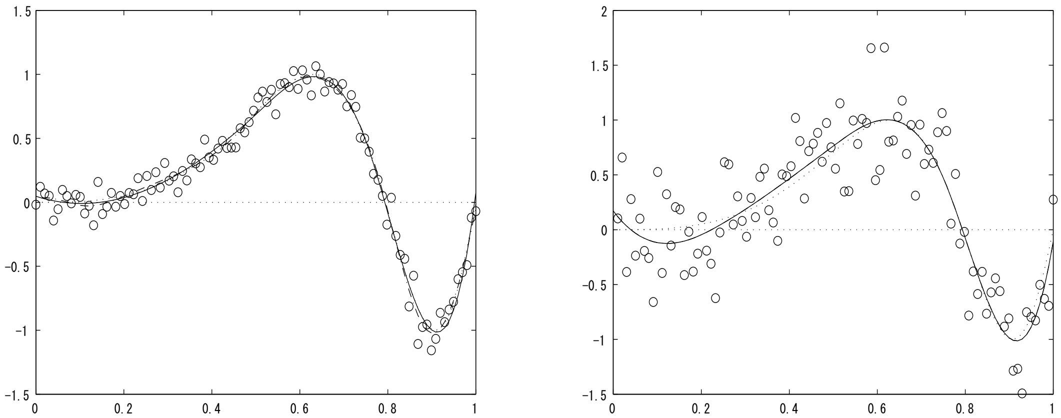


Figure 3: Examples of simulated data ($n = 100$; left: $\tau = 0.15R_y$; right: $\tau = 0.3R_y$): The dashed curve is the true regression curve $u(x) = \sin(2\pi x^3)$, while the solid curved and dot-dashed curvethe are estimated curve based on $\mathrm{PIC}_{\mathrm{MLE}}$ and $\mathrm{PIC}_{\mathrm{Mode}}$, respectively.

Table 1: $\tau^2 = 0.15$

Criterion	**Basis mean (SD)**	**hyper paramete mean (SD)**	**AMSE mean (SD)**	**APSE mean (SD)**
($n = 50$)				
GIC	8.37	3.03×10^{-4}	2.20×10^{-2}	1.19×10^{-1}
	(3.06)	(1.70×10^{-2})	(1.28×10^{-2})	(2.55×10^{-2})
mAIC	7.61	6.73×10^{-4}	2.04×10^{-2}	1.18×10^{-1}
	(2.79)	(2.70×10^{-3})	(1.22×10^{-1})	(2.48×10^{-2})
$\mathrm{PIC}_{\mathrm{MLE}}$	6.57	4.04×10^{-4}	1.79×10^{-2}	1.16×10^{-1}
	(2.12)	(2.00×10^{-3})	(1.11×10^{-2})	(2.45×10^{-2})
$\mathrm{PIC}_{\mathrm{Mode}}$	7.14	1.00×10^{-8}	1.93×10^{-2}	1.17×10^{-1}
	(2.38)	(6.29×10^{-23})	(1.19×10^{-2})	(2.45×10^{-2})
($n = 100$)				
GIC	7.88	3.03×10^{-4}	1.03×10^{-2}	1.076×10^{-1}
	(2.60)	(1.70×10^{-3})	(0.62-$\times 10^{-2}$)	(1.64-$\times 10^{-2}$)
mAIC	7.45	4.71×10^{-4}	1.00×10^{-2}	1.073×10^{-1}
	(2.47)	(2.10×10^{-1})	(6.30×10^{-3})	(1.67×10^{-2})
$\mathrm{PIC}_{\mathrm{MLE}}$	6.60	1.00×10^{-8}	9.20×10^{-3}	1.064×10^{-1}
	(1.68)	(6.29×10^{-23})	(5.50×10^{-3})	(1.66×10^{-2})
$\mathrm{PIC}_{\mathrm{Mode}}$	7.16	1.00×10^{-8}	9.60×10^{-3}	1.070×10^{-1}
	(2.14)	(6.29×10^{-23})	(5.90×10^{-3})	(1.69×10^{-2})
($n = 300$)				
GIC	7.53	3.36×10^{-5}	3.20×10^{-3}	1.018×10^{-1}
	(1.86)	(5.83×10^{-4})	(1.90×10^{-3})	(9.00×10^{-3})
mAIC	7.47	3.36×10^{-5}	3.20×10^{-3}	1.018×10^{-1}
	(1.76)	(5.83×10^{-4})	(1.90×10^{-3})	(9.00×10^{-3})
$\mathrm{PIC}_{\mathrm{MLE}}$	7.24	1.00×10^{-8}	3.10×10^{-3}	1.017×10^{-1}
	(1.52)	(6.29×10^{-23})	(1.80×10^{-3})	(8.90×10^{-3})
$\mathrm{PIC}_{\mathrm{Mode}}$	7.43	1.00×10^{-8}	3.20×10^{-3}	1.018×10^{-1}
	(1.71)	(6.29×10^{-23})	(1.90×10^{-3})	(9.00×10^{-3})

