A Bayesian Multiple Testing Paradigm for Model Selection in Inverse Regression Problems

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Abstract

Model selection in inverse regression problems where the objective is to infer about unobserved covariate values from observed responses and covariates, is almost non-existent in the statistical literature, a recent exception being consideration of pseudo-Bayes factors for such purpose (Chatterjee and Bhattacharya (2020a)).

In this article, we propose a novel Bayesian multiple testing formulation for model and variable selection in inverse setups, judiciously embedding the idea of inverse reference distributions proposed by Bhattacharya (2013) in a mixture framework consisting of the competing models. We develop the theory and methods in the general context encompassing parametric and nonparametric competing models, dependent data, as well as misspecifications. Our investigation shows that asymptotically the multiple testing procedure almost surely selects the best possible inverse model that minimizes the minimum Kullback-Leibler divergence from the true model. We also show that the error rates, namely, versions of the false discovery rate and the false non-discovery rate converge to zero almost surely as the sample size goes to infinity. Asymptotic α-control of versions of the false discovery rate and its impact on the convergence of false non-discovery rate versions, are also investigated.

With an aim to compare our multiple testing procedure with pseudo-Bayes factor, we consider the same simulation experiments with the same datasets reported in Chatterjee and Bhattacharya (2020a). The experiments involve small sample based selection among inverse Poisson log regression and inverse geometric logit and probit regression, where the regressions are either linear or based on Gaussian processes. Additionally, variable selection is also considered. Our multiple testing results turn out to be very encouraging in the sense of selecting the best models in all the cases and convincingly outperforming the pseudo-Bayes factors.

Keywords: Bayesian multiple testing; Forward and inverse regression; Importance Resampling MCMC; Kullback-Leibler divergence; Model and variable selection; Leave-one-out cross-validation.

1 Introduction

Model selection is arguably the most important area of statistics, which has received, and is continuing to receive, considerable attention. But in spite of immense importance and popularity of this field, the issue of model selection in the context of inverse regression problems has received almost no attention in either the classical or the Bayesian statistical literature.

In inverse regression problems the objective is to infer about unobserved covariate values from observed responses and covariates, and hence from the Bayesian perspective, a prior must be specified for the unknown covariate values. Thus, it is in contrast with the traditional forward regression problems where given some covariate values, the response needs to be predicted. An interesting motivation for the inverse regression setup is the quantitative palaeoclimate reconstruction problem where multivariate counts of a number of species are available along
with the observed climate values in modern times. Typically, data collected on or after the year 1950 are regarded as ‘modern data’. Also available are fossil assemblages of the same set of 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. Thus, the species count data, which are the response variables, are modeled as functions of the climate variables, which are the covariates in this case. But the interest lies in prediction of climate variables, given the species count data, thereby pointing towards the inverse nature of the problem. Chatterjee and Bhattacharya (2017) provide other examples of inverse regression problems.

As already mentioned, model selection in such inverse setups is almost non-existent in the statistical literature. A recent exception is the consideration of pseudo-Bayes factors for such purpose (Chatterjee and Bhattacharya (2020a)). Pseudo-Bayes factors seem to have been first constructed by Geisser and Eddy (1979) by combining the ideas of Bayes factor and cross-validation. Notably, although the Bayes factor approach is arguably the most principled and coherent approach to model comparison, Bayes factors are usually difficult to compute in practice and suffer from numerical instability. Moreover, they are well-known to suffer from the so-called Lindley’s paradox. The cross-validation idea proposed by Geisser and Eddy (1979) is to replace the marginal density of the entire dataset in Bayes factors with products of cross-validation densities of individual data points. This constitutes the pseudo-Bayes factors which are computationally far simpler and numerically much more stable than the corresponding Bayes factors. Furthermore, they are also immune to Lindley’s paradox. Recognizing the importance, Chatterjee and Bhattacharya (2020a) establish the asymptotic theory for pseudo-Bayes factors for both forward and inverse parametric and nonparametric regression problems in a very general setup that allows for dependent data and misspecified models. They illustrate their results with various theoretical examples and simulation experiments for small samples that even include simultaneous selection of models and covariates. The results of their simulation experiments, although interesting and insightful, do leave the scope for further improvement.

