Convergence of Pseudo-Bayes Factors in Forward and Inverse Regression Problems

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Abstract

In the Bayesian literature on model comparison, Bayes factors play the leading role. In the classical statistical literature, model selection criteria are often devised using cross-validation ideas. Amalgamating the ideas of Bayes factor and cross-validation Geisser and Eddy (1979) created the pseudo-Bayes factor. The usage of cross-validation inculcates several theoretical advantages, computational simplicity and numerical stability in Bayes factors as the marginal density of the entire dataset is replaced with products of cross-validation densities of individual data points.

However, the popularity of pseudo-Bayes factors is still negligible in comparison with Bayes factors, with respect to both theoretical investigations and practical applications. In this article, we establish almost sure exponential convergence of pseudo-Bayes factors for large samples under a general setup consisting of dependent data and model misspecifications. We particularly focus on general parametric and nonparametric regression setups in both forward and inverse contexts. In forward regression the goal is to predict the response given some observed value of the covariate and the rest of the data, while in inverse regression the objective is to infer about unobserved covariate values from observed responses and covariates. For the Bayesian treatment that we consider here, a prior for the unknown covariate value is needed.

Depending upon forward and inverse regression ideas, our asymptotic theory manifests itself in terms of almost sure exponential convergence of the pseudo-Bayes factor in terms of the Kullback-Leibler divergence rate or its integrated version, between the competing and the true models. Our asymptotic theory encompasses general model selection, variable selection and combinations of both.

We illustrate our theoretical results with various examples, providing explicit calculations. We also supplement our asymptotic theory with simulation experiments in small sample situations of Poisson log regression and geometric logit and probit regression, additionally addressing the variable selection problem. We consider both linear and nonparametric regression modeled by Gaussian processes for our purposes. Our simulation results provide quite interesting insights into the usage of pseudo-Bayes factors in forward and inverse setups.

Keywords: Forward and inverse regression; Kullback-Leibler divergence; Leave-one-out cross-validation; Pseudo-Bayes factor; Poisson and geometric regression; Posterior convergence.

1 Introduction

The Bayesian statistical literature on model selection is rich in its collection of innovative methodologies. Among them the most principled method of comparing different competing models seems to be offered by Bayes factors, through the ratio of the posterior and prior odds associated with the models under comparison, which reduces to the ratio of the marginal densities of the data under the two models. To illustrate, let us consider the problem of
comparing any two models \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) given data \( Y_n = \{y_1, y_2, \ldots, y_n\} \), where \( n \) is the sample size. Let \( \Theta_1 \) and \( \Theta_2 \) be the parameter spaces associated with \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \), respectively. For \( j = 1, 2 \), let the likelihoods, priors and the marginal densities for the two models be \( L_n(\theta_j|\mathcal{M}_j) \), \( \pi(\theta_j|\mathcal{M}_j) \) and \( m(Y_n|\mathcal{M}_j) = \int_{\Theta_j} L_n(\theta_j|\mathcal{M}_j) \pi(d\theta_j|\mathcal{M}_j) \), respectively. Then the Bayes factor (BF) of model \( \mathcal{M}_1 \) against \( \mathcal{M}_2 \) is given by

\[
BF^{(n)}(\mathcal{M}_1, \mathcal{M}_2) = \frac{m(Y_n|\mathcal{M}_1)}{m(Y_n|\mathcal{M}_2)}.
\]  

(1.1)

The above formula follows directly from the coherent procedure of Bayesian hypothesis testing of one model versus the other. In view of (1.1), \( BF^{(n)}(\mathcal{M}_1, \mathcal{M}_2) \) admits the interpretation as the quantification of the evidence of \( \mathcal{M}_1 \) against \( \mathcal{M}_2 \), given data \( Y_n \). A comprehensive account of BF and its various advantages are provided in Kass and Raftery (1995). BFs have interesting asymptotic convergence properties. Indeed, recently Chatterjee et al. (2018) establish the almost sure convergence theory of BF in the general setup that includes even dependent data and misspecified models. Their result depends explicitly on the average Kullback-Leibler (KL) divergence between the competing and the true models.

BFs are known to have several limitations. First, if the prior for the model parameter \( \theta_j \) is improper, then the marginal density \( m(\cdot|\mathcal{M}_j) \) is also improper and hence \( m(Y_n|\mathcal{M}_j) \) does not admit any sensible interpretation. Second, BFs suffer from the Jeffreys-Lindley-Bartlett paradox (see Jeffreys (1939), Lindley (1957), Bartlett (1957), Robert (1993), Villa and Walker (2015) for details and general discussions on the paradox). Furthermore, a drawback of BFs in practical applications is that the marginal density of the data \( Y_n \) is usually quite challenging to compute accurately, even with sophisticated simulation techniques based on importance sampling, bridge sampling and path sampling (see, for example, Meng and Wong (1996), Gelman and Meng (1998); see also Gronau et al. (2017) for a relatively recent tutorial and many relevant references), particularly when the posterior is far from normal and when the dimension of the parameter space is large. Moreover, the marginal density is usually extremely close to zero if \( n \) is even moderately large. This causes numerical instability in computation of the BF.

The problems of BFs regarding improper prior, Jeffreys-Lindley-Bartlett paradox, and general computational difficulties associated with the marginal density can be simultaneously alleviated if the marginal density \( m(Y_n|\mathcal{M}_j) \) for model \( \mathcal{M}_j \) is replaced with the product of leave-one-out cross-validation posteriors

\[
\pi(y_i|Y_{n,-i}, \mathcal{M}_j) = \prod_{i=1}^n \pi(y_i|Y_{n,-i}, \mathcal{M}_j),
\]

(1.2)

is the leave-one-out cross-validation posterior density evaluated at \( y_i \). In the above equation (1.2), \( f(y_i|\theta_j, y_1, \ldots, y_{i-1}, \mathcal{M}_j) \) is the density of \( y_i \) given model parameters \( \theta_j \) and \( y_1, \ldots, y_{i-1}; \pi(\theta_j|Y_{n,-i}, \mathcal{M}_j) \) is the posterior distribution of \( \theta_j \) given \( Y_{n,-i} \). Viewing \( \prod_{i=1}^n \pi(y_i|Y_{n,-i}, \mathcal{M}_j) \) as the surrogate for \( m(Y_n|\mathcal{M}_j) \), it seems reasonable to replace \( BF^{(n)}(\mathcal{M}_1, \mathcal{M}_2) \) with the corresponding pseudo-Bayes factor (PBF) given by

\[
PBF^{(n)}(\mathcal{M}_1, \mathcal{M}_2) = \frac{\prod_{i=1}^n \pi(y_i|Y_{n,-i}, \mathcal{M}_1)}{\prod_{i=1}^n \pi(y_i|Y_{n,-i}, \mathcal{M}_2)}.
\]

(1.3)

In the case of independent observations, the above formula and the terminology “pseudo-Bayes factor” seem to be first proposed by Geisser and Eddy (1979). Their motivation for PBF did not seem to arise as providing solutions to the problems of BFs, however, but rather the urge to exploit the concept of cross-validation in Bayesian model selection, which had been proved to be indispensable for constructing model selection criteria in the classical statistical paradigm. Below we argue how this cross-validation idea helps solve the aforementioned problems of BFs.
First note that the posterior $\pi(\theta_j|Y_{n,-i},\mathcal{M}_j)$ is usually proper even for improper prior for $\theta_j$ is $n$ is sufficiently large. Thus, $\pi(y_i|Y_{n,-i},\mathcal{M}_j)$ given by (1.2) is usually well-defined even for improper priors, unlike $m(Y_n|\mathcal{M}_j)$. So, even though BF is ill-defined for improper priors, PBF is usually still well-defined.

Second, a clear theoretical advantage of PBF over BF is that PBF is immune to the problem of Jeffreys-Lindley-Bartlett paradox (see Gelfand and Dey (1994) for example), while BF is certainly not.

Finally, PBF enjoys significant computational advantages over BF. Note that straightforward Monte Carlo averages of $f(y_i|\theta_j,y_1,\ldots,y_{i-1},\mathcal{M}_j)$ over realizations of $\theta$ obtained from $\pi(\theta|Y_{n,-i},\mathcal{M}_j)$ by simulation techniques is sufficient to ensure good estimates of the cross-validation posterior density $\pi(y_i|Y_{n,-i},\mathcal{M}_j)$. Since $\pi(y_i|Y_{n,-i},\mathcal{M}_j)$ is the density of $y_i$ individually, the estimate is also numerically stable compared to estimates of $m(Y_n|\mathcal{M}_j)$. Hence, the sum of logarithms of the estimates of $\pi(y_i|Y_{n,-i},\mathcal{M}_j)$, for $i = 1,\ldots,n$, results in quite accurate and stable estimates of $\log \left[ \prod_{i=1}^{n} \pi(y_i|Y_{n,-i},\mathcal{M}_j) \right]$. In other words, PBF is far simpler to compute accurately than BF and is numerically far more stable and reliable.

In spite of the advantages of PBF over BF, it seems to be largely ignored in the statistical literature, both theoretically and application-wise. Some asymptotic theory of PBF has been attempted by Gelfand and Dey (1994) using independent observations, Laplace approximations and some essentially ad-hoc simplifying approximations and arguments. Application of PBF has been considered in Bhattacharya (2008) for demonstrating the superiority of his new Bayesian nonparametric Dirichlet process model over the traditional Dirichlet process mixture model. But apart from these works we are not aware of any other significant research involving PBF.

In this article, we establish the asymptotic theory for PBF in the general setup consisting of dependent observations, model misspecifications as well as covariates; inclusion of covariates also validates our asymptotic theory in the variable selection framework. Judiciously exploiting the posterior convergence treatise of Shalizi (2009) we prove almost sure exponential convergence of PBF in favour of the true model, the convergence explicitly depending upon the KL-divergence rate from the true model. For any two models different from the true model, we prove almost sure exponential convergence of PBF in favour of the better model, where the convergence depends explicitly upon the difference between KL-divergence rates from the true model. Thus, our PBF convergence results agree with the BF convergence results established in Chatterjee et al. (2018).

An important aspect of our PBF research involves establishing its convergence properties even for “inverse regression problems”, and even if one of the two competing models involve “inverse regression” and the other “forward regression”. We distinguish forward and inverse regression as follows. In forward regression problems the goal is to predict the response from a given covariate value and the rest of the data. On the other hand, in inverse regression unknown values of the covariates are to be predicted given the observed response and the rest of the data. Crucially, Bayesian inverse regression problems require priors on the covariate values to be predicted. In our case, the inverse regression setup has been motivated by the quantitative paleoclimate reconstruction problem where ‘modern data’ consisting of multivariate counts of species are available along with the observed climate values. Also available are fossil assemblages of the same species, but deposited in lake sediments for past thousands of years. This is the fossil species data. However, the past climates corresponding to the fossil species data are unknown, and it is of interest to predict the past climates given the modern data and the fossil species data. Roughly, the species composition are regarded as functions of climate variables, since in general ecological terms, variations in climate drives variations in species, but not vice versa. However, since the interest lies in prediction of climate variables, the inverse nature of the problem is clear. The past climates, which must be regarded as random variables, may also be interpreted as unobserved covariate values. It is thus natural to put a prior probability distribution on the unobserved covariate values. Various other examples of inverse regression...
problems are provided in Chatterjee and Bhattacharya (2017).

In this article, we consider two setups of inverse regression and establish almost sure exponential convergence of PBF in general inverse regression for both the setups. These include situations where one of the competing models involve forward regression and the other is associated with inverse regression.

We illustrate our asymptotic results with various theoretical examples in both forward and inverse regression contexts, including forward and inverse variable selection problems. We also follow up our theoretical investigations with simulation experiments in small samples involving Poisson and geometric forward and inverse regression models with relevant link functions and both linear regression and nonparametric regression, the latter modeled by Gaussian processes. We also illustrate variable selection in the aforementioned setups with two different covariates. The results that we obtain are quite encouraging and illuminating, providing useful insights into the behaviour of PBF for forward and inverse parametric and nonparametric regression.

The roadmap for the rest of our paper is as follows. We begin our progress by discussing and formalizing the relevant aspects of forward and inverse regression problems and the associated pseudo-Bayes factors in Section 2. Then in Section 3 we include a brief overview of Shalizi’s approach to treatment of posterior convergence which we usefully exploit for our treatise of PBF asymptotics; further details are provided in Appendix A.1. Convergence of PBF in the forward regression context is established in Section 4, while in Sections 5 and 6 we establish convergence of PBF in the two setups related to inverse regression. In Sections 7 and 8 we provide theoretical illustrations of PBF convergence in forward and inverse setups, respectively, with various examples including variable selection. Details of our simulation experiments with small samples involving Poisson and geometric linear and Gaussian process regression for relevant link functions, under both forward and inverse setups, are reported in Section 9, which also includes experiments on variable selection. Finally, we summarize our contributions and provide future directions in Section 10.

2 Preliminaries and general setup for forward and inverse regression problems

Let us first consider the forward regression setup.

2.1 Forward regression problem

For \(i = 1, \ldots , n\), let observed response \(y_i\) be related to observed covariate \(x_i\) through

\[
y_1 \sim f(\cdot | \theta, x_1) \quad \text{and} \quad y_i \sim f(\cdot | \theta, x_i, Y^{(i-1)}) \quad \text{for} \quad i = 2, \ldots , n,
\]

(2.1)

where for \(i = 2, \ldots , n\), \(Y^{(i)} = \{y_1, \ldots , y_i\}\) and \(f(\cdot | \theta, x_1), f(\cdot | \theta, x_i, Y^{(i-1)})\) are known densities depending upon (a set of) parameters \(\theta \in \Theta\), where \(\Theta\) is the parameter space, which may be infinite-dimensional. For the sake of generality, we shall consider \(\theta = (\eta, \xi)\), where \(\eta\) is a function of the covariates, which we more explicitly denote as \(\eta(x)\). The covariate \(x \in \mathcal{X}\), \(\mathcal{X}\) being the space of covariates. The part \(\xi\) of \(\eta\) will be assumed to consist of other parameters, such as the unknown error variance. For Bayesian forward regression problems, some prior needs to be assigned on the parameter space \(\Theta\). For notational convenience, we shall denote \(f(\cdot | \theta, x_1)\) by \(f(\cdot | \theta, x_1, Y^{(0)})\), so that we can represent (2.1) more conveniently as

\[
y_i \sim f(\cdot | \theta, x_i, Y^{(i-1)}) \quad \text{for} \quad i = 1, \ldots , n.
\]

(2.2)
2.1.1 Examples of the forward regression setup

(i) \( y_i \sim Bernoulli(p_i) \), where \( p_i = H(\eta(x_i)) \), where \( H \) is some appropriate link function and \( \eta \) is some function with known or unknown form. For known, suitably parameterized form, the model is parametric. If the form of \( \eta \) is unknown, one may model it by a Gaussian process, assuming adequate smoothness of the function.

(ii) \( y_i \sim Poisson(\lambda_i) \), where \( \lambda_i = H(\eta(x_i)) \), where \( H \) is some appropriate link function and \( \eta \) is some function with known (parametric) or unknown (nonparametric) form. Again, in case of unknown form of \( \eta \), the Gaussian process can be used as a suitable model under sufficient smoothness assumptions.

(iii) \( y_i = \eta(x_i) + \epsilon_i \), where \( \eta \) is a parametric or nonparametric function and \( \epsilon_i \) are iid Gaussian errors. In particular, \( \eta(x_i) \) may be a linear regression function, that is, \( \eta(x_i) = \beta'x_i \), where \( \beta \) is a vector of unknown parameters. Non-linear forms of \( \eta \) are also permitted. Also, \( \eta \) may be a reasonably smooth function of unknown form, modeled by some appropriate Gaussian process.

2.2 Forward pseudo-Bayes factor

Letting \( Y_n = \{y_i : i = 1, \ldots, n\} \), \( X_n = \{x_i : i = 1, \ldots, n\} \), \( Y_{n,-i} = Y_n \setminus \{y_i\} \) and \( X_{n,-i} = X_n \setminus \{x_i\} \), let \( \pi(y_i|Y_{n,-i}, X_n, M) \) denote the posterior density at \( y_i \), given data \( Y_{n,-i}, X_n \) and model \( M \). Let the density of \( y_i \) given \( \theta \) and \( x_i \) under model \( M \) be denoted by \( f(y_i|\theta, x_i, Y^{(i-1)}M) \). Then note that

\[
\pi(y_i|Y_{n,-i}, X_n, M) = \int_\Theta f(y_i|\theta, x_i, Y^{(i-1)}M) d\pi(\theta|Y_{n,-i}, X_{n,-i}, M),
\]

where

\[
\pi(\theta|Y_{n,-i}, X_{n,-i}, M) \propto \pi(\theta) \prod_{j\neq i=1}^{n} f(y_j|\theta, x_j, Y^{(j-1)}M).
\]

For any two models \( M_1 \) and \( M_2 \), the forward pseudo Bayes factor (FPBF) of \( M_1 \) against \( M_2 \) based on the cross-validation posteriors of the form (2.3) is defined as follows:

\[
FPBF^{(n)}(M_1,M_2) = \frac{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_1)}{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_2)},
\]

and we are interested in studying the limit \( \lim_{n \to \infty} \frac{1}{n} \log FPBF^{(n)}(M_1,M_2) \) for almost all data sequences.

2.3 Inverse regression problem: first setup

In inverse regression, the basic premise remains the same as in forward regression detailed in Section 2.1. In other words, the distribution \( f(\cdot|\theta, x_i, Y^{(i-1)}) \), parameter \( \theta \), the parameter and the covariate space remain the same as in the forward regression setup. However, unlike in Bayesian forward regression problems where a prior needs to be assigned only to the unknown parameter \( \theta \), a prior is also required for \( \tilde{x} \), the unknown covariate observation associated with known response \( \tilde{y} \), say. Given the entire dataset and \( \tilde{y} \), the problem in inverse regression is to predict \( \tilde{x} \). Hence, in the Bayesian inverse setup, a prior on \( \tilde{x} \) is necessary. Given model \( M \) and the corresponding parameters \( \theta \), we denote such prior by \( \pi(\tilde{x} | \theta, M) \). For Bayesian cross-validation in inverse problems it is pertinent to successively leave out \((y_i, x_i) \); \( i = 1, \ldots, n \), and compute the posterior predictive distribution \( \pi(\tilde{x} | Y_n, X_{n,-i}) \), from \( y_i \) and the rest of the data \((Y_{n,-i}, X_{n,-i}) \) (see Bhattacharya and Haslett (2007)). But these posteriors are not useful for Bayes of pseudo-Bayes factors even for inverse regression setups. The reason is that the Bayes
factor for inverse regression is still the ratio of posterior odds and prior odds associated with the competing models, which as usual translates to the ratio of the marginal densities of the data under the two competing models. The marginal densities depend upon the prior for \((\theta, \tilde{x})\), however, under the competing models. The pseudo-Bayes factor for inverse models is then the ratio of products of the cross-validation posteriors of \(y_i\), where \(\theta\) and \(\tilde{x}\) are marginalized out. Details of such inverse cross-validation posteriors and the definition of pseudo-Bayes factors for inverse regression are given below.

### 2.3.1 Inverse pseudo-Bayes factor in this setup

In the inverse regression setup, first note that

\[
\begin{align*}
\pi(\tilde{x}_i, \theta|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M}) &= \pi(\tilde{x}_i, \theta|\mathcal{M}) \prod_{j \neq i=1}^{n} f(y_j|\theta, x_j, Y^{(j-1)}, \mathcal{M}) \\
&= \frac{\pi(\tilde{x}_i|\theta, \mathcal{M})\pi(\theta|\mathcal{M}) \prod_{j \neq i=1}^{n} f(y_j|\theta, x_j, Y^{(j-1)}, \mathcal{M})}{\int_{\Theta} \int_{X} \prod_{j \neq i=1}^{n} f(y_j|\theta, x_j, Y^{(j-1)}, \mathcal{M}) \pi(\theta|\mathcal{M}) d\theta d\pi} \\
&= \frac{\pi(\tilde{x}_i|\theta, \mathcal{M})\pi(\theta|\mathcal{M})}{\int_{\Theta} \int_{X} \prod_{j \neq i=1}^{n} f(y_j|\theta, x_j, Y^{(j-1)}, \mathcal{M}) \pi(\theta|\mathcal{M}) d\theta d\pi} \times \pi(\tilde{x}_i|\theta, \mathcal{M})\pi(\theta|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M}).
\end{align*}
\]

(2.6)

Using (2.6) we obtain

\[
\begin{align*}
\pi(y_i|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M}) &= \int_{\Theta} \int_{X} f(y_i|\theta, \tilde{x}_i, Y^{(i-1)}, \mathcal{M}) \pi(\tilde{x}_i|\theta, \mathcal{M}) d\pi \pi(\theta|\mathcal{M}) d\pi \\
&= \int_{\Theta} g(Y^{(i)}, \theta, \mathcal{M}) d\pi \pi(\theta|\mathcal{M}) d\pi,
\end{align*}
\]

where

\[
g(Y^{(i)}, \theta, \mathcal{M}) = \int_{\Theta} f(y_i|\theta, \tilde{x}_i, Y^{(i-1)}, \mathcal{M}) d\pi \pi(\theta|\mathcal{M}) d\pi.
\]

(2.7)

and \(\pi(\theta|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M})\) is the same as (2.4). For any two models \(\mathcal{M}_1\) and \(\mathcal{M}_2\), the inverse pseudo Bayes factor (IPBF) of \(\mathcal{M}_1\) against \(\mathcal{M}_2\) based on cross-validation posteriors of the form (2.7) is given by

\[
IPBF^{(n)}(\mathcal{M}_1, \mathcal{M}_2) = \prod_{i=1}^{n} \frac{\pi(y_i|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M}_1)}{\pi(y_i|Y_{n,\theta-i},X_{n,\theta-i},\mathcal{M}_2)}.
\]

(2.9)

and our goal is to investigate \(\lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n)}(\mathcal{M}_1, \mathcal{M}_2)\) for almost all data sequences.