Table 2: $\tau^2 = 0.3$

Criterion	**number mean(SD)**	**hyper parameter mean(SD)**	**AMSE mean(SD)**	**APSE mean(SD)**
$(n = 50)$				
GIC	8.46	1.60×10^{-3}	3.28×10^{-1}	1.8932
	(3.57)	(3.70×10^{-3})	(2.15×10^{-1})	(4.14×10^{-1})
mAIC	8.14	2.90×10^{-3}	2.85×10^{-1}	1.8539
	(3.53)	(4.60×10^{-3})	(1.87×10^{-1})	(3.88×10^{-1})
$\mathrm{PIC}_{\mathrm{MLE}}$	9.75	7.80×10^{-3}	2.47×10^{-1}	1.8197
	(4.08)	(6.80×10^{-3})	(1.28×10^{-1})	(3.73×10^{-1})
$\mathrm{PIC}_{\mathrm{Mode}}$	7.94	3.10×10^{-3}	2.69×10^{-1}	1.8397
	(3.54)	(4.70×10^{-3})	(1.80×10^{-1})	(3.86×10^{-1})
$(n = 100)$				
GIC	7.13	7.40×10^{-4}	1.42×10^{-1}	1.6976
	(3.04)	(2.60×10^{-3})	$(1.00\text{-}\times10^{-1})$	$(2.64\text{-}\times10^{-1})$
mAIC	6.77	9.09×10^{-4}	1.32×10^{-1}	1.6876
	(2.86)	(2.90×10^{-23})	(9.59×10^{-2})	(2.61×10^{-1})
$\mathrm{PIC}_{\mathrm{MLE}}$	6.93	2.00×10^{-3}	1.21×10^{-1}	1.6794
	(3.15)	(4.00×10^{-3})	(7.97×10^{-2})	(2.60×10^{-1})
$\mathrm{PIC}_{\mathrm{Mode}}$	6.55	7.40×10^{-4}	1.27×10^{-1}	1.6850
	(2.69)	(2.60×10^{-3})	(9.22×10^{-2})	(2.63×10^{-1})
$(n = 300)$				
GIC	6.98	1.50×10^{-4}	4.49×10^{-2}	1.6200
	(2.56)	(4.11×10^{-4})	(3.03×10^{-2})	(0.14)
mAIC	6.78	1.40×10^{-4}	4.37×10^{-2}	1.6199
	(2.46)	(3.90×10^{-4})	(2.88×10^{-2})	(0.14)
$\mathrm{PIC}_{\mathrm{MLE}}$	6.50	1.51×10^{-4}	4.14×10^{-2}	1.6178
	(2.20)	(4.61×10^{-4})	(2.77×10^{-2})	(0.14)
$\mathrm{PIC}_{\mathrm{Mode}}$	6.59	1.13×10^{-4}	4.26×10^{-2}	1.6188
	(2.2904)	(3.50×10^{-4})	(2.88×10^{-2})	(0.14)