The area of multiple hypotheses testing can be envisaged as a promising alternative to Bayes factors for model selection if properly formulated, and can bring about the aforementioned desired improvement in inverse model selection. Unfortunately, in spite of rising popularity of the multiple testing paradigm for general testing problems, its applicability and utility in general model selection problems remain yet to be thoroughly investigated. In the classical multiple comparison context, Shimodaira (1998) use the sampling error of the Akaike Information Criterion (AIC) to select a “confidence set of models” rather than a single model. The method requires computation of standardized difference of AIC for every pair of models. Since every pair of models is involved, clearly, for even a moderate number of competing models the computation becomes infeasible, and reliability of the proposed normal approximation need not be unquestionable in general situations. We are not aware of any other significant research on model selection in the multiple testing framework. Furthermore, multiple testing based model selection in inverse setups has not been hitherto even perceived.

In this article, for the first time ever, we propose and develop a Bayesian multiple testing paradigm for inverse model selection problems. Our starting point is the inverse reference distribution approach to Bayesian assessment of adequacy of inverse models introduced by Bhattacharya (2013). In a nutshell, the inverse model adequacy assessment idea is as follows. Given response data \( Y_n = \{y_1, \ldots, y_n\} \), covariate data \( X_n = \{x_1, \ldots, x_n\} \), and the Bayesian model for the data, consider the inverse leave-one-out cross-validation setup where for each \( i = 1, \ldots, n \), \( x_i \) needs to be predicted from the rest of the data and the underlying Bayesian model. Letting \( \tilde{x}_i \) denote the random variable corresponding to \( x_i \) when the latter is treated
as unknown, the interest is then in the cross-validation posteriors \( \pi(\tilde{x}_i | X_{n,-i}, Y_n); i = 1, \ldots, n \), where \( X_{n,-i} = \{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n\} \). Letting \( \tilde{X}_n = \{\tilde{x}_1, \ldots, \tilde{x}_n\} \), Bhattacharya (2013) considers the ‘inverse reference distribution’ of some suitable discrepancy measure \( T(\tilde{X}_n) \) where \( \tilde{x}_i \sim \pi(\cdot | X_{n,-i}, Y_n); i = 1, \ldots, n \). If the observed discrepancy measure \( T(X_n) \) falls within the desired \( 100(1 - \alpha)\% \) credible interval of \( T(\tilde{X}_n) \) where \( \alpha \in (0,1) \), then the underlying Bayesian model fits the data and not otherwise. Bhattacharya (2013) provides a Bayesian decision theoretic formalization of the above idea and investigates its theoretical and methodological properties, pointing out its advantages over existing ideas on forward Bayesian model assessment. The encouraging results obtained in simulation experiments and real data analyses reported in Bhattacharya (2013), Bhattacharya (2006) and Mukhopadhyay and Bhattacharya (2013) demonstrate the worth of the inverse model assessment idea using inverse reference distributions of appropriate discrepancy measures. Typical examples of discrepancy measures are given, for any \( n \)-dimensional vector \( v_n = (v_1, \ldots, v_n) \), by

\[
T_1(v_n) = \sum_{i=1}^{n} \frac{|v_i - E(\tilde{x}_i | X_{n,-i}, Y_n)|}{\sqrt{Var(\tilde{x}_i | X_{n,-i}, Y_n)}}
\]

and

\[
T_2(v_n) = \sum_{i=1}^{n} \frac{(v_i - E(\tilde{x}_i | X_{n,-i}, Y_n))^2}{Var(\tilde{x}_i | X_{n,-i}, Y_n)}.
\]