### 2.4 Inverse regression problem: second setup

In the inverse regression context, we consider another setup under which Chatterjee and Bhat-\text{tacharya} (2020) establish consistency of the inverse cross-validation posteriors of \(\tilde{x}_i\). Here we consider experiments with covariate observations \(x_1, x_2, \ldots, x_n\) along with responses \(Y_{nm} = \{y_{ij} : i = 1, \ldots, n, j = 1, \ldots, m\}\). In other words, the experiment considered here will allow us to have \(m\) samples of responses \(y_i = \{y_{i1}, y_{i2}, \ldots, y_{im}\}\) against each covariate observation \(x_i\), for \(i = 1, 2, \ldots, n\). Again, both \(x_i\) and \(y_{ij}\) are allowed to be multidimensional. Let \(Y_{nm,\theta-i} = Y_{nm}|\{y_i\}\).

For \(i = 1, \ldots, n\) consider the following general model setup: conditionally on \(\theta, x_i\) and
\( Y^{(i-1)}_j = \{ y_{ij}, \ldots, y_{i-1,j} \} \),

\[
y_{ij} \sim f \left( \cdot| \theta, x_i, Y^{(i-1)}_j \right); \quad j = 1, \ldots, m,
\]

independently, where \( f(\cdot| \theta, x_1, Y^{(0)}_j) = f(\cdot| \theta, x_1) \) as before.

### 2.4.1 Prior for \( \bar{x}_i \)

Following Chatterjee and Bhattacharya (2020), we consider the following prior for \( \bar{x}_i \): given \( \theta \),

\[
\bar{x}_i \sim U\left( B_{im}(\theta) \right),
\]

the uniform distribution on

\[
B_{im}(\theta) = \left\{ x : H(\eta(x)) \in \left[ \bar{y}_i - \frac{cs_i}{\sqrt{m}}, \bar{y}_i + \frac{cs_i}{\sqrt{m}} \right] \right\},
\]

where \( H \) is some suitable transformation of \( \eta(x) \). In (2.12), \( \bar{y}_i = \frac{1}{m} \sum_{j=1}^{m} y_{ij} \) and \( s_i^2 = \frac{1}{m-1} \sum_{j=1}^{m} (y_{ij} - \bar{y}_i)^2 \), and \( c \geq 1 \) is some constant. We denote this prior by \( \pi(\bar{x}_i|\eta) \). Chatterjee and Bhattacharya (2020) show that the density or any probability associated with \( \pi(\bar{x}_i|\eta) \) is continuous with respect to \( \eta \).

### 2.4.2 Examples of the prior

(i) \( y_{ij} \sim \text{Poisson} (\theta x_i) \), where \( \theta > 0 \) and \( x_i > 0 \) for all \( i \). Here, under the prior \( \pi(\bar{x}_i|\theta) \), \( \bar{x}_i \) has uniform distribution on the set \( B_{im}(\theta) = \left\{ x > 0 : \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}}}{\theta} \leq x \leq \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}}}{\theta} \right\} \).

(ii) \( y_{ij} \sim \text{Poisson} (\lambda_i) \), where \( \lambda_i = \lambda(x_i) \), with \( \lambda(x) = H(\eta(x)) \). Here \( H \) is a known, one-to-one, continuously differentiable function and \( \eta(\cdot) \) is an unknown function modeled by Gaussian process. Here, the prior for \( \bar{x}_i \) is the uniform distribution on

\[
B_{im}(\eta) = \left\{ x : \eta(x) \in H^{-1}\left\{ \left[ \bar{y}_i - \frac{cs_i}{\sqrt{m}}, \bar{y}_i + \frac{cs_i}{\sqrt{m}} \right] \right\} \right\}.
\]

(iii) \( y_{ij} \sim \text{Bernoulli}(p_i) \), where \( p_i = \lambda(x_i) \), with \( \lambda(x) = H(\eta(x)) \). Here \( H \) is a known, increasing, continuously differentiable, cumulative distribution function and \( \eta(\cdot) \) is an unknown function modeled by some appropriate Gaussian process. Here, the prior for \( \bar{x}_i \) is the uniform distribution on \( B_{im}(\eta) = \left\{ x : \eta(x) \in H^{-1}\left\{ \left[ \bar{y}_i - \frac{cs_i}{\sqrt{m}}, \bar{y}_i + \frac{cs_i}{\sqrt{m}} \right] \right\} \right\} \).

(iv) \( y_{ij} = \eta(x_i) + \epsilon_{ij} \), where \( \eta(\cdot) \) is an unknown function modeled by some appropriate Gaussian process, and \( \epsilon_{ij} \) are \( iid \) zero-mean Gaussian noise with variance \( \sigma^2 \). Here, the prior for \( \bar{x}_i \) is the uniform distribution on \( B_{im}(\eta) = \left\{ x : \eta(x) \in \left[ \bar{y}_i - \frac{cs_i}{\sqrt{m}}, \bar{y}_i + \frac{cs_i}{\sqrt{m}} \right] \right\} \).

If \( \eta(x_i) = \alpha + \beta x_i \), then the prior for \( \bar{x}_i \) is the uniform distribution on \([a, b]\), where \( a = \min \left\{ \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}} - \alpha}{\beta}, \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}} - \alpha}{\beta} \right\} \) and \( b = \max \left\{ \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}} + \alpha}{\beta}, \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}} + \alpha}{\beta} \right\} \).

Further examples of the prior in various other inverse regression models are provided in Sections 8 and 9.
2.4.3 Inverse pseudo-Bayes factor in this setup

For any two models $M_1$ and $M_2$ we define inverse pseudo-Bayes factor for model $M_1$ against model $M_2$, for any $k \geq 1$, as

$$IPBF^{(n,m,k)}(M_1,M_2) = \prod_{i=1}^n \pi(y_{ik}|Y_{nm,-i},X_{n,-i},M_1) / \prod_{i=1}^n \pi(y_{ik}|Y_{nm,-i},X_{n,-i},M_2)$$  \hspace{1cm} (2.13)$$

and study the limit $\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(M_1,M_2)$ for almost all data sequences. Note that since $\{y_{ik};k \geq 1\}$ are distributed independently as $f(\cdot|\theta,x_i,Y_{i-1}^{(i-1)})$ given any $\theta$ and $x_i$, it would follow that if the limit exists, it must be the same for all $k \geq 1$.

Suppose that the true data-generating parameter $\theta_0$ is not contained in $\Theta$, the parameter space considered. This is a case of misspecification that we must incorporate in our convergence theory of PBF. Our PBF asymptotics draws on posterior convergence theory for (possibly infinite-dimensional) parameters that also allows misspecification. In this regard, the approach presented in Shalizi (2009) seems to be very appropriate. Before proceeding further, we first provide a brief overview of this approach, which we conveniently exploit for our purpose.

3 A brief overview of Shalizi’s approach to posterior convergence

Let $Y_n = (Y_1,\ldots,Y_n)^T$, and let $f_\theta(Y_n)$ and $f_{\theta_0}(Y_n)$ denote the observed and the true likelihoods respectively, under the given value of the parameter $\theta$ and the true parameter $\theta_0$. We assume that $\theta \in \Theta$, where $\Theta$ is the (often infinite-dimensional) parameter space. However, we do not assume that $\theta_0 \in \Theta$, thus allowing misspecification. The key ingredient associated with Shalizi’s approach to proving convergence of the posterior distribution of $\theta$ is to show that the asymptotic equipartition property holds. To elucidate, let us consider the following likelihood ratio:

$$R_n(\theta) = \frac{f_\theta(Y_n)}{f_{\theta_0}(Y_n)}$$

Then, to say that for each $\theta \in \Theta$, the generalized or relative asymptotic equipartition property holds, we mean

$$\lim_{n \to \infty} \frac{1}{n} \log R_n(\theta) = -h(\theta),$$ \hspace{1cm} (3.1)

almost surely, where $h(\theta)$ is the KL-divergence rate given by

$$h(\theta) = \lim_{n \to \infty} \frac{1}{n} E_{\theta_0} \left( \log \frac{f_\theta(Y_n)}{f_{\theta_0}(Y_n)} \right),$$ \hspace{1cm} (3.2)

provided that it exists (possibly being infinite), where $E_{\theta_0}$ denotes expectation with respect to the true model. Let

$$h(A) = \text{ess inf}_{\theta \in A} h(\theta);$$

$$J(\theta) = h(\theta) - h(\Theta);$$

$$J(A) = \text{ess inf}_{\theta \in A} J(\theta).$$

Thus, $h(A)$ can be roughly interpreted as the minimum KL-divergence between the postulated and the true model over the set $A$. If $h(\Theta) > 0$, this indicates model misspecification. For $A \subset \Theta$, $h(A) > h(\Theta)$, so that $J(A) > 0$.

As regards the prior, it is required to construct an appropriate sequence of sieves $\mathcal{G}_n$ such
that $G_n \rightarrow \Theta$ and $\pi(G_n^c) \leq \alpha \exp(-\beta n)$, for some $\alpha > 0$.

With the above notions, verification of (3.1) along with several other technical conditions ensure that for any $A \subseteq \Theta$ such that $\pi(A) > 0$,

$$\lim_{n \to \infty} \pi(A|Y_n) = 0, \quad (3.3)$$

almost surely, provided that $h(A) > h(\Theta)$.

The seven assumptions of Shalizi leading to the above result, which we denote as (S1)--(S7), are provided in Appendix A.1. In what follows, we denote almost sure convergence by $\overset{a.s.}{\rightarrow}$, almost sure equality by $\overset{a.s.}{=}$, and weak convergence by $\overset{w}{\rightarrow}$.

4 Convergence of PBF in forward problems

Let $\mathcal{M}_0$ denote the true model which is also associated with parameter $\theta \in \Theta_0$, where $\Theta_0$ is a parameter space containing the true parameter $\theta_0$. Then the following result holds.

Theorem 1. Assume conditions (S1)--(S7) of Shalizi, and let the infimum of $h(\theta)$ over $\Theta$ be attained at $\tilde{\theta} \in \Theta$, where $\tilde{\theta} \neq \theta_0$. Also assume that $\Theta$ and $\Theta_0$ are complete separable metric spaces and that for $i \geq 1$, $f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M})$ and $f(y_i|\theta, x_i, Y^{(i-1)}, M_0)$ are bounded and continuous in $\theta$. Then,

$$\frac{1}{n} \log FPBF^{(n)}(\mathcal{M}, M_0) = \frac{1}{n} \log \left[ \prod_{i=1}^{n} \frac{\pi(y_i|Y_{n,-i}, X_n, \mathcal{M})}{\pi(y_i|Y_{n,-i}, X_n, M_0)} \right] \overset{a.s.}{\rightarrow} -h(\tilde{\theta}), \quad \text{as } n \to \infty, \quad (4.1)$$

where, for any $\theta$,

$$h(\theta) = \lim_{n \to \infty} \frac{1}{n} \log \left[ \sum_{i=1}^{n} \frac{f(y_i|\theta_0, x_i, Y^{(i-1)}, M_0)}{f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M})} \right]. \quad (4.2)$$

Proof. By the hypotheses, (3.3) holds, from which it follows that for any $\epsilon > 0$,

$$\lim_{n \to \infty} \pi(N_{\epsilon}^{(c)}|Y_{n,-i}, X_{n,-i}, M) = 0, \quad (4.3)$$

where $N_{\epsilon} = \{\theta : h(\theta) \leq h(\Theta) + \epsilon\}$.

Now, by hypothesis, the infimum of $h(\theta)$ over $\Theta$ be attained at $\tilde{\theta} \in \Theta$, where $\tilde{\theta} \neq \theta_0$. Then by (4.3), the posterior of $\theta$ given $Y_{n,-i}$ and $X_{n,-i}$, given by (2.4), concentrates around $\tilde{\theta}$, the minimizer of the limiting KL-divergence rate from the true distribution. Formally, given any neighborhood $U$ of $\tilde{\theta}$, the set $N_{\epsilon}$ is contained in $U$ for sufficiently small $\epsilon$. It follows that for any neighborhood $U$ of $\theta_0$, $\pi(U|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \to 1$, almost surely, as $n \to \infty$. Since $\Theta$ is a complete, separable metric space, it follows that (see, for example, Ghosh and Ramamoorthi (2003), Ghosal and van der Vaart (2017))

$$\pi(\cdot|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \overset{w}{\rightarrow} \delta_{\tilde{\theta}}(\cdot), \quad \text{almost surely, as } n \to \infty. \quad (4.4)$$

Then, due to (4.4) and the Portmanteau theorem, as $f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M})$ is bounded and continuous in $\theta$, it holds using (2.3), that

$$\pi(y_i|Y_{n,-i}, X_n, \mathcal{M}) \overset{a.s.}{\rightarrow} f(y_i|\tilde{\theta}, x_i, Y^{(i-1)}, \mathcal{M}), \quad \text{as } n \to \infty. \quad (4.5)$$

Now, due to (4.5),

$$\frac{1}{n} \sum_{i=1}^{n} \log \pi(y_i|Y_{n,-i}, X_n, \mathcal{M}) \overset{a.s.}{\rightarrow} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log f(y_i|\tilde{\theta}, x_i, Y^{(i-1)}, \mathcal{M}), \quad \text{as } n \to \infty. \quad (4.6)$$
Also, essentially the same arguments leading to (4.5) yield
\[ \pi(y_i|Y_{n,-i}, X_n, M_0) \xrightarrow{a.s.} f(y_i|\theta_0, x_i, Y^{(i-1)}, M_0), \text{ as } n \to \infty, \]
which ensures
\[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{1}{n} \sum_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_0) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log f(y_i|\theta_0, x_i, Y^{(i-1)}, M_0), \text{ as } n \to \infty. \quad (4.7) \]
From (4.6) and (4.7) we obtain
\[ \lim_{n \to \infty} \frac{1}{n} \log FPBF^{(n)}(M, M_0) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \frac{f(y_i|\tilde{\theta}, x_i, Y^{(i-1)}, M)}{f(y_i|\tilde{\theta}_0, x_i, Y^{(i-1)}, M_0)} \xrightarrow{a.s.} -h(\tilde{\theta}), \quad (4.8) \]
where the rightmost step of (4.8), given by (4.2), follows due to (3.1). Hence, the result is proved.

For postulated model \( M_j \), let the KL-divergence rate \( h \) in (3.2) be denoted by \( h_j \), for \( j \geq 1 \).

**Theorem 2.** For models \( M_0, M_1 \) and \( M_2 \) with complete separable parameter spaces \( \Theta_0, \Theta_1 \) and \( \Theta_2 \), assume conditions (S1)–(S7) of Shalizi, and for \( j = 1, 2 \), let the infimum of \( h_j(\theta) \) over \( \Theta_j \) be attained at \( \tilde{\theta}_j \in \Theta_j \), where \( \tilde{\theta}_j \neq \theta_0 \). Also assume that for \( i \geq 1 \), \( f(y_i|\theta, x_i, Y^{(i-1)}, M_j); j = 1, 2 \), and \( f(y_i|\theta, x_i, Y^{(i-1)}, M_j) \) are bounded and continuous in \( \theta \). Then,
\[ \frac{1}{n} \log FPBF^{(n)}(M_1, M_2) = \frac{1}{n} \log \left( \frac{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_1)}{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_2)} \right) \xrightarrow{a.s.} -h(\tilde{\theta}_1) - h(\tilde{\theta}_2), \text{ as } n \to \infty, \quad (4.9) \]
where, for \( j = 1, 2 \), and for any \( \theta \),
\[ h_j(\theta) = \lim_{n \to \infty} \frac{1}{n} E^{\theta_0} \left\{ \sum_{i=1}^{n} \log \frac{f(y_i|\theta, x_i, Y^{(i-1)}, M_0)}{f(y_i|\theta, x_i, Y^{(i-1)}, M_j)} \right\}. \quad (4.10) \]

**Proof.** The proof follows by noting that
\[ \frac{1}{n} \log FPBF^{(n)}(M_1, M_2) = \frac{1}{n} \log FPBF^{(n)}(M_1, M_0) - \frac{1}{n} \log FPBF^{(n)}(M_2, M_0), \]
and then using (4.1) for \( \frac{1}{n} \log FPBF^{(n)}(M_1, M_0) \) and \( \frac{1}{n} \log FPBF^{(n)}(M_2, M_0) \).

## 5 Convergence results for PBF in inverse regression: first setup

**Theorem 3.** Assume conditions (S1)–(S7) of Shalizi, and let the infimum of \( h(\theta) \) over \( \Theta \) be attained at \( \tilde{\theta} \in \Theta \), where \( \tilde{\theta} \neq \theta_0 \). Also assume that \( \Theta \) and \( \Theta_0 \) are complete separable metric spaces and that for \( i \geq 1 \), \( g(Y^{(i)}, \theta, M) \) and \( g(Y^{(i)}, \theta, M_0) \) are bounded and continuous in \( \theta \). Then,
\[ \frac{1}{n} \log IPBF^{(n)}(M, M_0) = \frac{1}{n} \log \left( \frac{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M)}{\prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_n, M_0)} \right) \xrightarrow{a.s.} -h^*(\tilde{\theta}), \text{ as } n \to \infty, \quad (5.1) \]
where, for any \( \theta \),
\[ h^*(\theta) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left( \frac{g(Y^{(i)}, \theta_0, M_0)}{g(Y^{(i)}, \theta, M)} \right), \]
provided that the limit exists.
Proof. Since \( \pi(\cdot|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \) remains the same as in Theorem 1, it follows as before that
\[
\pi(\cdot|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \xrightarrow{w} \delta_\theta(\cdot), \text{ almost surely, as } n \to \infty.
\]
Then, since \( g(y_i, \theta, \mathcal{M}) \) is bounded and continuous in \( \theta \), the above ensures in conjunction with the Portmanteau theorem using (2.7), that
\[
\pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \xrightarrow{a.s.} g(Y^{(i)}, \tilde{\theta}, \mathcal{M}), \text{ as } n \to \infty.
\]
(5.2)
Hence,
\[
\frac{1}{n} \sum_{i=1}^{n} \log \pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log g(Y^{(i)}, \tilde{\theta}, \mathcal{M}), \text{ as } n \to \infty.
\]
(5.3)
Similarly,
\[
\frac{1}{n} \sum_{i=1}^{n} \log \pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}_0) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log g(Y^{(i)}, \theta_0, \mathcal{M}_0), \text{ as } n \to \infty.
\]
(5.4)
Combining (5.3) and (5.4) yields
\[
\lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n)}(\mathcal{M}, \mathcal{M}_0) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{g(Y^{(i)}, \tilde{\theta}, \mathcal{M})}{g(Y^{(i)}, \tilde{\theta}, \mathcal{M}_0)} \right] = -h^*(\tilde{\theta}).
\]
Hence, the result is proved. \( \square \)

Remark 4. Observe that \( h^*(\tilde{\theta}) \) in Theorem 3 does not correspond to the KL-divergence rate given by (3.2), even though in the forward context, Theorem 1 shows almost convergence of \( \frac{1}{n} \log FPBF^{(n)} \) to \(-h(\tilde{\theta})\), where \( h(\tilde{\theta}) \) is the bona fide KL-divergence rate.