Table 3: $\tau^2 = 0.15$

Criterion	**number mean(SD)**	**hyper parameter mean(SD)**	**AMSE mean(SD)**	**APSE mean(SD)**
$(n = 50)$				
GIC	10.45	7.90×10^{-3}	2.10×10^{-3}	9.90×10^{-3}
	(3.08)	(2.38×10^{-2})	(9.78×10^{-4})	(2.10×10^{-3})
mAIC	9.68	1.57×10^{-2}	2.00×10^{-3}	9.80×10^{-3}
	(3.06)	(3.47×10^{-2})	(9.86×10^{-4})	(2.10×10^{-3})
PIC_{MLE}	7.89	1.00×10^{-8}	1.70×10^{-3}	9.50×10^{-3}
	(1.76)	(6.29×10^{-23})	(8.99×10^{-4})	(2.00×10^{-3})
PIC_{Mode}	9.04	1.00×10^{-8}	1.90×10^{-3}	9.80×10^{-3}
	(2.70)	(6.29×10^{-23})	(8.59×10^{-4})	(2.10×10^{-3})
$(n = 100)$				
GIC	9.70	4.10×10^{-3}	1.00×10^{-3}	9.00×10^{-3}
	(2.96)	(1.27×10^{-2})	(4.87×10^{-4})	(1.30×10^{-3})
mAIC	9.05	5.70×10^{-3}	1.00×10^{-3}	9.00×10^{-3}
	(2.82)	(1.64×10^{-2})	(4.90×10^{-4})	(1.30×10^{-3})
PIC_{MLE}	8.04	1.00×10^{-8}	9.11×10^{-4}	8.90×10^{-3}
	(1.99)	(6.29×10^{-23})	(4.6×10^{-4})	(1.30×10^{-3})
PIC_{Mode}	8.60	1.00×10^{-8}	9.56×10^{-4}	8.90×10^{-3}
	(2.49)	(6.29×10^{-23})	(4.73×10^{-4})	(1.40×10^{-3})
$(n = 300)$				
GIC	10.31	8.75×10^{-4}	3.87×10^{-4}	8.40×10^{-3}
	(2.96)	(3.60×10^{-3})	(1.54×10^{-4})	(7.49×10^{-4})
mAIC	9.86	9.76×10^{-4}	3.85×10^{-4}	8.40×10^{-3}
	(2.92)	(4.00×10^{-3})	(1.50×10^{-4})	(7.49×10^{-4})
PIC_{MLE}	9.41	1.00×10^{-8}	3.74×10^{-4}	8.40×10^{-3}
	(2.79)	(6.29×10^{-23})	(1.43×10^{-4})	(7.50×10^{-4})
PIC_{Mode}	9.70	1.00×10^{-8}	3.77×10^{-4}	8.40×10^{-3}
	(2.84)	(6.29×10^{-23})	(1.48×10^{-4})	(7.48×10^{-4})

Table 4: $\tau^2 = 0.3$

Criterion	number mean(SD)	hyper parameter mean(SD)	AMSE mean(SD)	APSE mean(SD)
($n = 50$)				
GIC	9.85	8.10×10^{-3}	2.89×10^{-2}	1.548×10^{-1}
	(2.95)	(1.48×10^{-2})	(1.55×10^{-2})	(3.28×10^{-2})
mAIC	9.80	1.41×10^{-2}	2.72×10^{-2}	1.534×10^{-1}
	(2.97)	(1.89×10^{-2})	(1.40×10^{-2})	(3.21×10^{-2})
PIC_{MLE}	13.95	1.32×10^{-2}	2.89×10^{-2}	1.548×10^{-1}
	(1.35)	(5.00×10^{-3})	(1.14×10^{-2})	(3.18×10^{-2})
PIC_{Mode}	11.84	8.10×10^{-3}	2.94×10^{-2}	1.553×10^{-1}
	(2.86)	(5.40×10^{-3})	(1.32×10^{-4})	(3.21×10^{-2})
($n = 100$)				
GIC	8.96	4.70×10^{-3}	1.38×10^{-2}	1.41×10^{-1}
	(2.68)	(9.70×10^{-3})	(7.90×10^{-3})	(2.18×10^{-2})
mAIC	8.88	6.20×10^{-3}	1.35×10^{-2}	1.40×10^{-1}
	(2.64)	(1.07×10^{-2})	(7.70×10^{-3})	(2.19×10^{-2})
PIC_{MLE}	13.21	9.60×10^{-3}	1.48×10^{-2}	1.41×10^{-1}
	(2.09)	(2.40×10^{-3})	(6.20×10^{-3})	(2.13×10^{-2})
PIC_{Mode}	10.22	4.90×10^{-3}	1.42×10^{-2}	1.41×10^{-1}
	(3.13)	(5.10×10^{-3})	(7.60×10^{-3})	(2.18×10^{-2})
($n = 300$)				
GIC	8.58	1.70×10^{-3}	2.20×10^{-3}	6.45×10^{-2}
	(2.45)	(4.40×10^{-3})	(1.20×10^{-3})	(5.80×10^{-3})
mAIC	8.50	2.00×10^{-3}	2.20×10^{-3}	6.44×10^{-2}
	(2.45)	(4.70×10^{-3})	(1.30×10^{-3})	(5.80×10^{-3})
PIC_{MLE}	7.74	1.00×10^{-8}	2.00×10^{-3}	6.43×10^{-2}
	(1.59)	(6.29×10^{-23})	(1.30×10^{-3})	(5.80×10^{-3})
PIC_{Mode}	7.84	1.00×10^{-8}	2.00×10^{-3}	6.43×10^{-2}
	(1.70)	(6.29×10^{-23})	(1.30×10^{-3})	(5.80×10^{-3})

6 Concluding Remarks

This article has proposed the nonlinear regression modeling based on basis expansion technique. We have introduced the information criterion for the Bayesian predictive distribution in nonlinear regression model based on basis expansion method. In particular, we derived PIC, when both of regression coefficient and regression variance are unknown.