Since the inverse reference distribution approach turned out to be useful for assessing adequacy of inverse models, it is natural to discern that such an approach would be valuable even for inverse model selection. This very perception provided the motivation for our Bayesian multiple testing approach to inverse model selection using inverse reference distributions. The key idea is to embed all the competing inverse regression models in a mixture setting to constitute a single model needed for multiple testing. In simple terms, each hypothesis of the multiple testing procedure then essentially tests if the inverse reference distribution of the corresponding inverse regression model gives high posterior probability to appropriate regions containing the observed discrepancy measure for the model, in addition to testing if the posterior model probability is sufficiently high. The best inverse model is expected to have the highest posterior probability with respect to the above and our multiple testing formalism is so designed that it renders this idea precise with relevant coherent supports.

Our theoretical and methodological development deals with parametric and nonparametric inverse competing models, allowing dependent data as well as misspecified models. In this highly general framework we show that our multiple testing procedure almost surely selects the best possible model, as the sample size tends tends to infinity. Here “best” is in terms of the minimizer of the minimum Kullback-Leibler (KL) divergence from the true model, concepts that will be subsequently clarified. Our investigation also brings out the desirable results that the error rates, namely, relevant versions of the false discovery rate and the false non-discovery rate, asymptotically converge to zero almost surely. Insightful theoretical results on asymptotic \( \alpha \)-control of versions of the false discovery rate and its impact on the convergence of versions of the false non-discovery rate, are also presented.

Monte Carlo based computations of the model-specific posterior probabilities associated with the inverse reference distributions proceed via fast and efficient Importance Re-sampling Markov Chain Monte Carlo (IRMCMC) (Bhattacharya and Haslett (2007)) aided by Transformation based Markov Chain Monte Carlo (TMCMC) (Dutta and Bhattacharya (2014)) for generation of MCMC samples from the cross-validation posterior distributions having excellent mixing properties. The posterior model probabilities are based on an efficient Gibbs sampling scheme that utilizes the forward pseudo-Bayes factors for sampling from the relevant full conditional distributions of the model indices. Thus, our entire computational methodology is fast and
efficient, more so because each hypothesis is associated with a single inverse model, and pairwise comparison as in Shimodaira (1998) is ruled out.

Recalling that one of our objectives behind development of this multiple testing paradigm is to obtain superior inverse model selection results compared to those obtained by Chatterjee and Bhattacharya (2020a) using pseudo-Bayes factors, we apply our multiple testing formalism to the same simulation experiments with the same datasets as in Chatterjee and Bhattacharya (2020a). The simulation experiments consist of two sets. In one set small sample based selection among inverse Poisson log regression and inverse geometric logit and probit regression is considered, where the regressions are either linear or based on Gaussian processes. In the other set, variable selection among two covariates is considered in addition to the aforementioned inverse model selection problem. We conduct the experiments in both non-misspecified and misspecified situations. Not only does our multiple testing procedure succeeds in selecting the best inverse models and variables in all the cases, it significantly outperforms the results yielded by the pseudo-Bayes factors.

The rest of our paper is structured as follows. We begin by distinguishing forward and inverse regression problems in Section 2. In Section 3 we introduce and develop our Bayesian multiple testing paradigm for inverse model selection. Then in Section 4 we include a brief overview of Shalizi’s approach (Shalizi (2009)) to dealing with posterior convergence which plays a significant role in the development of the asymptotic theory of our multiple testing procedure; further details are provided in Appendix A.1. We progress towards a general asymptotic theory by establishing in Section 5 the asymptotic properties of the posterior probabilities of the alternative hypotheses. Asymptotic optimality theory for our multiple testing procedure is then provided in Section 6, followed by convergence theory of the measures of error in Section 7. In Section 8 we recommend some judicious modifications of the hypotheses to suit practical implementation, and in Sections 9 and 10 we provide details on two sets of simulation experiments with small samples involving Poisson and geometric linear and Gaussian process regression for relevant link functions, the second set also including in addition the problem of variable selection involving two covariates. Non-misspecified and misspecified situations are addressed in both the simulation experiments. Finally, in Section 11, we summarize our contributions and discuss selection of inverse models in the context of two palaeoclimate reconstruction problems, recasting our previous results on inverse model assessment in the current multiple testing context.