In Theorem 3 we have assumed that for cross-validation even in the true model \( \mathcal{M}_0, x_i \) is assumed unknown, and that a prior has been placed on the corresponding unknown random quantity \( \tilde{x}_i \). If, on the other hand, \( x_i \) is considered known for cross-validation in \( \mathcal{M}_0 \), then we have the following theorem, which is an appropriately modified version of Theorem 3.

Theorem 5. Assume conditions (S1)-(S7) of Shalizi for models \( \mathcal{M}_0 \) and \( \mathcal{M} \), and let the infimum of \( h(\theta) \) over \( \Theta \) be attained at \( \tilde{\theta} \in \Theta \), where \( \tilde{\theta} \neq \theta_0 \). Also assume that \( \Theta \) and \( \Theta_0 \) are complete separable metric spaces and that for \( i \geq 1 \), \( g(Y^{(i)}, \theta, \mathcal{M}) \) and \( f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M}_0) \) are bounded and continuous in \( \theta \). Then the following result holds if \( x_i \) is assumed known for cross-validation with respect to \( \mathcal{M}_0 \):
\[
\frac{1}{n} \log IPBF^{(n)}(\mathcal{M}, \mathcal{M}_0) = \frac{1}{n} \log \left[ \prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}) \prod_{i=1}^{n} \pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}_0) \right] \xrightarrow{a.s.} -h^*(\tilde{\theta}), \text{ as } n \to \infty,
\]
(5.5)
where, for any \( \theta \),
\[
h^*(\theta) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_i|\theta_0, x_i, Y^{(i-1)}, \mathcal{M}_0)}{g(Y^{(i)}, \theta, \mathcal{M})} \right],
\]
provided that the limit exists.

Proof. In this case, for the true model \( \mathcal{M}_0 \), the cross-validation posterior \( \pi(y_i|Y_{n,-i}, X_{n,-i}, \mathcal{M}_0) \) is of the same form as (2.3) and hence, (4.7) holds. The rest of the proof remains the same as that of Theorem 3. \( \square \)
Remark 6. Observe that $h^*(\tilde{\theta})$ in Theorem 5 is a genuine KL-divergence rate. However, this is not the same as $h(\tilde{\theta})$ of Theorem 1, which is the KL-divergence rate between $M$ and $M_0$ when all the $x_i$ are known. Since cross-validation with all $x_i$ known can occur only in the forward regression setup, convergence rates of pseudo-Bayes factors in inverse regression problems can never be associated with $h$, even though the conditions of Theorem 5 show that $\tilde{\theta}$ is the minimizer of $h$.

Theorem 7. For models $M_0$, $M_1$ and $M_2$ with complete separable parameter spaces $\Theta_0$, $\Theta_1$ and $\Theta_2$, assume conditions (S1)–(S7) of Shalizi, and for $j = 1, 2$, let the infimum of $h_j(\theta)$ over $\Theta_j$ be attained at $\tilde{\theta}_j \in \Theta_j$, where $\tilde{\theta}_j \neq \theta_0$. Also assume that for $i \geq 1$, $g(Y(i), \theta, M_j)$; $j = 1, 2$, and $f(y_i|\theta, x_i, Y(i-1), M_0)$ are bounded and continuous in $\theta$. Then, if $x_i$ is assumed known for cross-validation with respect to $M_0$, the following holds:

$$
\frac{1}{n} \log IPBF(n)(M_1, M_2) = \frac{1}{n} \log \left[ \prod_{i=1}^{n} \frac{\pi(Y_{n-i}|x_i, M_1)}{\pi(Y_{n-i}|x_i, M_2)} \right] \overset{a.s.}{\to} - h^*(\tilde{\theta}_1) - h^*(\tilde{\theta}_2), \quad \text{as } n \to \infty,
$$

(5.6)

where, for $j = 1, 2$, and for any $\theta$,

$$
h^*_j(\theta) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_i|\theta, x_i, Y(i-1), M_0)}{g(Y(i), \theta, M_j)} \right],
$$

(5.7)

provided the limit exists.

Proof. The proof follows by noting that

$$
\frac{1}{n} \log IPBF(n)(M_1, M_2) = \frac{1}{n} \log IPBF(n)(M_1, M_0) - \frac{1}{n} \log IPBF(n)(M_2, M_0),
$$

and then using (5.5) for $\frac{1}{n} \log IPBF(n)(M_1, M_0)$ and $\frac{1}{n} \log IPBF(n)(M_2, M_0)$.

Remark 8. Note that the result of Theorem 7 holds without the assumption that $\Theta_0$ is complete separable and $f(y_i|\theta, x_i, Y(i-1), M_0)$ is bounded and continuous in $\theta$, irrespective of whether or not $x_i$ is treated as known in the case of cross-validation with respect to the true model $M_0$. Indeed, assuming the rest of the conditions of Theorem 7, it holds that

$$
\frac{1}{n} \log IPBF(n)(M_1, M_2) = \frac{1}{n} \log \left[ \prod_{i=1}^{n} \frac{\pi(Y_{n-i}|x_i, M_1)}{\pi(Y_{n-i}|x_i, M_2)} \right] \overset{a.s.}{\to} - h^*(\tilde{\theta}_1 - \tilde{\theta}_2), \quad \text{as } n \to \infty,
$$

where, for any $\theta_1, \theta_2$,

$$
h^*(\theta_1, \theta_2) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{g(Y(i), \theta_2, M_2)}{g(Y(i), \theta_1, M_1)} \right],
$$

provided that the limit exists. The proof follows in the same way as in Theorem 3 by replacing $M$ and $M_0$ with $M_1$ and $M_2$. Note that $h^*(\tilde{\theta}_1, \tilde{\theta}_2)$ above is the same as $h^*(\tilde{\theta}_1) - h^*(\tilde{\theta}_2)$ of Theorem 7, but the latter is interpretable as the difference between limiting KL-divergence rates for $M_1$ and $M_2$, while the former does not admit such desirable interpretation since without the assumptions $\Theta_0$ is complete separable and $f(y_i|\theta, x_i, Y(i-1), M_0)$ is bounded and continuous in $\theta$, the convergence

$$
\frac{1}{n} \sum_{i=1}^{n} \log \pi(Y_{n-i}|x_i, M_0) \overset{a.s.}{\to} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log f(y_i|\theta_0, x_i, Y(i-1), M_0), \quad \text{as } n \to \infty,
$$

need not hold, even if $x_i$ is considered known for cross-validation with respect to $M_0$.  


6 Convergence results for PBF in inverse regression: second setup

In the misspecified situation, \( \theta_0 \notin \Theta \), and \( \hat{\theta} \) is the minimizer of the limiting KL-divergence rate from \( \theta_0 \). If \( \theta \) is thus misspecified, then as \( m \to \infty \), \( B_{im}(\hat{\theta}) \overset{a.s.}{\to} \{x_i^*\} \) for some non-random \( x_i^* (\neq x_i) \) depending upon both \( \hat{\theta} \) and \( \theta_0 \). In other words, the prior distribution of \( \hat{\theta} \) and \( y_i \) concentrates around \( x_i^* \), as \( m \to \infty \). We now state and prove our result on IPBF convergence with respect to the prior (2.11).

**Theorem 9.** Assume conditions (S1)–(S7) of Shalizi. Let the infimum of \( h(\theta) \) over \( \Theta \) be attained at \( \hat{\theta} \in \Theta \), where \( \hat{\theta} \neq \theta_0 \). Assume that \( \hat{\theta} \) and \( \theta_0 \) are one-to-one functions. Also assume that \( \Theta \) and \( \Theta_0 \) are complete separable metric spaces and that for \( i \geq 1 \) and \( k \geq 1 \), \( f(y_{ik}|\theta, \tilde{x}_i, Y_k^{(i-1)}, M) \) and \( f(y_{ik}|\theta, \tilde{x}_i, Y_k^{(i-1)}, M_0) \) are bounded and continuous in \((\theta, \tilde{x}_i)\). Then, for prior (2.11) on \( \tilde{x}_i \), the following holds for any \( k \geq 1 \):

\[
\lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(M, M_0) = \lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log \left[ \prod_{i=1}^{m} \pi(y_{ik}|Y_{nm,-i}, X_{n,-i}, M) \right] \overset{a.s.}{=} -h^*(\hat{\theta}),
\]

where

\[
h^*(\hat{\theta}) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_{ik}|\theta_0, x_i, Y_k^{(i-1)}, M_0)}{f(y_{ik}|\theta, x_i, Y_k^{(i-1)}, M_0)} \right],
\]

provided that the limit exists.

**Proof.** It follows from (2.6) that \( \pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M) = \pi(\tilde{x}_i|\theta, M)\pi(\theta|Y_{nm,-i}, X_{n,-i}, M) \),

Hence, letting \( U_i \times V \) be any neighborhood of \((x_i^*, \theta)\), we have

\[
\pi(\tilde{x}_i \in U_i, \theta \in V|Y_{nm,-i}, X_{n,-i}, M) = \int_V \pi(\tilde{x}_i \in U_i|\theta, M)d\pi(\theta|Y_{nm,-i}, X_{n,-i}, M) \quad (6.2)
\]

Since \( \pi(\cdot|Y_{n,-i}, X_{n,-i}, M) \overset{w}{\to} \delta_{\hat{\theta}}(\cdot) \), as \( n \to \infty \), for any \( m \geq 1 \), and since \( \pi(\tilde{x}_i \in U_i|\theta, M) \) is bounded (since it is a probability) and continuous in \( \theta \) by Lemma 4.1 of Chatterjee and Bhattacharya (2020), by the Portmanteau theorem it follows from (6.2) that for \( m \geq 1 \),

\[
\pi(\tilde{x}_i \in U_i, \theta \in V|Y_{nm,-i}, X_{n,-i}, M) \overset{a.s.}{\to} \pi(\tilde{x}_i \in U_i|\hat{\theta}, M), \quad \text{as} \quad n \to \infty.
\]

(6.3)

Now, since \( B_{im}(\hat{\theta}) \overset{a.s.}{\to} \{x_i^*\} \) as \( m \to \infty \) since \( \hat{\theta} \) is one-to-one, it follows that there exists \( m_0 \geq 1 \) such that for \( m \geq m_0 \), \( B_{im}(\hat{\theta}) \subset U_i \). Hence,

\[
\pi(\tilde{x}_i \in U_i|\hat{\theta}, M) \overset{a.s.}{\to} 1, \quad \text{as} \quad m \to \infty.
\]

(6.4)

Combining (6.3) and (6.4) yields

\[
\pi(\tilde{x}_i \in U_i, \theta \in V|Y_{nm,-i}, X_{n,-i}, M) \overset{a.s.}{\to} 1, \quad \text{as} \quad m \to \infty, \quad n \to \infty.
\]

(6.5)

From (6.5) it follows thanks to complete separability of \( \mathcal{X} \) and \( \Theta \), that

\[
\pi(\cdot|Y_{nm,-i}, X_{n,-i}, M) \overset{w}{\to} \delta_{(x_i^*, \hat{\theta})}(\cdot), \quad \text{as} \quad m \to \infty, \quad n \to \infty.
\]

(6.6)

Since \( \pi(y_{ik}|Y_{nm,-i}, X_{n,-i}, M) = \int_{\mathcal{X}} \int_{\Theta} f(y_{ik}|\theta, \tilde{x}_i, Y_k^{(i-1)}, M)d\pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M), \) and \( f(y_{ik}|\theta, \tilde{x}_i, Y_k^{(i-1)}, M) \) is bounded and continuous in \((\theta, \tilde{x}_i)\), it follows using (6.6) and the Portmanteau theorem, that

\[
\pi(y_{ik}|Y_{nm,-i}, X_{n,-i}, M) \overset{a.s.}{\to} f(y_{ik}|\hat{\theta}, x_i^*, Y_k^{(i-1)}, M), \quad \text{as} \quad m \to \infty, \quad n \to \infty.
\]

(6.7)
Hence,
\[
\frac{1}{n} \sum_{i=1}^{n} \log \pi(y_{ik} | Y_{nm,-i}, X_{n,-i}, M) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log f(y_{ik} | \tilde{\theta}, x_i^*, Y_k^{(i-1)}, M), \text{ as } m \to \infty, n \to \infty.
\]  
(6.8)

In the same way,
\[
\frac{1}{n} \sum_{i=1}^{n} \log \pi(y_{ik} | Y_{nm,-i}, X_{n,-i}, M_0) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log f(y_{ik} | \theta_0, x_i, Y_k^{(i-1)}, M_0), \text{ as } m \to \infty, n \to \infty.
\]  
(6.9)

Combining (6.8) and (6.9) yields
\[
\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(M, M_0) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_{ik} | \tilde{\theta}, x_i^*, Y_k^{(i-1)}, M)}{f(y_{ik} | \theta_0, x_i, Y_k^{(i-1)}, M_0)} \right] = -h^*(\tilde{\theta}),
\]
thereby proving the result. □

**Remark 10.** Theorem 9 assumes that for $M_0$, cross-validation is carried out assuming $x_i$ is unknown. However, as is clear from the proof, the same result continues to hold even if $x_i$ is treated as known.

**Theorem 11.** For models $M_0$, $M_1$ and $M_2$ with complete separable parameter spaces $\Theta_0$, $\Theta_1$ and $\Theta_2$, assume conditions (S1)–(S7) of Shalizi and for $j = 1, 2$, let the infimum of $h_j(\theta)$ over $\Theta_j$ be attained at $\tilde{\theta}_j \in \Theta_j$, where $\tilde{\theta}_j \neq \theta_0$. Consider the prior (2.11) on $\tilde{\theta}_i$ and let $B_{lim}(\tilde{\theta}_j) \xrightarrow{a.s.} \{x^*_i\}$, for $j = 1, 2$. Also assume that for $i \geq 1$ and $k \geq 1$, $f(y_{ik} | \tilde{\theta}_i, X^{(i-1)}, M_j)$; $j = 1, 2$, and $f(y_{ik} | \tilde{\theta}_i, X_i, Y^{(i-1)}, M_0)$ are bounded and continuous in $(\theta, \tilde{\theta}_i)$, in addition to the conditions that $\theta_0$ and $\tilde{\theta}_j$; $j = 1, 2$, are one-to-one. Then, the following holds for any $k \geq 1$:

\[
\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(M_1, M_2)
= \lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log \left[ \prod_{i=1}^{n} \pi(y_{ik} | Y_{nm,-i}, X_{n,-i}, M_1) \right] \xrightarrow{a.s.} - \left[ h_1^*(\tilde{\theta}_1) - h_2^*(\tilde{\theta}_2) \right],
\]  
(6.10)

where, for $j = 1, 2$, and for any $\theta$,
\[
h_j^*(\theta) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_{ik} | \theta_0, x_i, Y_k^{(i-1)}, M_0)}{f(y_{ik} | \theta, x^*_i, Y_k^{(i-1)}, M_j)} \right],
\]  
(6.11)

provided the limit exists.

**Proof.** The proof follows by noting that
\[
\frac{1}{n} \log IPBF^{(n,m,k)}(M_1, M_2) = \frac{1}{n} \log IPBF^{(n,m,k)}(M_1, M_0) - \frac{1}{n} \log IPBF^{(n,m,k)}(M_2, M_0),
\]

and then using (6.1) for $\frac{1}{n} \log IPBF^{(n,m,k)}(M_1, M_0)$ and $\frac{1}{n} \log IPBF^{(n,m,k)}(M_2, M_0)$.

**Remark 12.** As in Remark 8 note that the result of Theorem 11 holds without the assumption that $\Theta_0$ is complete separable and $f(y_{ik} | \tilde{\theta}_i, X^{(i-1)}, M_0)$ is bounded and continuous in $(\theta, \tilde{\theta}_i)$ for $k \geq 1$, irrespective of whether or not $x_i$ is treated as known for cross-validation with respect to $M_0$. In this case, assuming the rest of the conditions of Theorem 11, it holds for any $k \geq 1$,.

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that

\[
\lim_{n \to \infty} \lim_{m \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(\mathcal{M}_1, \mathcal{M}_2) = \lim_{n \to \infty} \lim_{m \to \infty} \frac{1}{n} \log \left[ \prod_{i=1}^{n} \pi(y_{ik} | Y_{nm,-i}, X_{nm,-i}, \mathcal{M}_1) \right] \leq -h^*(\tilde{\theta}_1, \tilde{\theta}_2),
\]

where, for any \(\theta_1, \theta_2,\)

\[
h^*(\theta_1, \theta_2) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(y_{ik}|\theta_2, x_{i2}, Y_k^{(i-1)}, \mathcal{M}_2)}{f(y_{ik}|\theta_1, x_{i1}, Y_k^{(i-1)}, \mathcal{M}_1)} \right],
\]

provided that the limit exists. As in Remark 8, again \(h^*(\tilde{\theta}_1, \tilde{\theta}_2)\) above is the same as \(h^*(\tilde{\theta}_1) - h^*(\tilde{\theta}_2)\) of Theorem 11, although, unlike the latter, the former need not be interpretable as the difference between limiting KL-divergence rates for \(\mathcal{M}_1\) and \(\mathcal{M}_2\).

7 Illustrations of PBF convergence in forward regression problems

7.1 Forward linear regression model

Let

\[
\mathcal{M}_1 : y_i = \alpha + \beta x_i + \epsilon_i; \quad i = 1, \ldots, n, \tag{7.1}
\]

where \(\epsilon_i \sim N(0, \sigma^2)\) independently, for \(i = 1, \ldots, n\). Here \(\theta = (\alpha, \beta, \sigma^2)\) is the unknown set of parameters. Let the parameter space be \(\Theta = \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+\). Clearly, \(\Theta\) is complete and separable.

Also let

\[
\mathcal{M}_0 : y_i = \eta_0(x_i) + \epsilon_i; \quad i = 1, \ldots, n, \tag{7.2}
\]

where \(\eta_0(x)\) is the true, non-linear function of \(x\), which is also continuous, and \(\epsilon_i \sim N(0, \sigma_0^2)\) independently, for \(i = 1, \ldots, n\). In this case, the covariate space, is compact, under both \(\mathcal{M}_1\) and \(\mathcal{M}_0\).

7.1.1 Verification of the assumptions

From (7.1) it is clear that \(f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M}_1) = f(y_i|\theta, x_i, \mathcal{M}_1)\) is bounded and continuous in \(\theta\), and the true model \(f(y_i|x_i, Y^{(i-1)}, \mathcal{M}_0) = f(y_i|x_i, \mathcal{M}_0)\) is devoid of any parameters. Consequently, in this case, \(\pi(y_i|Y_{n,-i}, X_n, \mathcal{M}_0) \equiv f(y_i|x_i, \mathcal{M}_0)\).

We are now left to verify the seven assumptions of Shalizi. First note from the forms of (7.1) and (7.2) that measurability of \(R_n(\theta)\) clearly holds, so that the first assumption of Shalizi, namely, (S1) is satisfied.