7 Appendix

7.1 Derivation of PIC

As introduced by Kitagawa (1997), PIC is the derivation of our case is as follows:

$$\mathrm{PIC} = -2\log h(\boldsymbol{z}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star) + B_p(q(\cdot), \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star) \tag{26}$$

The log likelihood for the Bayesian predictive distribution, $\log h(\boldsymbol{z}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star)$ is given by

$$\log h(\boldsymbol{z}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\hat{\sigma}^2_\star I| - \frac{1}{2\hat{\sigma}^2_\star}(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)^T(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star). \tag{27}$$

Then, the diffence between the log likelihood for the Bayesian predictive distribution and expected loglikelihood is calcurated by

$$\begin{aligned}
&B_p(q(\cdot), \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star) \\
&= E_{q(\boldsymbol{y})}\left[\log h(\boldsymbol{y}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star) - E_{q(\boldsymbol{z})}\left[\log h(\boldsymbol{z}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}^2_\star)\right]\right] \\
&= -\frac{1}{2\hat{\sigma}^2_\star}\mathrm{tr}\left\{E_{q(\boldsymbol{y})}\left[(\boldsymbol{y} - B\hat{\boldsymbol{w}}_\star)(\boldsymbol{y} - B\hat{\boldsymbol{w}}_\star)^T - E_{q(\boldsymbol{z})}\left[(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)^T\right]\right]\right\}.
\end{aligned} \tag{28}$$

Moreover we assume that true distribution $q(\boldsymbol{z})$ is given by

$$q(\boldsymbol{z}) = f(\boldsymbol{z}|\boldsymbol{w}^*, \sigma^{2*}) \tag{29}$$

where, $\boldsymbol{w}^* \in R^m$, $\sigma^{2*} \in R^1$. Then we denoted this fact as

$$\boldsymbol{z}|\boldsymbol{w}^*, \sigma^{2*} \sim N(B\boldsymbol{w}^*, \sigma^{2*}I). \tag{30}$$

Futhermore, The expected that the value of the difference between the log-likelihood function and expected log-likelihood function is evaluated as

$$\begin{aligned}
E_{q(\boldsymbol{z})}\left\{(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)^T\right\} &= E_{f(\boldsymbol{z}|\boldsymbol{w}^*, \sigma^{2*})}\left\{(\boldsymbol{z} - B\boldsymbol{w}^*)(\boldsymbol{z} - B\boldsymbol{w}^*)^T\right\} \\
&\quad + (B\boldsymbol{w}^* - B\hat{\boldsymbol{w}}_\star)(B\boldsymbol{w}^* - B\hat{\boldsymbol{w}}_\star)^T.
\end{aligned} \tag{31}$$

Moreover, we have,

$$
\begin{aligned}
B\boldsymbol{w}^* - B\hat{\boldsymbol{w}}_\star &= (BB^T + n\lambda I_n)^{-1} BB^T (B\boldsymbol{w}^* - \boldsymbol{y}) + n\lambda (BB^T + n\lambda I_n)^{-1} B\boldsymbol{w}^* \\
\boldsymbol{y} - B\hat{\boldsymbol{w}}_\star &= n\lambda (B^T B + n\lambda I_m)^{-1} (\boldsymbol{y} - B\boldsymbol{w}^*) + n\lambda (B^T B + n\lambda I_m)^{-1} B\boldsymbol{w}^*. \qquad (32)
\end{aligned}
$$

Consequently, we correct bias term.

$$
\begin{aligned}
& E_{q(\boldsymbol{y})} \left[\log h(\boldsymbol{y}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}_\star^2) - E_{q(\boldsymbol{z})} \left[\log h(\boldsymbol{z}|\boldsymbol{y}, \hat{\boldsymbol{w}}_\star, \hat{\sigma}_\star^2) \right] \right] \\
&= -\frac{1}{2\hat{\sigma}^2} \mathrm{tr} \left[E_{q(\boldsymbol{y})} \left[(\boldsymbol{y} - B\hat{\boldsymbol{w}}_\star)(\boldsymbol{y} - B\hat{\boldsymbol{w}}_\star)^T - E_{q(\boldsymbol{z})} \left[(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)(\boldsymbol{z} - B\hat{\boldsymbol{w}}_\star)^T \right] \right] \right] \\
&= -\left(\frac{\sigma^{2*}}{\hat{\sigma}_\star^2} \right) \mathrm{tr} \left[B(B^T B + n\lambda I_m)^{-1} B^T \right]. \qquad (33)
\end{aligned}
$$

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