2 Distinction between forward and inverse regression problems

Here we essentially follow the discussion provided in Chatterjee and Bhattacharya (2020a).

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 \(x \in X\), \(X\) being the space of covariates. The part \(\xi\) of \(\theta\) 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
2.1.1 Examples of the forward regression setup

(i) \( y_i \sim \text{Bernoulli}(p_i) \), 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) \( y_i \sim \text{Poisson}(\lambda_i) \), 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 i.i.d 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 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 \( \mathcal{M} \) and the corresponding parameters \( \theta \), we denote such prior by \( \pi(\tilde{x} | \theta, \mathcal{M}) \).

2.3 Inverse regression problem: second setup

In the inverse regression context, we consider another setup under which Chatterjee and Bhattacharya (2020b) 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 \( Y_{nm,-i} = Y_{nm} \setminus \{y_i\} \).

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

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

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

2.3.1 Prior for \( \tilde{x}_i \)

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

\[
\tilde{x}_i \sim U(B_{im}(\theta)),
\]

so that we can represent (2.1) more conveniently as

\[
y_i \sim f(\cdot | \theta, x_i, Y^{(i-1)}) \text{ for } i = 1, \ldots, n. \tag{2.2}
\]
the uniform distribution on
\[
B_{im}(\theta) = \left\{ x : H(\eta(x)) \in \left[ \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}}}{\sqrt{m}}, \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}}}{\sqrt{m}} \right] \right\},
\]
where \( H \) is some suitable transformation of \( \eta(x) \). In (2.5), \( \bar{y}_i = \frac{1}{m} \sum_{j=1}^{m} y_{ij} \) 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 \( \pi(\tilde{x}_i|\eta) \). Chatterjee and Bhattacharya (2020b) show that the density or any probability associated with \( \pi(\tilde{x}_i|\eta) \) is continuous with respect to \( \eta \). Quite importantly, the prior form (2.4) leads to cross-validation posteriors that are consistent at \( x_i \); see Chatterjee and Bhattacharya (2020b).

2.3.2 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 \( \pi(\tilde{x}_i|\theta) \), \( \tilde{x}_i \) has uniform distribution on the set \( B_{im}(\theta) = \left\{ x > 0 : \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}}}{\sqrt{m}} \leq x \leq \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}}}{\sqrt{m}} \right\} \).

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

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

(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 \( \tilde{x}_i \) is the uniform distribution on \( B_{im}(\eta) = \left\{ x : \eta(x) \in \left[ \frac{\bar{y}_i - \frac{cs_i}{\sqrt{m}}}{\sqrt{m}}, \frac{\bar{y}_i + \frac{cs_i}{\sqrt{m}}}{\sqrt{m}} \right] \right\} \).

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

Further examples of the prior in various other inverse regression models are provided in Chatterjee and Bhattacharya (2020a); see also Sections 9 and 10. In this article, we shall throughout assume that the space of covariates \( X \) is compact.

3 A multiple testing framework for model selection in inverse regression problems

Let us consider models \( M_k \); \( k = 1, \ldots, K \), from among which the best model needs to be selected respecting the inverse perspective. In this article, we assume that \( 1 < K < \infty \). We allow the provision that the true, data-generating model is not contained in the set of models being considered. For \( k = 1, \ldots, K \), let \( \theta_k \) and \( \Theta_k \) denote the parameter set and the parameter space associated with model \( M_k \). Let \( \pi(\theta_k|M_k) \) denote the prior for \( \theta_k \) under model \( M_k \).