Now,

\[
\frac{1}{n} \log \prod_{i=1}^{n} f(y_i|\theta, x_i, \mathcal{M}_1) = -\frac{1}{2} \log 2\pi \sigma^2 - \frac{1}{2\sigma^2 n} \sum_{i=1}^{n} (y_i - \eta_0(x_i))^2 - \frac{1}{2\sigma^2 n} \sum_{i=1}^{n} (\eta_0(x_i) - \alpha - \beta x_i)^2
\]

\[
- \frac{1}{\sigma_0^2 n} \sum_{i=1}^{n} (y_i - \eta_0(x_i)) (\eta_0(x_i) - \alpha - \beta x_i). \tag{7.3}
\]

In (7.3),

\[
\frac{1}{n} \sum_{i=1}^{n} (y_i - \eta_0(x_i))^2 \xrightarrow{a.s.} \sigma_0^2, \quad \text{as } n \to \infty, \tag{7.4}
\]
and letting \(|\mathcal{X}|\) denote the Lebesgue measure of the compact space \(\mathcal{X}\),
\[
\frac{1}{n} \sum_{i=1}^{n} (\eta_0(x_i) - \alpha - \beta x_i)^2 \to |\mathcal{X}|^{-1} \int_{\mathcal{X}} (\eta_0(x) - \alpha - \beta x)^2 \, dx, \quad n \to \infty, \tag{7.5}
\]
since the former is a Riemann sum. Also, letting \(E_0\) and \(V_0\) denote the mean and variance under model \(\mathcal{M}_0\), we see that for all \(n \geq 1\),
\[
E_0 \left[ \frac{1}{n} \sum_{i=1}^{n} (y_i - \eta_0(x_i)) (\eta_0(x_i) - \alpha - \beta x_i) \right] = 0, \tag{7.6}
\]
and
\[
\sum_{i=1}^{\infty} V_0 \left[ \frac{(y_i - \eta_0(x_i)) (\eta_0(x_i) - \alpha - \beta x_i)}{\sigma_\theta^2} \right] \leq \sigma_\theta^2 \sup_{x \in \mathcal{X}} (\eta_0(x) - \alpha - \beta x)^2 \sum_{i=1}^{\infty} \frac{1}{\sigma_i^2} < \infty. \tag{7.7}
\]
From (7.6) and (7.7), it follows from Kolmogorov’s strong law of large numbers for independent but non-identical random variables,
\[
\frac{1}{n} \sum_{i=1}^{n} (y_i - \eta_0(x_i)) (\eta_0(x_i) - \alpha - \beta x_i) \overset{a.s.}{\longrightarrow} 0, \quad n \to \infty. \tag{7.8}
\]
Applying (7.4), (7.5) and (7.8) to (7.3) yields
\[
\frac{1}{n} \log \prod_{i=1}^{n} f(y_i|x_i, \mathcal{M}_1) \overset{a.s.}{\longrightarrow} - \frac{1}{2} \log 2\pi \sigma_\theta^2 - \frac{1}{2} \sup_{x \in \mathcal{X}} (\eta_0(x) - \alpha - \beta x)^2 \int_{\mathcal{X}} \, dx, \quad n \to \infty. \tag{7.9}
\]
Now observe that for the true model \(\mathcal{M}_0\),
\[
\frac{1}{n} \log \prod_{i=1}^{n} f(y_i|x_i, \mathcal{M}_0) = - \frac{1}{2} \log 2\pi \sigma_0^2 - \frac{1}{2} \sum_{i=1}^{n} (y_i - \eta_0(x_i))^2 \overset{a.s.}{\longrightarrow} - \frac{1}{2} \log 2\pi \sigma_0^2 - \frac{1}{2}, \quad n \to \infty. \tag{7.10}
\]
From (7.9) and (7.10) we have, for \(\theta \in \Theta\),
\[
\frac{1}{n} \log R_n(\theta) \overset{a.s.}{\longrightarrow} - h_1(\theta),
\]
where
\[
h_1(\theta) = \frac{1}{2} \log \left( \frac{\sigma_\theta^2}{\sigma_0^2} \right) + \frac{\sigma_0^2}{2\sigma_\theta^2} + \frac{|\mathcal{X}|^{-1}}{2\sigma_\theta^2} \int_{\mathcal{X}} (\eta_0(x) - \alpha - \beta x)^2 \, dx - \frac{1}{2}. \tag{7.11}
\]
Hence, (S3) of Shalizi holds.

It is easy to see by taking the limits of the expectations of \(\frac{1}{n} \log \prod_{i=1}^{n} f(y_i|x_i, \mathcal{M}_1)\) and \(\frac{1}{n} \log \prod_{i=1}^{n} f(y_i|x_i, \mathcal{M}_0)\), that the following also holds:
\[
\lim_{n \to \infty} \frac{1}{n} E_0 \left[ \log R_n(\theta) \right] = -h_1(\theta). \]
In other words, (S2) holds.

Note that \(h_1(\theta) < \infty\) almost surely if under the priors for \(\alpha, \beta, \sigma_\theta^2, |\alpha| < \infty, |\beta| < \infty\) and \(0 < \sigma_\theta^2 < \infty\), almost surely. Hence, (S4) holds.

Let
\[
\mathcal{G}_n = \left\{ \theta \in \Theta : |\alpha| \leq \exp (\gamma n), |\beta| \leq \exp (\gamma n), \sigma_\theta^{-2} \leq \exp (\gamma n) \right\}, \tag{7.12}
\]
where \(\gamma > 2h(\Theta)\). Then \(\mathcal{G}_n \uparrow \Theta\), as \(n \to \infty\).
Let us assume that the prior for \((\alpha, \beta, \sigma^{-2})\) is such that the prior expectations \(E(|\alpha|), E(|\beta|)\) and \(E(\sigma^{-2})\) are finite. Then under such priors, using Markov’s inequality, the probabilities \(P(|\alpha| > \exp(\gamma n))\), \(P(|\beta| > \exp(\gamma n))\) and \(P(\sigma^{-2} > \exp(\gamma n))\) are bounded above as follows:

\[
P(|\alpha| > \exp(\gamma n)) < E(|\alpha|) \exp(-\gamma n); \quad (7.13)
\]
\[
P(|\beta| > \exp(\gamma n)) < E(|\beta|) \exp(-\gamma n); \quad (7.14)
\]
\[
P(\sigma^{-2} > \exp(\gamma n)) < E(\sigma^{-2}) \exp(-\gamma n). \quad (7.15)
\]

From (7.12) and the inequalities (7.13), (7.14) and (7.15) it follows that

\[
\pi(G_n) \geq 1 - (P(|\alpha| > \exp(\gamma n)) + P(|\beta| > \exp(\gamma n)) + P(\sigma^{-2} > \exp(\gamma n))) \\
\geq 1 - (E(|\alpha|) + E(|\beta|) + E(\sigma^{-2})) \exp(-\gamma n). \quad (7.16)
\]

Thus, (S5)(1) holds.

The differential of \(\frac{1}{n} \log R_n(\theta)\) is continuous in \(\theta\), and since \(X\) is compact, it is easy to see that the differential is almost surely bounded on any compact subset \(G\) of \(\Theta\), as \(n \to \infty\). That is, \(\frac{1}{n} \log R_n(\theta)\) is almost surely Lipschitz, hence, equicontinuous on \(G\). Since \(\frac{1}{n} \log R_n(\theta)\) almost surely converges to \(-h_1(\theta)\) pointwise, as \(n \to \infty\), it holds due to the stochastic Ascoli lemma that

\[
\limsup_{n \to \infty} \sup_{\theta \in G} \left| \frac{1}{n} \log R_n(\theta) + h_1(\theta) \right| = 0, \text{ almost surely.} \quad (7.17)
\]

Since for any \(n \geq 1\), \(G_n\) is compact, (S5)(2) holds.

Since \(h_1(\theta)\) is continuous in \(\theta\), \(G_n\) is compact and \(h(G_n)\) is non-increasing in \(n\), (S5)(3) holds. Also, for any set \(A\) such that \(\pi(A) > 0\), since \(G_n \cap A\) increases to \(A\), it follows due to continuity of \(h_1(\theta)\) that \(h(G_n \cap A)\) decreases to \(h_1(A)\), so that (S7) holds.

Regarding verification of (S6), observe that the aim of assumption (S6) is to ensure that (see the proof of Lemma 7 of Shalizi (2009)) for every \(\varepsilon > 0\) and for all \(n\) sufficiently large,

\[
\frac{1}{n} \log \int_{G_n} R_n(\theta) d\pi(\theta) \leq -h(G_n) + \varepsilon, \text{ almost surely.}
\]

Since \(h(G_n) \to h(\Theta)\) as \(n \to \infty\), it is enough to verify that for every \(\varepsilon > 0\) and for all \(n\) sufficiently large,

\[
\frac{1}{n} \log \int_{G_n} R_n(\theta) d\pi(\theta) \leq -h(\Theta) + \varepsilon, \text{ almost surely.}
\]

In other words, it is sufficient to verify that

\[
\limsup_{n \to \infty} \frac{1}{n} \log \int_{G_n} R_n(\theta) \pi(\theta) d\theta \leq -h(\Theta), \text{ almost surely.} \quad (7.18)
\]

Theorem 27 stated and proved in Appendix B provides sufficient conditions for (7.18) to hold in general with proper priors on the parameters. We now make use of Theorem 27 of Appendix B to validate (S6) of Shalizi. For any function \(g(x)\) on \(X\), let us consider the notation

\[
E_X [g(X)] = |X|^{-1} \int_X g(x) dx. \quad (7.19)
\]

Note that (7.19) is indeed the expectation of \(g(X)\) with respect to the uniform distribution on the compact set \(X\).
Now observe that \( h_1(\theta) \) is uniquely minimized by
\[
\hat{\beta} = \frac{E_X [(X - E_X(X))((\eta_0(X) - E(\eta_0(X)))]}{E_X(X - E_X(X))^2}; \quad (7.20)
\]
\[
\hat{\alpha} = E_X(\eta_0(X)) - \hat{\beta}E_X(X); \quad (7.21)
\]
\[
\hat{\sigma}_\epsilon^2 = \sigma_0^2 + E_X \left( \eta_0(X) - \hat{\alpha} - \hat{\beta}X \right)^2. \quad (7.22)
\]

Now, letting \( \bar{x}_n = \frac{\sum_{i=1}^n x_i}{n}, \bar{y}_n = \frac{\sum_{i=1}^n y_i}{n} \) and \( \bar{\eta}_n = \frac{\sum_{i=1}^n \eta_i(x_i)}{n} \), we see that \( \frac{1}{n} \log R_n(\theta) \) is minimized at
\[
\tilde{\beta}_n = \frac{\sum_{i=1}^n (y_i - \bar{y}_n)(x_i - \bar{x}_n)}{\sum_{i=1}^n (x_i - \bar{x}_n)^2}, \quad (7.23)
\]
\[
\tilde{\alpha}_n = \bar{y}_n - \tilde{\beta}_n \bar{x}_n; \quad (7.24)
\]
\[
\tilde{\sigma}_n^2 = \frac{1}{n} \left[ \sum_{i=1}^n (y_i - \eta_0(x_i))^2 + \sum_{i=1}^n (\eta_0(x_i) - \tilde{\alpha}_n - \tilde{\beta}_n x_i)^2 \right. \]
\[
\left. + 2 \sum_{i=1}^n (y_i - \eta_0(x_i))(\eta_0(x_i) - \tilde{\alpha}_n - \tilde{\beta}_n x_i) \right]. \quad (7.25)
\]

Using Kolmogorov’s strong law of large numbers and Riemann sum convergence, we see that
\[
\tilde{\beta}_n \xrightarrow{a.s.} \tilde{\beta}; \quad (7.26)
\]
where \( \tilde{\beta} \) is given by (7.20).

By (7.26), and since \( \bar{y}_n \xrightarrow{a.s.} E_X(\eta_0(X)), \bar{x}_n \rightarrow E_X(X) \), it follows that
\[
\tilde{\alpha}_n \xrightarrow{a.s.} \tilde{\alpha}, \quad (7.27)
\]
where \( \tilde{\alpha} \) is given by (7.21).

For the convergence of \( \tilde{\sigma}_n^2 \) given by (7.25), first observe that the first term on the right hand side of (7.25) converges almost surely to \( \sigma_0^2 \). The \( i \)-th term of the second term on the right hand side converges to \((\eta_0(x_i) - \tilde{\alpha} - \tilde{\beta}x_i)^2 \) almost surely, so that the second term converges to \( E_X(\eta_0(X) - \tilde{\alpha} - \tilde{\beta}X)^2 \). The \( i \)-th term of the third term on the right hand side converges almost surely to \( 2(y_i - \eta_0(x_i))(\eta_0(x_i) - \tilde{\alpha} - \tilde{\beta}x_i) \), so that the third term converges to zero almost surely due to (7.8). It follows that
\[
\tilde{\sigma}_n^2 \xrightarrow{a.s.} \tilde{\sigma}_\epsilon^2, \quad (7.28)
\]
where \( \tilde{\sigma}_\epsilon^2 \) is given by (7.22). Combining (7.26), (7.27) and (7.28) yields
\[
\tilde{\theta}_n = \left( \tilde{\alpha}_n, \tilde{\beta}_n, \tilde{\sigma}_n^2 \right) \xrightarrow{a.s.} \left( \tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}_\epsilon^2 \right) = \tilde{\theta}, \text{ as } n \rightarrow \infty. \quad (7.29)
\]

In other words, we have shown that conditions (i) and (ii) of Theorem 27 hold. Since we have already shown pointwise almost sure convergence of \( \frac{1}{n} \log R_n(\theta) \) to \( -h_1(\theta) \) in the context of verifying (S3) and stochastic equicontinuity of \( \frac{1}{n} \log R_n(\theta) \) on compact subsets of \( \Theta \) in the context of verifying (S5)(2), all the conditions of Theorem 27 go through with proper prior for \( \theta \). Hence (7.18), and consequently, (S6), holds.

With these, it is seen that the conditions of Theorem 1 are satisfied, which leads to the following specialized version of the theorem:

**Theorem 13.** Consider the linear regression model \( M_1 \) given by (7.1) and the true, non-linear model \( M_0 \) given by (7.2). Assume the parameter space \( \Theta \) associated with model \( M_1 \) be \( \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+ \), and let the covariate space \( X \) be compact. Then (4.1) holds for \( \frac{1}{n} \log FPBF^{(n)}(M_1, M_0) \),
where for $\theta \in \Theta$, $h(\theta) = h_1(\theta)$ is given by (7.11), and $\tilde{\theta} = (\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}_\epsilon^2)$, where $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\sigma}_\epsilon^2$ are given by (7.21), (7.20) and (7.22), respectively.

7.2 Forward quadratic regression model

Now consider the following model on quadratic regression which may be regarded as a competitor to linear regression:

$$M_2 : y_i = \alpha + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i; \quad i = 1, \ldots, n,$$

(7.30)

where $\epsilon_i \sim N(0, \sigma^2_\epsilon)$ independently, for $i = 1, \ldots, n$. Here $\theta = (\alpha, \beta_1, \beta_2, \sigma^2_\epsilon)$ is the unknown set of parameters, and the parameter space is $\Theta = \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+.$

In this case,

$$\frac{1}{n} \log R_n(\theta) \xrightarrow{a.s.} -h_2(\theta),$$

where

$$h_2(\theta) = \frac{1}{2} \log \left( \frac{\sigma^2_\epsilon}{\sigma^2_0} \right) + \frac{\sigma^2_0}{2\sigma^2_\epsilon} + \frac{|\mathcal{X}|^{-1}}{2\sigma^2_\epsilon} \int_{\mathcal{X}} (\eta_0(x) - \alpha - \beta_1 x - \beta_2 x^2)^2 dx - \frac{1}{2},$$

(7.31)

It is easy to see that $h_2(\theta)$ is uniquely minimized at $\tilde{\theta} = (\tilde{\alpha}, \tilde{\beta}_1, \tilde{\beta}_2)$, given by

$$\tilde{\vartheta} = A^{-1} b,$$

(7.32)

where

$$A = \begin{pmatrix} 1 & E_X(X) & E_X(X^2) \\ E_X(X) & E_X(X^2) & E_X(X^3) \\ E_X(X^2) & E_X(X^3) & E_X(X^4) \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} E_X(\eta_0(X)) \\ E_X(X\eta_0(X)) \\ E_X(X^2\eta_0(X)) \end{pmatrix},$$

(7.33)

and

$$\tilde{\sigma}_\epsilon^2 = \sigma^2_0 + E_X \left( \eta_0(X) - \tilde{\alpha} - \tilde{\beta}_1 X - \tilde{\beta}_2 X^2 \right)^2.$$

(7.34)

That $A$ in (7.33) is invertible, will be shown shortly.

The maximizer of $\frac{1}{n} \log R_n(\theta)$ here is given by the least squares estimators $\tilde{\vartheta}_n^* = (\tilde{\alpha}_n, \tilde{\beta}_1^*_n, \tilde{\beta}_2^*_n)$ given by

$$\tilde{\vartheta}_n^* = A_n^{-1} b_n,$$

(7.35)

where

$$A_n = n^{-1} \begin{pmatrix} \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 \\ \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 & \sum_{i=1}^n x_i^4 \\ \sum_{i=1}^n x_i^3 & \sum_{i=1}^n x_i^4 & \sum_{i=1}^n x_i^5 \end{pmatrix} \quad \text{and} \quad b_n = n^{-1} \begin{pmatrix} \sum_{i=1}^n \eta_0(x_i) \\ \sum_{i=1}^n x_i \eta_0(x_i) \\ \sum_{i=1}^n x_i^2 \eta_0(x_i) \end{pmatrix},$$

(7.36)

and

$$\tilde{\sigma}_n^2 = \frac{1}{n} \left[ \sum_{i=1}^n (y_i - \eta_0(x_i))^2 + \sum_{i=1}^n \left( \eta_0(x_i) - \tilde{\alpha}_n - \tilde{\beta}_1^*_n x_i - \tilde{\beta}_2^*_n x_i^2 \right)^2 
+ 2 \sum_{i=1}^n (y_i - \eta_0(x_i)) \left( \eta_0(x_i) - \tilde{\alpha}_n - \tilde{\beta}_1^*_n x_i - \tilde{\beta}_2^*_n x_i^2 \right) \right].$$

(7.37)

Now note that $A_n$ in (7.36) corresponds to the so-called Vandermonde design matrix (see, for example, Macon and Spitzbart (1958)) associated with the least squares quadratic regression. The design matrix if of full rank if all the $x_i$ are distinct, which we assume. Hence, for all $n \geq 3$, $A_n$ is invertible, which makes the least squares estimators $\tilde{\vartheta}_n^*$, given by (7.35), well-defined, for
all $n \geq 3$. Now observe that by Riemann sum convergence,
\begin{align}
A_n & \xrightarrow{a.s.} A, \text{ as } n \to \infty, \text{ and } \\
b_n & \xrightarrow{a.s.} b, \text{ as } n \to \infty.
\end{align} \tag{7.38}
(7.39)

Since $A_n$ is invertible for every $n \geq 3$, $A$ must also be invertible, since (7.38) holds. Hence, $\tilde{\vartheta}$ given by (7.32), is well-defined.

Now, thanks to (7.38) and (7.39), we have
\[\tilde{\vartheta}^* \xrightarrow{a.s.} \vartheta, \text{ as } n \to \infty,\]
and also in the same way as for model $M_1$, here also,
\[\tilde{\sigma}^2 \xrightarrow{a.s.} \tilde{\sigma}^2, \text{ as } n \to \infty.\]
In other words,
\[\tilde{\theta}^* \xrightarrow{a.s.} \tilde{\theta}, \text{ as } n \to \infty,\]
even for model $M_2$.

For this quadratic regression model, let
\[G_n = \{ \theta \in \Theta : |\alpha| \leq \exp(\gamma n), |\beta_1| \leq \exp(\gamma n), |\beta_2| \leq \exp(\gamma n), \sigma^2 \leq \exp(\gamma n) \},\]
where $\gamma > 2h(\Theta)$. Then $G_n \uparrow \Theta$, as $n \to \infty$, and the rest of the assumptions of Shalizi are easily seen to be satisfied. The condition of boundedness and continuity of $f(y_i|\theta, x_i, M_2)$ are also clearly satisfied.

We summarize our results on FPBF consistency in favour of $M_0$ when the data is modeled by $M_2$ as follows.

**Theorem 14.** Consider the quadratic regression model $M_2$ given by (7.30) and the true, non-linear model $M_0$ given by (7.2). Assume the parameter space $\Theta$ associated with model $M_2$ be $\mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+$, and let the covariate space $\mathcal{X}$ be compact. Also assume that $x_i; i \geq 1$ are all distinct. Then (4.1) holds for $\frac{1}{n} \log FPBF(\mathcal{M}_2, \mathcal{M}_0)$, where for $\theta \in \Theta$, $h(\theta) = h_2(\tilde{\theta})$ is given by (7.31), and $\tilde{\theta} = (\tilde{\alpha}, \tilde{\beta}_1, \tilde{\beta}_2, \tilde{\sigma}^2)$, where $\tilde{\alpha}, \tilde{\beta}_1, \tilde{\beta}_2$ and $\tilde{\sigma}^2$ are given by (7.32) and (7.34).