For our multiple testing treatise, we shall consider the second inverse regression setup detailed in Section 2.3. As such, for \( n > 1 \) and \( m > 1 \), let \( Y_{nn} \) be generated from the marginal distribution of \( M_0 \), the true model having parameters \( \theta_0 \) with prior \( \pi(\theta_0|M_0) \) on parameter space \( \Theta_0 \). Note that \( \pi(\theta_0|M_0) \) may even be the point mass on some element of \( \Theta_0 \).
The dimensions of the parameter spaces $\Theta_0, \Theta_1, \ldots, \Theta_K$ may all be different. We shall consider the consistent prior for $\tilde{x}_i$ detailed in Section 2.3.1.

Now, for $k = 1, \ldots, K$, let $f(Y_{nm}|X_n, \theta_k, \mathcal{M}_k)$ denote the density of $Y_{nm}$ under model $\mathcal{M}_k$. We combine the competing models in the following mixture form:

$$f(Y_{nm}|X_n, \theta) = \sum_{k=1}^{K} p_k f(Y_{nm}|X_n, \theta_k, \mathcal{M}_k),$$  \hspace{1cm} (3.1)

where $\theta = (\theta_1, \ldots, \theta_K)$, $0 \leq p_k \leq 1$, for $k = 1, \ldots, K$ and $\sum_{k=1}^{K} p_k = 1$. Letting $\zeta$ denote the allocation variable (model index), with $P(\zeta = k) = p_k$, note that $f(Y_{nm}|X_n, \theta, \zeta = k) = f(Y_{nm}|X_n, \theta_k, \mathcal{M}_k)$. Now let $\Theta_k$ be a proper subset of $\Theta_k$ assumed to contain the minimizer of the KL-divergence from the true model $\mathcal{M}_0$.

Let $\pi(\tilde{x}_i|\theta_k, \mathcal{M}_k)$ be the prior for $\tilde{x}_i$ given $\theta_k$, under $\mathcal{M}_k$. This yields the familiar (see, for example, Bhattacharya and Haslett (2007), Chatterjee and Bhattacharya (2020b)) inverse cross-validation posterior for $\tilde{x}_i$ given $X_{n,-i}$ and $Y_{nm}$ given by

$$\pi(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k) = \int_{\Theta_k} \pi(\tilde{x}_i|\theta_k, y_i, \mathcal{M}_k)d\pi(\theta_k|X_{n,-i}, Y_{nm}).$$

However, if $\theta_k$ is restricted to $\tilde{\Theta}_k$, then we obtain the following $\tilde{\Theta}_k$-restricted inverse cross-validation posterior for $\tilde{x}_i$ given $X_{n,-i}$ and $Y_{nm}$:

$$\pi(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k) = \frac{\int_{\tilde{\Theta}_k} \pi(\tilde{x}_i|\theta_k, y_i, \mathcal{M}_k)d\pi(\theta_k|X_{n,-i}, Y_{nm})}{\pi(\tilde{\Theta}_k|X_{n,-i}, Y_{nm})}. \hspace{1cm} (3.2)$$

In the misspecified situation, $\theta_0 \notin \Theta_k$, and $\tilde{\theta}_k$ is the minimizer of the limiting KL-divergence rate from $\mathcal{M}_0$. Thus, in the case of misspecification of $\theta_k$, $B_{im}(\tilde{\theta}_k) \xrightarrow{a.s.} \{x^*_ik\}$ as $m \to \infty$, for some non-random $x^*_ik$ ($\neq x_i$), depending upon model $\mathcal{M}_k$. In other words, the prior distribution of $\tilde{x}_i$ given $\theta_k$ and $y_i$ concentrates around $x^*_ik$, as $m \to \infty$. In Theorem 2 we show that the cross-validation posterior of $\tilde{x}_i$ also concentrates around $x^*_ik$. Note that $x^*_ik$ depends upon both $\tilde{\theta}_k$ and $\theta_0$, apart from $x_i$ (and perhaps $x_j$ for some $j \neq i$).

For any $n$-dimensional vector $v_n = (v_1, \ldots, v_n)$, and for some $c > 0$, define

$$T_1^{(k)}(v_n) = \frac{1}{n} \sum_{i=1}^{n} \frac{|v_i - E(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k)|}{\sqrt{Var(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k) + c}}. \hspace{1cm} (3.3)$$

Similarly, let

$$T_2^{(k)}(v_n) = \frac{1}{n} \sum_{i=1}^{n} \frac{(v_i - E(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k))^2}{Var(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k) + c}. \hspace{1cm} (3.4)$$

In (3.3) and (3.4), $\tilde{x}_i$ has the cross-validation posterior distribution (3.2), for $i = 1, \ldots, n$. The positive constant $c$ is not only needed for asymptotics, it plays the role of maintaining stability of the discrepancy measures when $Var(\tilde{x}_i|X_{n,-i}, Y_{nm}, \mathcal{M}_k, \tilde{\Theta}_k)$ is close to zero for some $i \geq 1$. Various other measures of discrepancy can be defined (see Bhattacharya (2013) for a discussion on such discrepancy measures; see also Mukhopadhyay and Bhattacharya (2013)), but for brevity we focus on these two measures in this paper. For a given discrepancy measure $T^{(k)}$, let $[\hat{\ell}_{k\alpha}, \hat{u}_{k\alpha}]$ denote the 100$(1 - \alpha)$% credible interval for the posterior distribution of $T^{(k)}(X_n)$ for any desired $\alpha \in (0, 1)$. In Theorem 5 we
show that for any \( \varepsilon > 0 \), the posterior probability of the event
\[
\left\{ T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \right\}
\]
tends to one almost surely as \( m \to \infty \) and \( n \to \infty \). Here \( a_k \) are positive constants reflecting misspecification. If there is no misspecification, then \( a_k = 0 \).

With the above notions and ideas it seems reasonable to formulate the following multiple testing problem for inverse model selection. For given \( \varepsilon > 0 \) and \( \eta > 0 \), and given discrepancy measure \( T^{(k)} \), consider testing
\[
H_{0k}: p_k > 1 - \eta, \theta_k \in \Theta_k, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon]
\]
versus
\[
H_{1k}: \left\{ p_k \leq 1 - \eta \right\} \cup \left\{ p_k > 1 - \eta, \theta_k \in \tilde{\Theta}_k \right\} \cup \left\{ p_k > 1 - \eta, \theta_k \in \Theta_k, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \right\}.
\]
The positive constants \( a_k \) in the hypotheses should be perceived as analogous to \( a_{1k} \) and \( a_{2k} \) in (5.15) and (5.16).

However, the above multiple testing formulation depends upon the choice of \( \eta \). More importantly, even though the posterior probability of \( \zeta = \tilde{k} \) goes to 1 asymptotically for the best model \( \mathcal{M}_{\tilde{k}} \), that of \( \{ p_k > 1 - \eta \} \), for any \( \eta > 0 \), does not tend to one for any prior on \( (p_1, \ldots, p_K) \). For example, for a Dirichlet prior with parameters \( (\alpha_1, \ldots, \alpha_K) \), where \( a_k > 0 \) for \( k = 1, \ldots, K \), the posterior distribution of \( (p_1, \ldots, p_K) \) given \( \zeta \), the other parameters and the data, is Dirichlet with parameters \( (\alpha_1 + I(\zeta = 1), \ldots, \alpha_K + I(\zeta = K)) \), where for any \( k, I(\zeta = k) = 1 \) if \( \zeta = k \) and zero otherwise. Thus, even if \( \zeta = k \) with posterior probability tending to one, asymptotically the posterior distribution of \( p_k \) does not converge to one. It is thus necessary to modify the above multiple testing formulation, replacing the statements involving \( p_k \) with those involving \( \zeta \). Specifically, we re-write the hypotheses as follows:
\[
H_{0k}: \zeta = k, \theta_k \in \tilde{\Theta}_k, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \quad (3.5)
\]
versus
\[
H_{1k}: \{ \zeta \neq k \} \cup \{ \zeta = k, \theta_k \in \tilde{\Theta}_k \} \cup \{ \zeta = k, \theta_k \in \tilde{\Theta}_k, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \} \quad (3.6)
\]
Henceforth, unless stated otherwise, we shall refer to (3.5) and (3.6) for our multiple testing purpose.