**7.3 Asymptotic comparison of forward linear and quadratic models with FPBF**

Theorems 13 and 14 show almost sure exponential convergence of FPBF in favour of the true model $M_0$ given by (7.2) when the postulated models are either the forward linear or quadratic regression model. Now, if the goal is to make asymptotic comparison between the linear and quadratic regression models, then the aforementioned theorems ensure the following result:

**Theorem 15.** Let the true model be given by $M_0$ formulated in (7.2). Assuming that the covariate observations $x_i; i \geq 1$ are all distinct and that the covariate space $\mathcal{X}$ is compact, consider comparison of the linear and quadratic regression models $M_1$ and $M_2$ given by (7.1) and (7.30), respectively. Let $\tilde{\theta}_1$ and $\tilde{\theta}_2$ be the unique minimizers of $h_1$ and $h_2$. Then,
\[
\frac{1}{n} \log FPBF(\mathcal{M}_1, \mathcal{M}_2) \xrightarrow{a.s.} - \left( h_1(\tilde{\theta}_1) - h_2(\tilde{\theta}_2) \right), \text{ as } n \to \infty.
\]
7.4 FPBF asymptotics for variable selection in autoregressive time series regression

Let us consider the following first order autoregressive (AR(1)) time series linear regression as model $M_1$:

$$y_t = \rho_1 y_{t-1} + \beta_1 x_t + \epsilon_{1t}; \quad t = 1, \ldots, n,$$

(7.40)

where $y_0 \equiv 0$; $t = 1, \ldots, n$ are covariate observations associated with variable $x$ and $\epsilon_{1t} \overset{iid}{\sim} N(0, \sigma_1^2)$. Here $\theta_1 = (\rho_1, \beta_1, \sigma_1^2)$ is the set of unknown parameters and $\Theta_1 = \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+$ is the parameter space. We might wish to compare this model with another AR(1) regression model with covariate $z$ different from $x$. This model, which we refer to as $M_2$, is given as follows:

$$y_t = \rho_2 y_{t-1} + \beta_2 z_t + \epsilon_{2t}; \quad t = 1, \ldots, n,$$

(7.41)

where $y_0 \equiv 0$; $t = 1, \ldots, n$ are observations associated with covariate $z$ different from $x$ and $\theta_2 = (\rho_2, \beta_2, \sigma_2^2)$ is the set of parameters and the parameter space $\Theta_2 = \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+$ remains the same as $\Theta_1$. Here, for $t = 1, \ldots, n$, $\epsilon_{2t} \overset{iid}{\sim} N(0, \sigma_2^2)$. Let the true model $M_0$ be given by

$$y_t = \rho_0 y_{t-1} + \beta_0 (x_t + z_t) + \epsilon_{0t}; \quad t = 1, \ldots, n,$$

(7.42)

where $|\rho_0| < 1$ and $\epsilon_{0t} \overset{iid}{\sim} N(0, \sigma_0^2)$, for $t = 1, \ldots, n$.

Our goal in this example is to compare models $M_1$ and $M_2$ using FPBF. Note that if we use the same priors for $\theta_1$ and $\theta_2$, this boils down to selection of either covariate $x$ or $z$ in the AR(1) regression. Hence, variable selection constitutes an important ingredient in this FPBF convergence example. Note that both the models $M_1$ and $M_2$ are wrong with respect to the true model $M_0$ which consists of both $x$ and $z$. The purpose of variable selection here is then to select the more important variable among $x$ and $z$ when none of the available models considers both $x$ and $z$.

We make the following assumptions that are analogous to the AR(1) regression example considered in Chandra and Bhattacharya (2020):

(A1)

$$
\frac{1}{n} \sum_{t=1}^{n} x_t \to 0, \quad \frac{1}{n} \sum_{t=1}^{n} z_t \to 0; \\
\frac{1}{n} \sum_{t=1}^{n} x_t z_t \to 0; \quad \frac{1}{n} \sum_{t=1}^{n} x_{t+k} z_t \to 0; \quad \frac{1}{n} \sum_{t=1}^{n} x_t z_{t+k} \to 0 \text{ for any } k \geq 1; \\
\frac{1}{n} \sum_{t=1}^{n} x_{t+k} x_t \to 0 \text{ and } \frac{1}{n} \sum_{t=1}^{n} z_{t+k} z_t \to 0 \text{ for any } k \geq 1; \\
\frac{1}{n} \sum_{t=1}^{n} x_t^2 \to \sigma_x^2 \text{ and } \frac{1}{n} \sum_{t=1}^{n} z_t^2 \to \sigma_z^2,
$$

as $n \to \infty$. In the above, $\sigma_x^2$ and $\sigma_z^2$ are positive quantities.

(A2) $\sup_{t \geq 1} |x_t \beta_0| < C$ and $\sup_{t \geq 1} |z_t \beta_0| < C$, for some $C > 0$.

Let $\frac{1}{n} \log R_n^{(1)}(\theta)$ and $\frac{1}{n} \log R_n^{(2)}(\theta)$ stand for $\frac{1}{n} \log R_n(\theta)$ for models $M_1$ and $M_2$, respectively. Also let $\sigma_{x+z}^2 = \sigma_x^2 + \sigma_z^2$. Then proceeding in the same way as in Chandra and Bhattacharya
it can be shown that
\[
\lim_{n \to \infty} \frac{1}{n} \log R_n^{(1)}(\theta) \overset{a.s.}{=} -h_1(\theta), \text{ for all } \theta \in \Theta_1; \quad (7.43)
\]
\[
\lim_{n \to \infty} \frac{1}{n} \log R_n^{(2)}(\theta) \overset{a.s.}{=} -h_2(\theta), \text{ for all } \theta \in \Theta_2, \quad (7.44)
\]
and the above convergences are uniform on compact subsets of \( \Theta_1 \) and \( \Theta_2 \), respectively. In the above,
\[
h_1(\theta) = \log \left( \frac{\sigma}{\sigma_0} \right) + \left( 1 - \frac{1}{2\sigma^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0} + \frac{\rho_0}{\sigma_0} \right) + \left( \frac{\rho_0^2}{2\sigma^2} - \frac{\rho_0^2}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0} + \frac{\rho_0}{\sigma_0} \right)
+ \frac{1}{2\sigma^2} \beta^2 \sigma_{x+z}^2 - \frac{1}{2\sigma_0^2} \beta_0^2 \sigma_{x+z}^2 \left( \frac{\rho}{\sigma^2} - \frac{\rho_0}{\sigma_0^2} \right) + \frac{1}{2\sigma^2} \beta^2 \sigma_{x+z}^2 \beta_0 + \frac{2\sigma^2 \beta (2\beta_0 - \beta)}{2\sigma^2}.
(7.45)
\]
and
\[
h_2(\theta) = \log \left( \frac{\sigma}{\sigma_0} \right) + \left( 1 - \frac{1}{2\sigma^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0} + \frac{\rho_0}{\sigma_0} \right) + \left( \frac{\rho_0^2}{2\sigma^2} - \frac{\rho_0^2}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0} + \frac{\rho_0}{\sigma_0} \right)
+ \frac{1}{2\sigma^2} \beta^2 \sigma_{x+z}^2 - \frac{1}{2\sigma_0^2} \beta_0^2 \sigma_{x+z}^2 \left( \frac{\rho}{\sigma^2} - \frac{\rho_0}{\sigma_0^2} \right) + \frac{1}{2\sigma^2} \beta^2 \sigma_{x+z}^2 \beta_0 + \frac{2\sigma^2 \beta (2\beta_0 - \beta)}{2\sigma^2}.
(7.46)
\]

For \( i = 1, 2 \), for model \( M_i \), let
\[
G_n^{(i)} = \{ \theta \in \Theta : |\rho| \leq \exp(\gamma_i n), |\beta| \leq \exp(\gamma_i n), \sigma^{-2} \leq \exp(\gamma_i n) \}, 
(7.47)
\]
where \( \gamma_i > 2h_i(\Theta_i) \). Then \( G_n^{(i)} \uparrow \Theta_i \), as \( n \to \infty \). Let us assume that under both \( M_1 \) and \( M_2 \), the prior for \( (\rho, \beta, \sigma^{-2}) \) is such that the prior expectations \( E(|\rho|), E(|\beta|) \) and \( E(\sigma^{-2}) \) are finite.

With these, conditions (S1)–(S5) and (S7) of Shalizi hold for \( M_1 \) and \( M_2 \) in the same way as the AR(1) regression example of Chandra and Bhattacharya (2020). Thus verification of (S6) only remains, for which we begin with the following result.

**Theorem 16.** The functions \( \frac{1}{n} \log R_n^{(1)}(\theta) \) and \( \frac{1}{n} \log R_n^{(2)}(\theta) \) are asymptotically concave in \( \theta \).

**Proof.** The proof follows in the same line as that of Theorem 17 of Chandra and Bhattacharya (2020).
\[
\square
\]
It is also easy to see that both \( h_1(\theta) \) and \( h_2(\theta) \) given by (7.45) and (7.46) are convex in \( \theta \). Hence, there exist unique minimizers \( \bar{\theta}_1 \) and \( \bar{\theta}_2 \), respectively, of \( h_1 \) and \( h_2 \). Theorem 17 shows consistency of the unique roots of \( \frac{1}{n} \log R_n^{(1)}(\theta) \) and \( \frac{1}{n} \log R_n^{(2)}(\theta) \) for \( \bar{\theta}_1 \) and \( \bar{\theta}_2 \), respectively.

**Theorem 17.** Given any \( \eta > 0 \), \( \frac{1}{n} \log R_n^{(1)}(\theta) \) and \( \frac{1}{n} \log R_n^{(2)}(\theta) \) have their unique roots in the \( \eta \)-neighbourhood of \( \bar{\theta}_1 \) and \( \bar{\theta}_2 \), respectively, almost surely, for large \( n \).

**Proof.** See Appendix C.
\[
\square
\]
For \( i = 1, 2 \), let \( \bar{\theta}_n^{(i)} \) stand for the unique maximizer of \( \frac{1}{n} \log R_n^{(i)}(\theta) \). By Theorem 17
\[
\bar{\theta}_n^{(i)} \overset{a.s.}{\rightarrow} \bar{\theta}^{(i)}, \text{ for } i = 1, 2,
\]
which, in turn implies thanks to Theorem 27, that (7.18), and hence (S6) of Shalizi, holds for both \( M_1 \) and \( M_2 \).
In other words, models $\mathcal{M}_1$ and $\mathcal{M}_2$ satisfy conditions (S1)–(S7) of Shalizi. We summarize below our results on variable selection in forward AR(1) regression framework.

**Theorem 18 (FPBF consistency for $\mathcal{M}_1$ versus $\mathcal{M}_0$).** Consider the AR(1) regression models $\mathcal{M}_1$ and $\mathcal{M}_0$ given by (7.40) and (7.42). Then under assumptions (A1) and (A2),

$$
\lim_{n \to \infty} \frac{1}{n} \log \text{FPBF}^{(n)}(\mathcal{M}_1, \mathcal{M}_0) \overset{a.s.}{=} -h_1(\tilde{\theta}_1),
$$

where $h_1$ is given by (7.45) and $\tilde{\theta}_1$ is its unique minimizer.

**Theorem 19 (FPBF consistency for $\mathcal{M}_2$ versus $\mathcal{M}_0$).** Consider the AR(1) regression models $\mathcal{M}_2$ and $\mathcal{M}_0$ given by (7.41) and (7.42). Then under assumptions (A1) and (A2),

$$
\lim_{n \to \infty} \frac{1}{n} \log \text{FPBF}^{(n)}(\mathcal{M}_2, \mathcal{M}_0) \overset{a.s.}{=} -h_2(\tilde{\theta}_2),
$$

where $h_1$ is given by (7.46) and $\tilde{\theta}_2$ is its unique minimizer.

**Theorem 20 (FPBF convergence for $\mathcal{M}_1$ versus $\mathcal{M}_2$).** Consider the AR(1) regression models $\mathcal{M}_1$ and $\mathcal{M}_2$ given by (7.40) and (7.41) and the true model $\mathcal{M}_0$ given by (7.42). Then under assumptions (A1) and (A2),

$$
\lim_{n \to \infty} \frac{1}{n} \log \text{FPBF}^{(n)}(\mathcal{M}_1, \mathcal{M}_2) \overset{a.s.}{=} - \left( h_1(\tilde{\theta}_1) - h_2(\tilde{\theta}_2) \right),
$$

where $h_1$ and $h_2$ are given by (7.45) and (7.46) and $\tilde{\theta}_1$ and $\tilde{\theta}_2$ are their respective unique minimizers.

### 8 Illustrations of PBF convergence in inverse regression problems

First note that if $f(y_i|\theta, \bar{x}_i, Y^{(i-1)}, \mathcal{M})$ is bounded and continuous in $(\theta, \bar{x}_i)$, then in inverse regression setups, $g(y_i, \theta, \mathcal{M})$ is bounded and continuous in $\theta$ if $\pi(\bar{x}_i|\theta, \mathcal{M})$ is bounded and continuous in $(\theta, \bar{x}_i)$. Here continuity of $g(Y^{(i)}, \theta, \mathcal{M})$ follows by the dominated convergence theorem. Thus, whenever $f(y_i|\theta, x_i, Y^{(i-1)}, \mathcal{M}_0)$ are also bounded and continuous in $\theta$ and conditions (S1)–(S7) of Shalizi are verified, almost sure exponential convergence of IPBF also hold, provided that $h^*(\theta)$ exists. But existence of $h^*(\theta)$ requires existence of the limit of $n^{-1}\sum_{i=1}^n g(Y^{(i)}, \theta, \mathcal{M})$. Although this is expected to exist, it is not straightforward to guarantee this rigorously for general regression problems.

However, in practice, simple approximations may be used. For example, if $\mathcal{M}$ stands for simple linear regression, then let us consider a uniform prior for $\bar{x}_i$ on $X = [-a, a]$, for some $a > 0$. Then

$$
g(Y^{(i)}, \theta, \mathcal{M}) = \int_{-a}^a \frac{1}{\sigma_\epsilon \sqrt{2\pi}} \exp \left\{ -\frac{1}{2\sigma_\epsilon^2} (y_i - \alpha - \beta \bar{x}_i)^2 \right\} \, d\bar{x}_i \overset{a.s.}{\to} |\beta|^{-1}, \quad \text{as } a \to \infty.
$$

Thus for sufficiently large $a$, $g(Y^{(i)}, \hat{\theta}, \mathcal{M})$ can be approximated by $|\hat{\beta}|^{-1}$, which is independent of $i$. Thus, for large enough $a$, the limit of $n^{-1}\sum_{i=1}^n \log g(Y^{(i)}, \hat{\theta}, \mathcal{M})$ can be approximated by $|\beta|^{-1}$. But in general non-linear regression, such simple approximations are not available.

The setup where $y_i = \{y_{i1}, \ldots, y_{iim}\}$, is far more flexible in this regard. Let us illustrate this with respect to the models $\mathcal{M}_0$, $\mathcal{M}_1$ and $\mathcal{M}_2$ considered in Section 7. Assuming invertibility of $\eta_0$ in addition to continuity, we assume the prior

$$
\pi(\bar{x}_i|\eta_0, \mathcal{M}_0) \equiv U \left( B_{im}^{(0)}(\eta_0) \right) \quad \text{(8.1)}
$$
under model $\mathcal{M}_0$, where

$$B^{(0)}_{im}(\eta_0) = \left\{ x : \eta_0(x) \in \left[ \bar{y}_i - \frac{cs_i}{\sqrt{m}}, \bar{y}_i + \frac{cs_i}{\sqrt{m}} \right] \right\}. \quad (8.2)$$

In the case of the linear regression model $\mathcal{M}_1$, we set

$$\pi(\tilde{x}_i|\theta, \mathcal{M}_1) \equiv U\left(B^{(1)}_{im}(\theta)\right) \quad (8.3)$$

where

$$B^{(1)}_{im}(\theta) = \left[ \frac{\bar{y}_i - \alpha - \frac{cs_i}{\beta}}{\frac{cs_i}{\beta}} \frac{\bar{y}_i - \alpha - \frac{cs_i}{\beta}}{\frac{cs_i}{\beta}} + \frac{cs_i}{\beta} \right]. \quad (8.4)$$

For the quadratic model $\mathcal{M}_2$, note that even if the true model is quadratic, then it is not one-to-one. Hence the general form of the prior considered in Section 2.4.1 is not applicable here. In this case, we propose the following prior for $\tilde{x}_i$ under the quadratic model $\mathcal{M}_2$:

$$\pi(\tilde{x}_i|\theta, \mathcal{M}_2) \equiv U\left(B^{(2)}_{im}(\theta)\right) \quad (8.5)$$

where

$$B^{(2)}_{im}(\theta) = \left[ \frac{\bar{y}_i - \alpha - \frac{cs_i}{\beta_1} \bar{y}_i - \alpha - \frac{cs_i}{\beta_1} + \frac{cs_i}{\beta_1} \right]. \quad (8.6)$$

Note that the prior depends upon $x_i$ itself, which is the truth in this case. It is unusual in Bayesian inference to make the prior depend upon the truth. Indeed, the true parameter is always unknown; had it been known, then one would give full prior probability to the true parameter. In our case $x_i$ is actually known but a prior is needed for $\tilde{x}_i$ for the sake of cross-validation. Moreover, the prior does not consider $x_i$ to be known as long as the sample sizes $n$ and $m$ remain finite and $\theta$ is unknown or takes false values. The prior has substantial variance in these cases. Hence, although unusual, such a prior on $\tilde{x}_i$ is not untenable for inverse cross-validation.

Now observe that $\tilde{\theta}_1$ and $\tilde{\theta}_2$ associated with models $\mathcal{M}_1$ and $\mathcal{M}_2$ remain the same as those in Section 7. Also note that when the true model is $\mathcal{M}_0$ and when $\tilde{\theta}_1$ is associated with $\mathcal{M}_1$, then

$$B^{(1)}_{im}(\tilde{\theta}_1) \xrightarrow{a.s.} \{ x^{*}_{i1} \}, \text{ as } m \to \infty, \quad (8.7)$$

where

$$x^{*}_{i1} = \frac{\eta_0(x_i) - \tilde{\alpha}}{\beta}. \quad (8.7)$$

Similarly, when the true model is $\mathcal{M}_0$ and when $\tilde{\theta}_2$ is associated with $\mathcal{M}_2$, then

$$B^{(2)}_{im}(\tilde{\theta}_2) \xrightarrow{a.s.} \{ x^{*}_{i2} \}, \text{ as } m \to \infty, \quad (8.8)$$

where

$$x^{*}_{i2} = \frac{\eta_0(x_i) - \tilde{\alpha} - \tilde{\beta} x^2_{i2}}{\beta_1}. \quad (8.8)$$

Since $x^{*}_{i1}$ and $x^{*}_{i2}$ given by (8.7) and (8.8) are both continuous in $x_i$, the asymptotic calculations of $\frac{1}{n} \log \prod_{i=1}^{n} f(y_{ik}|\tilde{\theta}_1, x^{*}_{i1}, \mathcal{M}_1)$ and $\frac{1}{n} \log \prod_{i=1}^{n} f(y_{ik}|\tilde{\theta}_1, x^{*}_{i2}, \mathcal{M}_2)$ remain the same as $\frac{1}{n} \log \prod_{i=1}^{n} f(y_{i1}|\tilde{\theta}_1, x_i, \mathcal{M}_1)$ and $\frac{1}{n} \log \prod_{i=1}^{n} f(y_{i2}|\tilde{\theta}_1, x_i, \mathcal{M}_2)$, respectively, detailed in Section 7. Hence, the final asymptotic results for IPBF remain the same for FPBF with respect to the models $\mathcal{M}_0$, $\mathcal{M}_1$ and $\mathcal{M}_2$. Also note that here the cross-validation posterior for $\mathcal{M}_0$ is given by

$$\pi(y_{ik}|Y_{nm,-i}, X_{n,-i}) = \int_{\mathcal{X}} f(y_{ik}|\tilde{x}_i, \mathcal{M}_0) d\pi(\tilde{x}_i|\mathcal{M}_0) \xrightarrow{a.s.} f(y_{ik}|x_i), \text{ as } m \to \infty,$$
since $D_{m}^{(0)}(\eta_{h}) \xrightarrow{a.s.} \{x_{i}\}$, as $m \to \infty$. Hence, the final asymptotic results do not depend upon whether or not $x_{i}$ is considered known or the prior $\pi(\tilde{x}_{i}|\eta_{h}, \mathcal{M}_{0})$ is used treating it as unknown, when cross-validating for $\mathcal{M}_{0}$. Appealing to Theorem 9, Remark 10 and Theorem 11 we thus summarize our results for IPBF concerning $\mathcal{M}_{0}$, $\mathcal{M}_{1}$ and $\mathcal{M}_{2}$ as follows.

**Theorem 21 (IPBF convergence for linear regression).** Assume the setup where data \{\(y_{ij}; i = 1, \ldots, n; j = 1, \ldots, m\)\} are available. In this setup consider the linear regression model $\mathcal{M}_{1}$ given by (7.1) and the true, non-linear model $\mathcal{M}_{0}$ given by (7.2). Let the parameter space $\Theta$ associated with model $\mathcal{M}_{1}$ be $\mathbb{R} \times \mathbb{R} \times \mathbb{R}^{+}$, and let the covariate space $X$ be compact. Assume the priors (8.1) and (8.3) on $\tilde{x}_{i}$ under the models $\mathcal{M}_{0}$ and $\mathcal{M}_{1}$, respectively. Then

$$\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log \text{IPBF}^{(n, m, k)}(\mathcal{M}_{1}, \mathcal{M}_{0}) \xrightarrow{a.s.} -h_{1}(\tilde{\theta}_{1}),$$

where for $\theta \in \Theta$, $h_{1}(\theta)$ is given by (7.11), and $\tilde{\theta}_{1} = (\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}^{2})$, where $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\sigma}^{2}$ are given by (7.24), (7.23) and (7.25), respectively. The result remains unchanged if $x_{i}$ is treated as known for cross-validation with respect to $\mathcal{M}_{0}$.

**Theorem 22 (IPBF convergence for quadratic regression).** Assume the setup where data \{\(y_{ij}; i = 1, \ldots, n; j = 1, \ldots, m\)\} are available. In this setup consider the quadratic regression model $\mathcal{M}_{2}$ given by (7.2) and the true, non-linear model $\mathcal{M}_{0}$ given by (7.2). Let the parameter space $\Theta$ associated with model $\mathcal{M}_{2}$ be $\mathbb{R} \times \mathbb{R} \times \mathbb{R}^{+}$, and let the covariate space $X$ be compact. Also assume that $x_{i}; i \geq 1$ are all distinct. Assume the priors (8.1) and (8.5) on $\tilde{x}_{i}$ under the models $\mathcal{M}_{0}$ and $\mathcal{M}_{2}$, respectively. Then

$$\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log \text{IPBF}^{(n, m, k)}(\mathcal{M}_{2}, \mathcal{M}_{0}) \xrightarrow{a.s.} -h_{2}(\tilde{\theta}_{2}),$$

where for $\theta \in \Theta$, $h_{2}(\theta)$ is given by (7.31), and $\tilde{\theta}_{2} = (\tilde{\alpha}, \tilde{\beta}_{1}, \tilde{\beta}_{2}, \tilde{\sigma}^{2})$, where $\tilde{\alpha}$, $\tilde{\beta}_{1}$, $\tilde{\beta}_{2}$ and $\tilde{\sigma}^{2}$ are given by (7.32), (7.33) and (7.34). The result remains unchanged if $x_{i}$ is treated as known for cross-validation with respect to $\mathcal{M}_{0}$.

**Theorem 23 (Comparison between linear and quadratic regressions).** Assume the setup where data \{\(y_{ij}; i = 1, \ldots, n; j = 1, \ldots, m\)\} are available. Let the true model be given by $\mathcal{M}_{0}$ formulated in (7.2). Assuming that the covariate observations $x_{i}; i \geq 1$ are all distinct and that the covariate space $X$ is compact, consider comparison of the linear and quadratic regression models $\mathcal{M}_{1}$ and $\mathcal{M}_{2}$ given by (7.1) and (7.30), respectively, using IPBF. Assume the priors (8.1), (8.3) and (8.5) on $\tilde{x}_{i}$ under the models $\mathcal{M}_{0}$, $\mathcal{M}_{1}$ and $\mathcal{M}_{2}$, respectively. Then,

$$\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log \text{IPBF}^{(n, m, k)}(\mathcal{M}_{1}, \mathcal{M}_{2}) \xrightarrow{a.s.} -(h_{1}(\tilde{\theta}_{1}) - h_{2}(\tilde{\theta}_{2}))$$

where $h_{1}(\tilde{\theta}_{1})$ and $h_{2}(\tilde{\theta}_{2})$ are the same as in Theorems 21 and 22, respectively. The result remains unchanged if $\tilde{x}_{i}$ is treated as known for cross-validation with respect to $\mathcal{M}_{0}$.

### 8.1 IPBF asymptotics for variable selection in AR(1)

Now let us reconsider the AR(1) regression setup described by the competing models $\mathcal{M}_{1}$ (7.40), $\mathcal{M}_{2}$ (7.41) and the true model $\mathcal{M}_{0}$ (7.42), along with assumptions (A1) and (A2). But now we reformulate the models as follows to suit the second setup of inverse regression.

$$y_{tj} = \rho_{1}y_{t-1,j} + \beta_{1}x_{t} + \epsilon_{t,j}, \quad t = 1, \ldots, n; \quad j = 1, \ldots, m,$$  (8.9)
where \( y_{t,j} \equiv 0 \) for \( j = 1, \ldots, m \) and \( \epsilon_{t,j} \overset{iid}{\sim} N(0, \sigma_j^2) \), for \( t = 1, \ldots, n \) and \( j = 1, \ldots, m \). Similarly, \( M_2 \) is now given by

\[
y_{t,j} = \rho_2 y_{t-1,j} + \beta_2 z_t + \epsilon_{2t,j}; \quad t = 1, \ldots, n; \quad j = 1, \ldots, m,
\]

where \( \epsilon_{2t,j} \overset{iid}{\sim} N(0, \sigma_j^2) \), for \( t = 1, \ldots, n \) and \( j = 1, \ldots, m \).

The true model \( M_0 \) be given by

\[
y_{t,j} = \rho_0 y_{t-1,j} + \beta_0 (x_t + z_t) + \epsilon_{0t,j}; \quad t = 1, \ldots, n; \quad j = 1, \ldots, m,
\]

where \( |\rho_0| < 1 \) and \( \epsilon_{0t,j} \overset{iid}{\sim} N(0, \sigma_j^2) \), for \( t = 1, \ldots, n \) and \( j = 1, \ldots, m \).

For \( t = 1, \ldots, n \), let \( \bar{y}_t = \frac{1}{m} \sum_{j=1}^{m} y_{t,j} \) and \( s_t^2(\rho) = \frac{1}{m} \left( (y_{t,j} - \bar{y}_t)^2 - \rho (y_{t-1,j} - \bar{y}_{t-1})^2 \right) \). We consider the following priors for \( \tilde{x}_t \) and \( \tilde{z}_t \) associated with \( M_1 \) and \( M_2 \):

\[
\pi(\tilde{x}_t|\theta_1, M_1) \equiv U \left( B_{tm}^{(1)}(\theta_1) \right);
\]

\[
\pi(\tilde{z}_t|\theta_2, M_2) \equiv U \left( B_{tm}^{(2)}(\theta_1) \right),
\]

where

\[
B_{tm}^{(1)}(\theta_1) = \frac{\bar{y}_t - \rho_1 \bar{y}_{t-1}}{\beta_1} + \frac{cs_t(p_1)}{\beta_1 |\beta_1| \sqrt{m}};
\]

\[
B_{tm}^{(2)}(\theta_2) = \frac{\bar{y}_t - \rho_2 \bar{y}_{t-1}}{\beta_2} + \frac{cs_t(p_2)}{\beta_2 |\beta_2| \sqrt{m}}.
\]

Note that

\[
B_{tm}^{(1)}(\tilde{\theta}_1) \xrightarrow{a.s.} \{x_t^*\} \text{ as } m \to \infty;
\]

\[
B_{tm}^{(2)}(\tilde{\theta}_2) \xrightarrow{a.s.} \{z_t^*\} \text{ as } m \to \infty,
\]

where

\[
x_t^* = \frac{\beta_0 \sum_{k=1}^{t-1} \rho^{t-k} x_k - \beta_0 \tilde{\rho}_1 \sum_{k=1}^{t-1} \rho^{t-k} x_k}{\beta_1};
\]

\[
z_t^* = \frac{\beta_0 \sum_{k=1}^{t-1} \rho^{t-k} z_k - \beta_0 \tilde{\rho}_2 \sum_{k=1}^{t-1} \rho^{t-k} z_k}{\beta_2}.
\]

Direct calculations reveal that

\[
\frac{1}{n} \sum_{t=1}^{n} x_t^* \to 0; \quad \frac{1}{n} \sum_{t=1}^{n} x_t^{*2} \to \sigma_x^2 \beta_0^2 (1 - \tilde{\rho}_1)^2 / \beta_1^2 (1 - \rho_0^2), \text{ as } n \to \infty;
\]

\[
\frac{1}{n} \sum_{t=1}^{n} z_t^* \to 0; \quad \frac{1}{n} \sum_{t=1}^{n} z_t^{*2} \to \sigma_z^2 \beta_0^2 (1 - \tilde{\rho}_2)^2 / \beta_2^2 (1 - \rho_0^2), \text{ as } n \to \infty.
\]

Hence, for the final IPBF calculations associated with \( h_1 \) and \( h_2 \) for this example, we need to replace \( x_t, z_t, \sigma_x^2 \) and \( \sigma_z^2 \) in (A1) with \( x_t^*, z_t^*, \sigma_x^2 \) and \( \sigma_z^2 \), respectively, for models \( M_1 \) and \( M_2 \).
In this regard, let
\begin{align*}
h_1^*(\theta) &= \log \left( \frac{\sigma}{\sigma_0} \right) + \left( \frac{1}{2\sigma^2} - \frac{1}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0^2} + \beta_0^2 \sigma_{x+z}^2 \right) + \left( \frac{\rho^2}{2\sigma^2} - \frac{\rho_0^2}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0^2} + \beta_0^2 \sigma_{z}^2 \right) \\
&+ \frac{1}{2\sigma^2} \beta_0^2 \sigma_{x+z}^2 - \frac{1}{2\sigma_0^2} \beta_0^2 \sigma_{x+z}^2 - \left( \frac{\rho}{\sigma} - \frac{\rho_0}{\sigma_0} \right) \left( \frac{\rho_0 \sigma_0^2}{1 - \rho_0^2} + \rho_0^2 \frac{\beta_0 \sigma_{z}^2}{1 - \rho_0^2} \right) - \left( \frac{\beta}{\sigma} - \frac{\beta_0}{\sigma_0} \right) \sigma_{x+z}^2 \beta_0 \\
&+ \frac{\sigma_0^2 \beta (\beta_0 - \beta)}{\sigma^2} + \frac{\beta^2}{2\sigma^2} \left( \sigma_{x+z}^2 + \sigma_{z}^2 - \frac{2\beta_0 \sigma_{z}^2}{\beta_1} \right).
\end{align*}

and
\begin{align*}
h_2^*(\theta) &= \log \left( \frac{\sigma}{\sigma_0} \right) + \left( \frac{1}{2\sigma^2} - \frac{1}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0^2} + \beta_0^2 \sigma_{x+z}^2 \right) + \left( \frac{\rho^2}{2\sigma^2} - \frac{\rho_0^2}{2\sigma_0^2} \right) \left( \frac{\sigma_0^2}{1 - \rho_0^2} + \beta_0^2 \sigma_{z}^2 \right) \\
&+ \frac{1}{2\sigma^2} \beta_0^2 \sigma_{x+z}^2 - \frac{1}{2\sigma_0^2} \beta_0^2 \sigma_{x+z}^2 - \left( \frac{\rho}{\sigma} - \frac{\rho_0}{\sigma_0} \right) \left( \frac{\rho_0 \sigma_0^2}{1 - \rho_0^2} + \rho_0^2 \frac{\beta_0 \sigma_{z}^2}{1 - \rho_0^2} \right) - \left( \frac{\beta}{\sigma} - \frac{\beta_0}{\sigma_0} \right) \sigma_{x+z}^2 \beta_0 \\
&+ \frac{\sigma_0^2 \beta (\beta_0 - \beta)}{\sigma^2} + \frac{\beta^2}{2\sigma^2} \left( \sigma_{x+z}^2 + \sigma_{z}^2 - \frac{2\beta_0 \sigma_{z}^2}{\beta_2} \right).
\end{align*}

If cross-validation is considered with respect to the true model \( M_0 \) with a prior on the covariates, then since \( x_t \) and \( z_t \) are not separately identifiable in \( M_0 \), let \( u_t = x_t + z_t \) and consider a prior on \( \tilde{u}_t \) as follows:
\begin{equation}
\pi(\tilde{u}_t|\theta_0, M_0) \equiv U \left( B_{tm}^{(0)}(\theta_0) \right),
\end{equation}
where
\begin{equation}
B_{tm}^{(0)}(\theta_0) = \left[ \frac{\bar{y}_t - \rho_0 \bar{y}_{t-1}}{\beta_0} \right] - \frac{c_{st}(\rho_0)}{\beta_0 \sqrt{m}} \bar{y}_t - \frac{c_{st}(\rho_0)}{\beta_0 \sqrt{m}}.
\end{equation}

Note that \( B_{tm}^{(0)}(\theta_0) \xrightarrow{a.s.} \{ u_t \} \), as \( m \to \infty \). Let \( U_{n,-t} = \{ u_1, \ldots , u_n \} \setminus \{ u_t \} \). As before, it follows that \( \pi (y_{tk}|Y_{am,-t}, U_{n,-t}) \xrightarrow{a.s.} f(y_{tk}|u_t, y_{t-1,k}) \), as \( m \to \infty \). Hence, the final asymptotic results do not depend upon whether or not \( u_t \) is considered known or the prior (8.24) is used for \( \tilde{u}_t \) treating \( u_t \) it as unknown, when cross-validating for the true model \( M_0 \).

We summarize our results on variable selection in the inverse AR(1) regression framework as follows.

Theorem 24 (IPBF consistency for \( M_1 \) versus \( M_0 \)). Consider comparing model \( M_1 \) (8.9) against the true model \( M_0 \) (8.11). Assume the priors (8.12) and (8.24) on \( \tilde{x}_t \) and \( \tilde{u}_t \) under the models \( M_1 \) and \( M_0 \), respectively. Then
\begin{equation}
\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m)}(M_1, M_0) \xrightarrow{a.s.} -h_1^*(\tilde{\theta}_1),
\end{equation}
where for \( \theta \in \Theta_1 \), \( h_1^*(\theta) \) is given by (8.22), and \( \tilde{\theta}_1 \) is the unique minimizer of \( h_1 \) given by (7.45). The result remains unchanged if \( u_t \) is treated as known for cross-validation with respect to \( M_0 \).

Theorem 25 (IPBF consistency for \( M_2 \) versus \( M_0 \)). Consider comparing model \( M_2 \) (8.10) against the true model \( M_0 \) (8.11). Assume the priors (8.13) and (8.24) on \( \tilde{x}_t \) and \( \tilde{u}_t \) under the models \( M_2 \) and \( M_0 \), respectively. Then
\begin{equation}
\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m)}(M_1, M_0) \xrightarrow{a.s.} -h_2^*(\tilde{\theta}_2),
\end{equation}
where for \( \theta \in \Theta_2 \), \( h_2^*(\theta) \) is given by (8.23), and \( \tilde{\theta}_2 \) is the unique minimizer of \( h_2 \) given by (7.46). The result remains unchanged if \( u_t \) is treated as known for cross-validation with respect to \( M_0 \).
Theorem 26 (IPBF convergence for $M_1$ versus $M_2$). Consider comparing models $M_1$ (8.9) against model $M_2$ (8.10). Assume the priors (8.12) and (8.13) on $\tilde{x}_i$ and $\tilde{z}_i$ under the models $M_1$ and $M_2$, respectively. Then

$$\lim_{m \to \infty} \lim_{n \to \infty} \frac{1}{n} \log IPBF^{(n,m,k)}(M_1, M_2) \overset{a.s.}{\to} -\left(h^*_1(\tilde{\theta}_1) - h^*_2(\tilde{\theta}_2)\right),$$

where $h^*_1$ and $h^*_2$ are given by (8.22) and (8.23). In the above, $\tilde{\theta}_1$ and $\tilde{\theta}_2$ are the unique minimizers of $h_1$ of $h_2$ given by (7.45) and (7.46), respectively. The result remains unchanged if $u_i$ is treated as known for cross-validation with respect to $M_0$.

8.2 Discussion of FPBF and IPBF convergence for nonparametric regression models

Chatterjee and Bhattacharya (2019a) investigate posterior convergence for Gaussian and general stochastic process regression under suitable assumptions while posterior convergence for binary and Poisson nonparametric regression based on Gaussian process modeling of the regression function are addressed in Chatterjee and Bhattacharya (2019b). In all these nonparametric setups, the authors verified assumptions (S1)–(S7) of Shalizi. Here it is important to point out that Theorem 27 used to verify assumption (S6) of Shalizi in our parametric setups, is not valid in infinite-dimensional nonparametric models since without further assumptions on model sparsity, $\tilde{\theta}_n$ can not converge to $\tilde{\theta}$. That is, condition (ii) of Theorem 27 does not hold in general for nonparametric models. Moreover, enforcing sparsity conditions to general stochastic processes, such as Gaussian processes, need not be desirable. Chatterjee and Bhattacharya (2019a) and Chatterjee and Bhattacharya (2019b) propose a general sufficient condition for verification of (S6) of Shalizi, which is appropriate for nonparametric models, and use that condition for their purposes.

The point of the above discussion is that assumptions (S1)–(S7) are already verified by Chatterjee and Bhattacharya (2019a) and Chatterjee and Bhattacharya (2019b) for nonparametric Bayesian regression models, and since boundedness and continuity of $f(y_i|\theta, M)$ also hold for such models $M$, our asymptotic results on almost sure exponential convergence of FPBF and IPBF are directly applicable to such models. For IPBF convergence in nonparametric situations, the priors for $\tilde{x}_i$ proposed in Section 2.4.2 for nonparametric cases (ii)–(iv) are appropriate.

Note that parametric and nonparametric models can also be compared asymptotically using our FPBF and IPBF theory.

9 Simulation experiments

So far we have investigated large sample properties of FPBF and IPBF. However, for all practical purposes it is important to provide insights into small sample behaviours of such versions of pseudo-Bayes factor. In this section we undertake such small sample study with the help of simulation experiments. Specifically, we set $n = m = 10$ and generate data from relevant Poisson distribution with the log-linear link function and consider modeling the data with Poisson and geometric distributions with log, logit and probit links for linear models as well as nonparametric regression modeled by Gaussian process having linear mean function and squared exponential covariance. We also consider variable selection in these setups with respect to two different covariates. We report both FPBF and IPBF results for the experiments. Details follow.
9.1 Poisson versus geometric linear and nonparametric regression models when the true model is Poisson linear regression

9.1.1 True distribution

Let us first consider the case where the true data-generating distribution is \( y_{ij} \sim \text{Poisson}(\lambda(x_i)) \), with \( \lambda(x) = \exp(\alpha + \beta x) \). We generate the data by simulating \( \alpha_0 \sim U(-1, 1) \), \( \beta_0 \sim U(-1, 1) \) and \( x_i \sim U(-1, 1); \ i = 1, \ldots, n \), and then finally simulating \( y_{ij} \sim \text{Poisson}(\lambda(x_i)); \ j = 1, \ldots, m \), \( i = 1, \ldots, n \).

To model the data generated from the true distribution, we consider both Poisson and geometric distributions and both linear and Gaussian process based nonparametric regression for such models. Let us begin with the Poisson setup.

9.2 Competing forward and inverse Poisson regression models

9.2.1 Forward Poisson linear regression model

In this setup we model the data as follows: \( y_{ij} \sim \text{Poisson}(\lambda(x_i)) \), with \( \lambda(x) = \exp(\alpha + \beta x) \), and set the prior \( \pi(\alpha, \beta) = 1 \), for \(-\infty < \alpha, \beta < \infty\). For the forward setup, this completes the model and prior specifications. Denoting this by model \( \mathcal{M} \), we compute the forward cross-validation posterior of the form

\[
\pi(y_{i1}|Y_{n,-i}, X_n, \mathcal{M}) = \int_{\Theta} f(y_{i1}|\theta, x_i, Y^{(i-1)}_n, \mathcal{M}) d\pi(\theta|Y_{n,-i}, X_n, \mathcal{M}),
\]

by taking Monte Carlo averages of \( f(y_{i1}|\theta, x_i, Y^{(i-1)}_n, \mathcal{M}) \) over realizations of \( \theta \) from \( \pi(\theta|Y_{n,-i}, X_n, \mathcal{M}) \). In our case this is the Monte Carlo average of the relevant Poisson probability of \( y_{i1} \) given \( x_i \) over realizations of \( \theta = (\alpha, \beta) \). Samples of \( \theta \) are obtained approximately from the posterior distribution of \( \pi(\theta|Y_{nm,-i}, X_{n,-i}) \) by first generating realizations from the “importance sampling density” \( \pi(\theta|Y_{nm}, X_n) \) using transformation based Markov chain Monte Carlo (TMCMC) (Dutta and Bhattacharya (2014)) and then re-using the realizations with importance weights to obtain the desired Monte Carlo averages. The rationale behind the choice of the full posterior \( \pi(\theta|Y_{nm}, X_n) \) associated with the full data set as the importance sampling density is that it is not significantly different from the posterior \( \pi(\theta|Y_{nm,-i}, X_{n,-i}) \) associated with leaving out a single data point. This choice is also quite popular in the literature; see, for example, Gelfand (1996). In our examples, we generate 30,000 TMCMC samples from \( \pi(\theta|Y_{nm}, X_n) \) of which we discard the first 10,000 as burn-in, and re-sample 1000 \( \theta \)-realizations without replacement from the remaining 20,000 realizations. We re-use each re-sampled \( \theta \)-value 100 times and compute the Monte Carlo average over such 1000 \( \times \) 100 = 100,000 realizations. The re-use of each re-sampled \( \theta \)-value corresponds to importance re-sampling MCMC (IRMCMC) of Bhattacharya and Haslett (2007). Although IRMCMC is meant for cross-validation in inverse problems, the idea carries over to forward problems as well. We finally compute \( \frac{1}{n} \sum_{i=1}^{n} \log \pi(y_{i1}|Y_{nm,-i}, X_n, \mathcal{M}) \) for model \( \mathcal{M} \).

9.2.2 Inverse Poisson linear regression model

With the same Poisson linear regression model as in the forward case, we now put a prior on \( \tilde{x}_i \) corresponding to \( x_i \). In our case, it follows from Section 2.4.2 that \( \pi(\tilde{x}_i|\alpha, \beta) \equiv U(a, b) \), where

\[
a = \min \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha \right), \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha \right) \right\} \quad (9.2)
\]

and

\[
b = \max \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha \right), \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha \right) \right\}. \quad (9.3)
\]
We set $c_1 = 1$ and $c_2 = 100$, for ensuring positive value of $\tilde{y}_i - \frac{c_2 x_i}{\sqrt{m}}$ (so that logarithm of this quantity is well-defined) and a reasonably large support of the prior for $\tilde{x}_i$. We then compute

$$
\pi(y_{1i}|Y_{nm,-i}, X_{n,-i}, M) = \int \int f(y_{1i}|\theta, \tilde{x}_i, Y_1^{(i-1)}, M) d\pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M)
$$

by Monte Carlo averaging of the relevant Poisson probability of $y_{1i}$ over realizations of $(\tilde{x}_i, \theta) = (\tilde{x}_i, (\alpha, \beta))$ generated from $\pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M)$. Since it follows from (2.6) that $\pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M) = \pi(\tilde{x}_i|\theta, M)\pi(\theta|Y_{nm,-i}, X_{n,-i}, M)$, and since realizations of $\theta$ from $\pi(\theta|Y_{nm,-i}, X_{n,-i}, M)$ are already available in the forward context, we simply generate $\tilde{x}_i$ given $\theta$ from the prior for $\tilde{x}_i$ to obtain realizations from $\pi(\tilde{x}_i, \theta|Y_{nm,-i}, X_{n,-i}, M)$. Note that for different $i$, only sub-samples of $\theta$ of size 1000 from the original sample of size 20,000 from the full posterior of $\theta$ are available, and each $\theta$ is repeated 100 times. However, realizations of $\tilde{x}_i$ are all distinct in spite of repetitions of $\theta$-values.

Once for each $i = 1, \ldots, n$, the Monte Carlo estimates of $\pi(y_{1i}|Y_{nm,-i}, X_{n,-i}, M)$ are available, we finally obtain the estimate of $\frac{1}{n} \sum_{i=1}^n \log \pi(y_{1i}|Y_{nm,-i}, X_{n,-i}, M)$ using the individual Monte Carlo estimates.

### 9.2.3 Forward Poisson nonparametric regression model

We now consider the case where $y_{ij} \sim \text{Poisson}(\lambda(x_i))$, where $\lambda(x) = \exp(\eta(x))$, where $\eta(\cdot)$ is a Gaussian process with mean function $\mu(x) = \alpha + \beta x$ and covariance $\text{Cov}(\eta(x_1), \eta(x_2)) = \sigma^2 \exp\{-(x_1 - x_2)^2\}$, where $\sigma$ is unknown. For our convenience, we reparameterize $\sigma^2$ as $\exp(\omega)$, where $-\infty < \omega < \infty$. For the prior on the parameters, we set $\pi(\alpha, \beta, \omega) = 1$, for $-\infty < \alpha, \beta, \omega < \infty$.

In the inverse case, for the reason of prior specification, we linearize $\eta(\tilde{x}_i)$ as $\alpha + \beta \tilde{x}_i$; see Section 9.2.4. Hence, for comparability with the inverse counterpart, we set $\eta(x_i) = \alpha + \beta x_i$. Thus, in the forward case, $\theta = (\alpha, \beta, \eta(x_1), \ldots, \eta(x_{i-1}), \eta(x_{i+1}), \ldots, \eta(x_n), \omega)$. We obtain $\frac{1}{n} \sum_{i=1}^n \log \pi(y_{1i}|Y_{nm,-i}, X_n, M)$ using the same method of Monte Carlo averaging described in Section 9.2.1, where $\theta$ is again first generated using TCMC from the full posterior of $\theta$ by discarding the first 10,000 iterations and retaining the next 20,000 for inference, which are reused to approximate the desired posteriors $\pi(\theta|Y_{nm,-i}, X_{n,-i}, M)$. As before, we obtain Monte Carlo averages over 100,000 realizations of $\theta$.

### 9.2.4 Inverse Poisson nonparametric regression model

The model in this case remains the same as that in Section 9.2.3, but now a prior on $\tilde{x}_i$ is needed. However, note that the prior for $\tilde{x}_i$, which is uniform on $B_{m}(\eta) = \{x : \eta(x) \in \log\left\{\left[\tilde{y}_i - \frac{c_2 x_i}{\sqrt{m}}, \tilde{y}_i + \frac{c_2 x_i}{\sqrt{m}}\right]\right\}\}$, does not have a closed form, since the form of $\eta(x)$ is unknown. However, if $m$ is large, the interval $\log\left\{\left[\tilde{y}_i - \frac{c_2 x_i}{\sqrt{m}}, \tilde{y}_i + \frac{c_2 x_i}{\sqrt{m}}\right]\right\}$ is small, and $\eta(x)$ falling in this small interval can be reasonably well-approximated by a straight line. Hence, we set $\eta(x) = \mu(x) = \alpha + \beta x$, for $\eta(x)$ falling in this interval. Thus it follows that $\pi(\tilde{x}_i|\eta) \equiv U(a, b)$, where $a$ and $b$ are given by (9.2) and (9.3), respectively. Hence, we obtain the same prior for $\tilde{x}_i$ as in the case of linear Poisson regression described in Section 9.2.2. As before we set $c_1 = 1$ and $c_2 = 100$.

The method for obtaining $\frac{1}{n} \sum_{i=1}^n \log \pi(y_{1i}|Y_{nm,-i}, X_{n,-i}, M)$ remains the same as discussed in Section 9.2.2.
9.3 Competing forward and inverse geometric regression models

We also report results of our simulation experiments where data generated from Poisson linear regression is modeled by geometric regression models of the form

$$f(y_{ij} | \theta, x_i) = (1 - p(x_i))^{y_{ij}} p(x_i),$$

(9.4)

where $p(x_i)$ is modeled as logit or probit linear or nonparametric regression. In other words, we consider the following possibilities of modeling $p(x_i)$:

$$\log \left( \frac{p(x)}{1 - p(x)} \right) = \alpha + \beta x; \quad \log \left( \frac{p(x)}{1 - p(x)} \right) = \eta(x);$$

$$p(x) = \Phi (\alpha + \beta x); \quad p(x) = \Phi (\eta(x)),$$

where $\Phi$ is the cumulative distribution function of the standard normal distribution. In the above, $\eta$ is again modeled by a Gaussian process with mean function $\mu(x) = \alpha + \beta x$ and covariance function given by $\text{Cov}(\eta(x_1), \eta(x_2)) = \sigma^2 \exp \{- (x_1 - x_2)^2 \}$. We again set $\sigma^2 = \exp(\omega)$, where $-\infty < \omega < \infty$, and consider the prior $\pi(\alpha, \beta, \omega) = 1$ for $-\infty < \alpha, \beta, \omega < \infty$.

In the inverse setup we assign prior on $\tilde{x}_i$ such that the mean of the geometric distribution, namely, $\frac{1 - p(x)}{p(x)}$, lies in $[\tilde{y}_i - \frac{c_1 s_i}{\sqrt{m}} , \tilde{y}_i + \frac{c_2 s_i}{\sqrt{m}}]$. Using the same principles as before it follows that for the logit link, either for linear or Gaussian process regression, the prior for $\tilde{x}_i$ is $U(a_1, b_1)$, where

$$a_1 = \min \left\{ -\beta^{-1} \left( \log \left( \tilde{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha \right) , -\beta^{-1} \left( \log \left( \tilde{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha \right) \right\}$$

(9.5)

and

$$b_1 = \max \left\{ -\beta^{-1} \left( \log \left( \tilde{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha \right) , -\beta^{-1} \left( \log \left( \tilde{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha \right) \right\}.$$ (9.6)

We set $c_1 = 1$ and $c_2 = 100$, as before.

For geometric probit regression, first let $\ell_{im} = \tilde{y}_i - \frac{c_1 s_i}{\sqrt{m}}$ and $u_{im} = \tilde{y}_i + \frac{c_2 s_i}{\sqrt{m}}$. Let

$$a_2 = \min \left\{ \frac{\Phi^{-1} \left( \frac{1}{\sqrt{m+1}} \right) - \alpha}{\beta} , \frac{\Phi^{-1} \left( \frac{1}{\sqrt{m+1}} \right) - \alpha}{\beta} \right\};$$

(9.7)

and

$$b_2 = \max \left\{ \frac{\Phi^{-1} \left( \frac{1}{\sqrt{m+1}} \right) - \alpha}{\beta} , \frac{\Phi^{-1} \left( \frac{1}{\sqrt{m+1}} \right) - \alpha}{\beta} \right\};$$

(9.8)

Then the prior for $\tilde{x}_i$ is $U(a_2, b_2)$, for both linear and Gaussian process based geometric probit regression.

The rest of the methodology for computing FPBF and IPBF for geometric regression remains the same as for Poisson regression described in Section 9.2.

9.3.1 Results of the simulation experiment for model selection

For $n = m = 10$, when the true model is Poisson with log-linear regression, the last two columns of Table 9.1 provide the forward and inverse estimates of $\frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, M)$ and $\frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, -i, M)$, respectively, for Poisson and geometric linear and Gaussian process regression with different link functions, using which the models can be easily compared with respect to both forward and inverse perspectives using FPBF and IPBF. Note that forward and inverse perspectives can also be compared.

Observe that the forward Poisson log-linear regression turns out to be the best model as expected, since this corresponds to the true, data-generating distribution. The Gaussian process
based Poisson inverse regression model is the next best, followed closely by the Poisson log-linear inverse regression model, and then comes the Gaussian process based Poisson forward regression model. This order of model selection can be explained as follows. First, the inverse cases involve more uncertainties than the corresponding forward models, since these cases treat $x_{j}$ as unknown. Hence, expectedly the Poisson log-linear forward regression model outperforms the inverse counterpart. But the inverse Gaussian process regression performs marginally better than the inverse linear model and more significantly better than the forward Gaussian process model. This merits an interesting explanation. Recall that in the inverse Gaussian process model $\eta(\tilde{x}_i)$ has been linearized for constructing the prior for $\tilde{x}_i$, so that this part is equivalent to the linear model, which explains why the difference between the inverse linear and Gaussian process models is not significant. However, the linear part of the Gaussian process model is of course influenced by the additional Gaussian process part associated with the other data points, unlike the linear regression models. The posterior dependence structure, in conjunction with the posterior distribution of $\tilde{x}_i$, can yield better regression estimates $\eta(\tilde{x}_i)$ for the $i$-th data point in a substantial number of Monte Carlo iterations. Since the Gaussian process model includes the linear model as a special case (that is, it is not a case of misspecification), this explains why the inverse Gaussian process regression performs marginally better than the inverse linear model. In the forward Gaussian process regression, even though we have linearized $\eta(x_i)$ for comparability with the inverse model, $x_i$ is fixed. Thus, when the $i$-th regression part is not well-estimated in the Monte Carlo simulations, there is no further scope for improvement in this part. However, in the inverse Gaussian process regression, $x_i$ is replaced with the random $\tilde{x}_i$, which, though its posterior simulations, can improve upon the $i$-th regression part with positive probability, even if the regression coefficients are not well-estimated. Thus, the inverse Gaussian process regression model can significantly outperform the forward counterpart, as we observe here.

The geometric logit and probit linear and Gaussian process regressions are examples of model misspecifications since the true, data-generating model is the Poisson log-linear regression model. Accordingly, both the forward and inverse setups perform worse than the Poisson regression setups. Among the forward and inverse cases for geometric regression, the probit linear model performs the best, followed closely by the logit linear model, then by the forward logit Gaussian process and then by the forward probit Gaussian process – all the inverse regression models perform worse than the worse of the forward regression models. This is not surprising since all these models are cases of misspecifications and given the data generated from the true model, the inverse models here only increase the uncertainty regarding $x_{j}$ compared to the forward models without any positive effect. However, note that the inverse logit Gaussian process model significantly outperforms the inverse logit linear model thanks to its better flexibility and similar prior structure for $\tilde{x}_i$ as in the case of the true log-linear Poisson regression whose positive effects carry over to this case from the first two rows of the last column of Table 9.1. But the same phenomenon of superiority of the inverse probit Gaussian process over inverse probit linear model is not at all visible since the prior structure of $\tilde{x}_i$ in this misspecified case is completely different from that of the true Poisson log-linear model, and indeed, inconsistent.

9.4 Variable selection in Poisson and geometric linear and nonparametric regression models when true model is Poisson linear regression

Rather than a single covariate $x$ in the previous examples, let us now consider covariates $x$ and $z$, where the true data-generating distribution is $y_{ij} \sim Poisson(\lambda(x_i, z_i))$, with $\lambda(x, z) = \exp(a_0 + \beta_0 x + \gamma_0 z)$. We generate the data by simulating $a_0, \beta_0, \gamma_0 \sim U(-1, 1)$, independently; and $x_i \sim U(-1, 1), z_i \sim U(0, 2); i = 1, \ldots, n$, and then finally simulating $y_{ij} \sim Poisson(\lambda(x_i, z_i)); j = 1, \ldots, m, i = 1, \ldots, n$.

We model the data $y_{ij}; i = 1, \ldots, n; j = 1, \ldots, m$ with both Poisson and geometric models as before with the regression part consisting of either $x$ or $z$, or both. We denote the linear
regression coefficients of the intercept, $x$ and $z$ as $\alpha$, $\beta$ and $\gamma$, respectively, and give the improper prior density 1 to $(\alpha, \beta)$, $(\alpha, \gamma)$ and $(\alpha, \beta, \gamma)$ when the models consist of these combinations of parameters. For Gaussian process regression with both $x$ and $z$, we let $\eta(x, z)$ be the regression function modeled by a Gaussian process with mean $\mu(x, z) = \alpha + \beta x + \gamma z$ and covariance function $\text{Cov}(\eta(x_1, z_1), \eta(x_2, z_2)) = \exp(\omega) \exp\left(-\{(x_1 - x_2)^2 + (z_1 - z_2)^2\}\right)$, and we assign prior mass 1 to $(\alpha, \beta, \omega)$, $(\alpha, \gamma, \omega)$ and $(\alpha, \beta, \gamma, \omega)$ when the models consist of the covariates $x$, $z$ or both. Using FPBF and IPBF we then compare the different models, along with the covariates associated with them. In the inverse cases, where the model consists of the single covariate $x$ or $z$, then the priors for $\tilde{x}_i$ and $\tilde{z}_i$ remain the same as in the previous cases.

But wherever the models consist of both the covariates $x$ and $z$, we need to assign priors for both $\tilde{x}_i$ and $\tilde{z}_i$, in addition to requiring that $E(y_{ij} | \theta, x_i, z_i)$ under the postulated model fall in $\left[\bar{y}_i - \frac{c_1 s_i}{\sqrt{m}}, \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}}\right]$. The same priors for $\tilde{x}_i$ and $\tilde{z}_i$ as the previous situations where the models consisted of single covariates, will not be consistent in these situations. For consistent priors we adopt the following strategy. Letting $\alpha$ be the intercept, $\beta$ and $\gamma$ the coefficients of $x_i$ and $z_i$ respectively in the regression forms, we envisage the following priors for $\tilde{x}_i$ and $\tilde{z}_i$.

9.4.1 Prior for $\tilde{x}_i$ and $\tilde{z}_i$ for Poisson regression

For the Poisson linear or Gaussian process regression model with log link consisting of both the covariates $x$ and $z$, we set $\tilde{x}_i \sim U(a_x^{(1)}, b_x^{(1)})$ and $\tilde{z}_i \sim U(a_z^{(1)}, b_z^{(1)})$, where

$$a_x^{(1)} = \min \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha - \gamma z_i \right), \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha - \gamma z_i \right) \right\},$$

$$b_x^{(1)} = \max \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha - \gamma z_i \right), \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha - \gamma z_i \right) \right\},$$

$$a_z^{(1)} = \min \left\{ \gamma^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right), \gamma^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right) \right\},$$

and

$$b_z^{(1)} = \max \left\{ \gamma^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right), \gamma^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right) \right\}.$$

Note that the priors for $\tilde{x}_i$ and $\tilde{z}_i$ depend upon $z_i$ and $x_i$ respectively. This is somewhat in keeping with (8.6) where the prior for $\tilde{x}_i$ depends upon $x_i$ itself. The discussion following (8.6) is enough to justify that the priors for $\tilde{x}_i$ and $\tilde{z}_i$ in the current situation do make sense.
from ensuring consistency.

9.4.2 Prior for \( \tilde{x}_i \) and \( \tilde{z}_i \) for geometric regression with logit link

For the geometric linear or Gaussian process regression model with logit link consisting of both the covariates \( x \) and \( z \), we set \( \tilde{x}_i \sim U \left( a_x^{(2)}, b_x^{(2)} \right) \) and \( \tilde{z}_i \sim U \left( a_z^{(2)}, b_z^{(2)} \right) \), where

\[
a_x^{(2)} = \min \left\{ -\beta^{-1} \left( \log \left( \frac{\bar{y}_i - c_1 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right), -\beta^{-1} \left( \log \left( \frac{\bar{y}_i + \delta s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) \right\},
\]

\[
b_x^{(2)} = \max \left\{ -\beta^{-1} \left( \log \left( \frac{\bar{y}_i - c_1 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right), -\beta^{-1} \left( \log \left( \frac{\bar{y}_i + \delta s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) \right\},
\]

\[
a_z^{(2)} = \min \left\{ -\gamma^{-1} \left( \log \left( \frac{\bar{y}_i - c_1 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right), -\gamma^{-1} \left( \log \left( \frac{\bar{y}_i + \delta s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) \right\}
\]

and

\[
b_z^{(2)} = \max \left\{ -\gamma^{-1} \left( \log \left( \frac{\bar{y}_i - c_1 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right), -\gamma^{-1} \left( \log \left( \frac{\bar{y}_i + \delta s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) \right\}.
\]

9.4.3 Prior for \( \tilde{x}_i \) and \( \tilde{z}_i \) for geometric regression with probit link

For the geometric linear or Gaussian process regression model with probit link consisting of both the covariates \( x \) and \( z \), we set \( \tilde{x}_i \sim U \left( a_x^{(3)}, b_x^{(3)} \right) \) and \( \tilde{z}_i \sim U \left( a_z^{(3)}, b_z^{(3)} \right) \), where

\[
a_x^{(3)} = \min \left\{ \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \gamma z_i, \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \gamma z_i \right\},
\]

\[
b_x^{(3)} = \max \left\{ \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \gamma z_i, \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \gamma z_i \right\},
\]

\[
a_z^{(3)} = \min \left\{ \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \beta x_i, \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \beta x_i \right\}
\]

and

\[
b_z^{(3)} = \max \left\{ \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \beta x_i, \Phi^{-1} \left( \frac{1}{\tau_{im+1}} \right) - \alpha - \beta x_i \right\}.
\]

9.4.4 Results of the simulation experiment for model and variable selection

For \( n = m = 10 \), when the true model is Poisson with log-linear regression on both the covariates \( x \) and \( z \), the last two columns of Table 9.2 provide the estimates of \( \frac{1}{n} \sum_{i=1}^{n} \log \pi(y_1 | Y_{nm-i}, X_{n}, M) \) and \( \frac{1}{n} \sum_{i=1}^{n} \log \pi(y_1 | Y_{nm-i}, X_{n-i}, M) \) for Poisson and geometric linear and Gaussian process regression on either \( x_i \) or \( z_i \) or both, with different link functions. Thus, the models, along with the associated covariates can be compared with respect to both forward and inverse perspectives.

Table 9.2 shows that the correct Poisson log-linear model with both the covariates \( x \) and \( z \) has turned out to be the third best, after the inverse Poisson log-linear model with covariate
and the forward Poisson log-linear model with covariate $z$. However, the difference between the latter and the correct model is not substantial and may perhaps be attributed to Monte Carlo sampling fluctuations. So, considering only the forward setup, it is difficult to rule out the possibility of the correct Poisson log-linear model with both the covariates $x$ and $z$ from being the best.

That the inverse Poisson log-linear model with covariate $x$ seems to perform so well can be attributed to significant variability of the prior for $\tilde{x}_i$ which goes on to account for the missing $z_i$ as well in the additive model. Since the additive model is not identifiable when both $x_i$ and $z_i$ are unknown, the significant prior variability of $\tilde{x}_i$ compensates for non-inclusion of $z_i$ in the model, given the data that has arisen from the true model consisting of both $x$ and $z$. The same argument is valid for good performance of the inverse Poisson log-linear model with covariate $z$, where the prior variance for $\tilde{z}_i$ compensates for non-inclusion of $x_i$. However, note that the performance of the inverse Poisson log-linear model deteriorates significantly when the regression consists of both $x$ and $z$. This is of course the consequence of the priors for both $\tilde{x}_i$ and $\tilde{z}_i$, whose variances get added up in the linear model. For small $n$ and $m$ as in our examples, the true values $x_i$ and $z_i$ fail to get enough posterior weight, an issue that gets reflected in the Monte Carlo simulations where the true regression is not represented in sufficiently large proportion.

For Poisson Gaussian process regression, the inverse models outperform their forward counterparts by large margins. This admits similar explanation provided in Section 9.3.1 for the superiority of the inverse Poisson Gaussian process model compared to its forward counterpart as visible in Table 9.1.

For geometric linear regression, the forward models emerge the winners in all the cases, as opposed to the inverse counterparts and also outperform the Gaussian geometric process regression models. Among the geometric models, the probit linear model with both the covariates $x$ and $z$, turns out to be the best. That the corresponding inverse counterparts perform worse can be explained as in Section 9.3.1 that these are instances of model misspecification, and here the inverse models only increase uncertainty by treating $x_i$ and $z_i$ as unknown, without any beneficial effect.

In geometric Gaussian process regression, the inverse models perform better than the corresponding forward ones in most cases. In these cases, given the data generated from the true model, the Gaussian process dependence combined with the prior variability render the inverse models somewhat less misspecified than the forward models with no prior associated with the covariates.

Also observe that given either forward or inverse setups, the linear models perform better than the corresponding Gaussian process models, for both Poisson and geometric cases. Since the true regression is linear, this seems to provide an internal consistency. However, this phenomenon is somewhat different from that observed in Table 9.1 where the Gaussian process model performed better than the linear regression model for Poisson and geometric logit models. The reason for this is inconsistency of the prior for $\tilde{x}_i$ when covariate $z$ is ignored and that of the prior for $\tilde{z}_i$ when covariate $x$ is ignored in the postulated model. Indeed, Table 9.2 shows that in these cases, the inverse linear models outperform the Gaussian process models by considerably large margins. In these cases the Gaussian process priors only increase uncertainties without adding any value, since the priors for $\tilde{x}_i$ and $\tilde{z}_i$ are inconsistent. On the other hand, note that when both $x$ and $z$ are incorporated in the inverse models, the linear models perform only marginally better than the Gaussian process models in the cases of inverse Poisson and inverse geometric logit models. This is because the priors of $\tilde{x}_i$ and $\tilde{z}_i$ are consistent in such cases, and moreover, the prior structures of $\tilde{x}_i$ and $\tilde{z}_i$ are similar for Poisson and geometric logit regressions. For geometric probit regression, the prior structures are entirely different from those of the correct Poisson model and in fact inconsistent, and as in Table 9.1, here also inverse geometric probit Gaussian process regression performs much worse than inverse
geometric probit linear regression.

Table 9.2: Results of our simulation study for model and variable selection using FPBF and IPBF. The last two columns show the estimates of $\frac{1}{n} \sum_{i=1}^{n} \log p(y_{ni}|\mathbf{Y}_{n_{m-1}}, \mathbf{X}_{n|\mathbf{M}})$ and $\frac{1}{n} \sum_{i=1}^{n} \log p(y_{ni}|\mathbf{Y}_{n_{m-1}}, \mathbf{X}_{n|\mathbf{M}})$, respectively, for forward and inverse setups.

| Covariates | Model               | Link function | Regression form   | Forward | Inverse |
|------------|---------------------|---------------|------------------|---------|---------|
| $x_i$      | Poisson($\lambda(x_i)$) | log           | linear           | -8.618  | -8.388  |
| $z_i$      | Poisson($\lambda(z_i)$) | log           | linear           | -8.834  | -8.739  |
| $(x_i, z_i)$ | Poisson($\lambda(x_i, z_i)$) | log | linear | -8.686  | -13.257 |
| $x_i$      | Poisson($\lambda(x_i)$) | log           | Gaussian process | -31.834 | -9.136  |
| $z_i$      | Poisson($\lambda(z_i)$) | log           | Gaussian process | -31.213 | -10.052 |
| $(x_i, z_i)$ | Geometric($p(x_i)$)   | logit         | linear           | -9.784  | -10.526 |
| $z_i$      | Geometric($p(z_i)$)   | logit         | linear           | -9.673  | -12.629 |
| $(x_i, z_i)$ | Geometric($p(x_i, z_i)$) | logit | linear | -11.806 | -15.478 |
| $x_i$      | Geometric($p(x_i)$)   | logit         | Gaussian process | -26.232 | -21.161 |
| $z_i$      | Geometric($p(z_i)$)   | logit         | Gaussian process | -19.391 | -29.388 |
| $(x_i, z_i)$ | Geometric($p(x_i, z_i)$) | logit | Gaussian process | -17.128 | -15.686 |
| $x_i$      | Geometric($p(x_i)$)   | probit        | linear           | -9.543  | -11.671 |
| $z_i$      | Geometric($p(z_i)$)   | probit        | linear           | -9.401  | -16.183 |
| $(x_i, z_i)$ | Geometric($p(x_i, z_i)$) | probit | linear | -9.606  | -13.839 |
| $x_i$      | Geometric($p(x_i)$)   | probit        | Gaussian process | -23.538 | -16.460 |
| $z_i$      | Geometric($p(z_i)$)   | probit        | Gaussian process | -20.522 | -17.099 |
| $(x_i, z_i)$ | Geometric($p(x_i, z_i)$) | probit | Gaussian process | -20.102 | -20.501 |

10 Summary and future direction

The importance of PBF in Bayesian model and variable selection seems to have been overlooked in the statistical literature. In this article we have pointed out the theoretical and computational advantages of PBF over BF, and investigated the asymptotic convergence properties of PBF in general forward and inverse regression setups. Since the inverse regression problem requires a prior on the covariate value to be predicted, this makes the treatise of PBF distinct from the forward regression problems. Specifically, we considered two setups for inverse regression. One setup is the same as that of forward regression except a prior for the relevant covariate value $\hat{x}_i$. Although the priors in this case can not guarantee consistency of the posterior for $\hat{x}_i$, we show that the corresponding PBF still converges exponentially and almost surely in favour of the better model, in the same way as for forward regression. However, for the inverse case, the convergence depends upon an integrated version of the KL-divergence, rather than KL-divergence as in the forward case. In another inverse regression setup, we consider $m$ responses corresponding to each covariate value, and assign the general prior for $\hat{x}_i$ constructed by Chatterjee and Bhattacharya (2020). This prior guarantees consistency for the posterior of $\hat{x}_i$ when $m$ tends to infinity, along with the sample size. For this inverse setup, PBF has convergence results similar to that of forward regression which is also applicable to this setup, except that no prior is associated with the covariates.

Our results on PBF for forward regression are in agreement with the general BF convergence theory established in Chatterjee et al. (2018), as both are the same almost sure sure exponential convergence depending upon the KL-divergence from the true model. Now there might arise the question if PBF and BF convergence agree even for inverse regression setups. To clarify, first recall that BF is the ratio of the marginal densities of the data. Now for forward regression, the marginal density of the data $\mathbf{Y}_n$ depends upon the observed covariates $\mathbf{X}_n$. For model
\( \mathcal{M}_j; j = 1, 2 \), let us denote this marginal by \( m(Y_n|X_n, M_j) \). In the inverse setup, we need to treat \( X_n \) as unknown, and replace this with \( \tilde{X}_n = (\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n) \) having some relevant prior, which may even follow from some stochastic process specification for \( \tilde{X}_\infty = (\tilde{x}_1, \tilde{x}_2, \ldots) \). If \( L(\theta_j|Y_n, X_n, M_j) \) denotes the likelihood of \( \theta_j \) for fully observed data, then the marginal density of \( Y_n \) in the inverse situation is given by

\[
\tilde{m}(Y_n|M_j) = \int_{\Theta_j} \int_{X^n} L(\theta_j|Y_n, \tilde{X}_n, M_j) d\pi(\tilde{X}_n|\theta_j, M_j) d\pi(\theta_j|M_j)
\]

where

\[
\tilde{L}(\theta_j|Y_n, M_j) = \int_{X^n} L(\theta_j|Y_n, \tilde{X}_n, M_j) d\pi(\tilde{X}_n|\theta_j, M_j).
\]

Letting

\[
\tilde{\pi}(\theta_j|Y_n, M_j) = \frac{\tilde{L}(\theta_j|Y_n, M_j) \pi(\theta_j|M_j)}{\tilde{m}(Y_n|M_j)}
\]

we have for all \( \theta_j \in \Theta_j \),

\[
\log \tilde{m}(Y_n|M_j) = \log \tilde{L}(\theta_j|Y_n, M_j) + \log \pi(\theta_j|M_j) - \log \tilde{\pi}(\theta_j|Y_n, M_j),
\]

which reduces the inverse marginal to the same form as that used by Chatterjee et al. (2018) for establishing their almost sure exponential BF convergence result which depends explicitly on the KL-divergence rate between the postulated and the true models. Hence, even in both the inverse setups that we consider, our PBF and BF convergence results agree.

We have illustrated our general asymptotic results for PBF with several theoretical examples, including linear, quadratic, AR(1) regression and variable selection, providing the explicit theoretical calculations for both forward and inverse setups. Our AR(1) regression results validate our general PBF convergence theory in a dependent data setup.

We also conducted extensive simulation experiments with small simulated datasets comparing Poisson log regression and geometric logit and probit regressions, where the regressions are modeled by straight lines as well as Gaussian process based nonparametric functions. Both forward and inverse setups are undertaken, which include, in addition, variable selection among two possible covariates. Among several insightful revelations, our results demonstrate that the inverse regression can outperform the forward counterpart when the regression considered is nonparametric.

Thus, overall the premise for PBF investigation seems promising enough to pursue further research. In particular, we shall address PBF based variable selection in both forward and inverse regression contexts in the so-called “large \( p \), small \( n \)” framework, where the number of variables considered increases with sample size with various rates, crucially, at rates faster than the sample size. Various complex and high-dimensional real data based applications shall also be considered for model and variable selection using forward and inverse PBF. More sophisticated computational methods combining advanced versions of TMCMC, bridge sampling and path sampling may need to be created for accurate estimations of PBF in such real situations. These ideas will be communicated elsewhere.
Appendix

A Preliminaries for ensuring posterior consistency under general setup

Following Shalizi (2009) we consider a probability space $(\Omega, \mathcal{F}, P)$, and a sequence of random variables $y_1, y_2, \ldots$, taking values in some measurable space $(\Xi, \mathcal{Y})$, whose infinite-dimensional distribution is $P$. Let $Y_n = \{y_1, \ldots, y_n\}$. The natural filtration of this process is $\sigma(Y_n)$, the smallest $\sigma$-field with respect to which $Y_n$ is measurable.

We denote the distributions of processes adapted to $\sigma(Y_n)$ by $F_{\theta}$, where $\theta$ is associated with a measurable space $(\Theta, \mathcal{T})$, and is generally infinite-dimensional. For the sake of convenience, we assume, as in Shalizi (2009), that $P$ and all the $F_{\theta}$ are dominated by a common reference measure, with respective densities $f_{\theta_0}$ and $f_{\theta}$. The usual assumptions that $P \in \Theta$ or even $P$ lies in the support of the prior on $\Theta$, are not required for Shalizi’s result, rendering it very general indeed.

A.1 Assumptions and theorems of Shalizi

(S1) Consider the following likelihood ratio:

$$R_n(\theta) = \frac{f_{\theta}(Y_n)}{f_{\theta_0}(Y_n)}.$$ 

Assume that $R_n(\theta)$ is $\sigma(Y_n) \times \mathcal{T}$-measurable for all $n > 0$.

(S2) For every $\theta \in \Theta$, the KL-divergence rate

$$h(\theta) = \lim_{n \to \infty} \frac{1}{n} E\left( \log \frac{f_{\theta_0}(Y_n)}{f_{\theta}(Y_n)} \right),$$

exists (possibly being infinite) and is $\mathcal{T}$-measurable.

(S3) For each $\theta \in \Theta$, the generalized or relative asymptotic equipartition property holds, and so, almost surely,

$$\lim_{n \to \infty} \frac{1}{n} \log R_n(\theta) = -h(\theta).$$

(S4) Let $I = \{\theta : h(\theta) = \infty\}$. The prior $\pi$ satisfies $\pi(I) < 1$.

(S5) There exists a sequence of sets $G_n \to \Theta$ as $n \to \infty$ such that:

1. $\pi(G_n) \geq 1 - \zeta \exp(-\gamma n)$, for some $\zeta > 0$, $\gamma > 2h(\Theta)$;  
2. The convergence in (S3) is uniform in $\theta$ over $G_n \setminus I$.
3. $h(G_n) \to h(\Theta)$, as $n \to \infty$.

For each measurable $A \subseteq \Theta$, for every $\delta > 0$, there exists a random natural number $\tau(A, \delta)$ such that

$$n^{-1} \log \int_A R_n(\theta) \pi(\theta)d\theta \leq \delta + \limsup_{n \to \infty} n^{-1} \log \int_A R_n(\theta) \pi(\theta)d\theta,$$

for all $n > \tau(A, \delta)$, provided $\limsup_{n \to \infty} n^{-1} \log \pi(1_A R_n) < \infty$. Regarding this, the following assumption has been made by Shalizi:
(S6) The sets $G_n$ of (S5) can be chosen such that for every $\delta > 0$, the inequality $n > \tau(G_n, \delta)$ holds almost surely for all sufficiently large $n$.

(S7) The sets $G_n$ of (S5) and (S6) can be chosen such that for any set $A$ with $\pi(A) > 0$,

$$h(G_n \cap A) \rightarrow h(A),$$

as $n \rightarrow \infty$.

**B A result on sufficient condition for (S6) of Shalizi**

**Theorem 27.** Consider the following assumptions:

(i) Let $\tilde{\theta} = \arg \min_{\theta \in \Theta} h(\theta)$ be the unique minimizer of $h(\theta)$ on $\Theta$.

(ii) Let $\tilde{\theta}_n^* = \arg \max_{\theta \in \Theta} \frac{1}{n} \log R_n(\theta)$, and assume that $\tilde{\theta}_n^* \xrightarrow{a.s.} \tilde{\theta}$, as $n \rightarrow \infty$.

(iii) $\frac{1}{n} \log R_n(\theta)$ is stochastically equicontinuous on compact subsets of $\Theta$.

(iv) For all $\theta$ in such compact subsets,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log R_n(\theta) = h(\theta),$$

almost surely.

(v) The prior $\pi$ on $\Theta$ is proper.

Then (7.18) holds.

**Proof.** Note that

$$\frac{1}{n} \log \int_{G_n} R_n(\theta) \pi(\theta) d\theta \leq \frac{1}{n} \log \left( \sup_{\theta \in G_n} R_n(\theta) \right) + \frac{1}{n} \log \pi(G_n)
= \sup_{\theta \in G_n} \frac{1}{n} \log R_n(\theta) + \frac{1}{n} \log \pi(G_n)
= \frac{1}{n} \log R_n(\tilde{\theta}_n^*) + \frac{1}{n} \log \pi(G_n).$$

(B.2)

Since by condition (ii), $\tilde{\theta}_n^* \xrightarrow{a.s.} \tilde{\theta}$ as $n \rightarrow \infty$, for any $\epsilon > 0$, there exists $n_0(\epsilon) \geq 1$ such that for $n \geq n_0(\epsilon)$,

$$\tilde{\theta}_n^* \in (\tilde{\theta} - \epsilon, \tilde{\theta} + \epsilon),$$

almost surely.

(B.3)

Conditions (iii) and (iv) validate the stochastic Ascoli lemma, and hence, for any compact subset $G$ of $\Theta$ that contains $(\tilde{\theta} - \epsilon, \tilde{\theta} + \epsilon)$,

$$\lim_{n \rightarrow \infty} \sup_{\theta \in G} \left| \frac{1}{n} \log R_n(\theta) + h(\theta) \right| = 0,$$

almost surely.

Hence, for any $\xi > 0$, for all $\theta \in G$, almost surely,

$$\frac{1}{n} \log R_n(\theta) \leq -h(\theta) + \eta \leq -h(\Theta) + \eta,$$

for sufficiently large $n$.

(B.4)

Since $G$ contains $(\tilde{\theta} - \epsilon, \tilde{\theta} + \epsilon)$, which, in turn contains $\tilde{\theta}_n^*$ for sufficiently large $n$, due to (B.3), it follows from (B.4), that for any $\xi > 0$,

$$\frac{1}{n} \log R_n(\tilde{\theta}_n^*) \leq -h(\Theta) + \eta,$$

for sufficiently large $n$.

(B.5)
The proof follows by combining (B.2) and (B.5), and noting that $\frac{1}{n} \log \pi(G_n) < 0$ for all $n \geq 1$, since $0 < \pi(G_n) < 1$ for proper priors.

\section*{C Proof of Theorem 17}

Our proof uses concepts that are broadly similar to that of Theorem 10 of Chandra and Bhattacharya (2020). Here we shall provide the proof for $\frac{1}{n} \log R_n(\theta)$ since that for $\frac{1}{n} \log R_n^{(2)}(\theta)$ is exactly the same. For notational convenience, we denote $\frac{1}{n} \log R_n^{(1)}(\theta)$ by $\frac{1}{n} \log R_n(\theta)$, $h_1(\theta)$ by $h(\theta)$, $\tilde{\theta}$ by $\tilde{\theta}$ and $\Theta_1$ by $\Theta$.

Since $h(\theta)$ is convex, $\tilde{\theta}$ must be an interior point of $\Theta$. Hence, there exists a compact set $G \subset \Theta$ such that $\tilde{\theta}$ is interior to $G$. From convergence (7.43) which is also uniform on compact sets, it follows that

$$\lim_{n \to \infty} \sup_{\theta \in G} \left| \frac{1}{n} \log R_n(\theta) + h(\theta) \right| = 0. \tag{C.1}$$

For any $\eta > 0$, we define

$$N_\eta(\tilde{\theta}) = \{ \theta : \| \tilde{\theta} - \theta \| < \eta \}; \quad N_\eta'(\tilde{\theta}) = \{ \theta : \| \tilde{\theta} - \theta \| = \eta \}; \quad \overline{N_\eta}(\tilde{\theta}) = \{ \theta : \| \tilde{\theta} - \theta \| \leq \eta \}.$$

Note that for sufficiently small $\eta$, $\overline{N_\eta}(\tilde{\theta}) \subset G$. Let $H = \inf_{\theta \in N_\eta'(\tilde{\theta})} h(\theta)$. Since $h(\theta)$ is minimum at $\theta = \tilde{\theta}$, $H > 0$. Let us fix an $\varepsilon$ such that $0 < \varepsilon < H$. Then by (C.1), for large enough $n$ all $\theta \in N_\eta'(\tilde{\theta})$,

$$\frac{1}{n} \log R_n(\theta) < -h(\tilde{\theta}) + \varepsilon < -h(\tilde{\theta}) + \varepsilon. \tag{C.2}$$

Since by (7.43) $\frac{1}{n} \log R_n(\tilde{\theta}) > -h(\tilde{\theta}) - \varepsilon$ for sufficiently large $n$, it follows from this and (C.2) that

$$\frac{1}{n} \log R_n(\theta) < \frac{1}{n} \log R_n(\tilde{\theta}) + 2\varepsilon, \tag{C.3}$$

for sufficiently large $n$. Since $0 < \varepsilon < H$ is arbitrary, it follows that for all $\theta \in N_\eta'(\tilde{\theta})$, for large enough $n$,

$$\frac{1}{n} \log R_n(\theta) < \frac{1}{n} \log R_n(\tilde{\theta}), \tag{C.4}$$

which shows that for large enough $n$, the maximum of $\frac{1}{n} \log R_n(\theta)$ is not attained at the boundary $N_\eta'(\tilde{\theta})$. Hence, the maximum must occur in the interior of $\overline{N_\eta}(\tilde{\theta})$ when $n$ is sufficiently large. That the maximizer is unique is guaranteed by Theorem 16. Hence, the result is proved.

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