### 3.1 Further discussion of the multiple testing formulation

To select the best model from an inverse perspective we first need to choose a model \( f(Y_{nm}|X_n, \theta_{\tilde{k}}, \mathcal{M}_{\tilde{k}}) \) indexed by \( \zeta = \tilde{k} \) which has high marginal posterior probability. But this is not enough as the inverse context is not reflected in this selection. Indeed, such a selection is the same as in the forward context.

Thus, in addition to selecting such a \( \tilde{k} \), we demand that for such model
\[
T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon]. \quad (3.7)
\]
This reflects the inverse perspective. We further demand that this holds for \( \tilde{X}_n \) associated with some region \( \tilde{\Theta}_k \) of the parameter space that contains the minimizer of the KL-divergence of
\( f(Y_{nm}|X_n, \theta_k, \mathcal{M}_k) \) from the true model. The reason for this is that \( \tilde{\Theta}_k \) is the region that has the highest posterior probability, at least asymptotically, which we shall subsequently establish. Moreover, it follows from Chatterjee and Bhattacharya (2020b) that \( \pi(\theta_k|X_n, Y_{nm}, \mathcal{M}_k) \) and \( \pi(\theta_k|X_{n-i}, Y_{nm}, \mathcal{M}_k) \) are asymptotically the same for any \( i \geq 1 \), for any \( m \geq 1 \). Hence the event (3.7) associated with \( \tilde{\Theta}_k \) for \( k = \tilde{k} \), is expected to be reliable.

We shall also show that asymptotically the posterior probability of the best model, \( \zeta = \tilde{k} \), tends to 1 almost surely. As already mentioned, here the notion the best model is with respect to minimization of the minimum KL-divergence rate from the true model. We shall show that for this \( \tilde{k} \), the posterior probability of \( H_{\tilde{0}k} \) goes to 1 asymptotically, for any \( \varepsilon > 0 \) in (3.7). That is, asymptotically, only one inverse model, namely, the best inverse model satisfying the conditions of \( H_{\tilde{0}k} \), will be selected.

It is useful to remark here that the KL-divergence rate referred to above is completely in the forward sense, where all the \( x_i; i \geq 1 \), are assumed to be known. Hence, the above arguments and our subsequent theoretical underpinnings show that the asymptotic theory is dominated by the forward perspective. In fact, any consistent prior for \( \tilde{x}_i \) would asymptotically lead to the best forward model. However, the above can not be guaranteed in any non-asymptotic sense. The model \( \mathcal{M}_k \) with high posterior probability of \( \{\zeta = \tilde{k}\} \) may have low posterior probability of \( (\tilde{X}_n - T^{(k)}(X_n)) \in [\tilde{\ell}_{knm} - a_k - \varepsilon, \tilde{u}_{knm} - a_k + \varepsilon] \), which may result in overall lower posterior probability of \( H_{\tilde{0}k} \) compared to \( H_{\tilde{0}k} \) for several \( k \neq \tilde{k} \). In such situations, \( \mathcal{M}_k \) will not be the best choice non-asymptotically. Thus, the inverse perspective is particularly important in realistic, non-asymptotic situations. An appropriate Bayesian multiple testing procedure is expected to yield the best possible inference regarding inverse model selection in both asymptotic and non-asymptotic situations, which we now devise.

### 3.2 The Bayesian multiple testing procedure

Chandra and Bhattacharya (2019) proposed a novel Bayesian non-marginal testing procedure for testing general dependent hypotheses. We first briefly discuss their method and then consider a special case of their idea to be applied to inverse model selection context.

Let

\[
  d_k = \begin{cases} 
    1 & \text{if the } k\text{-th hypothesis is rejected;} \\
    0 & \text{otherwise;} 
  \end{cases}
\]

\[
  r_k = \begin{cases} 
    1 & \text{if } H_{1k} \text{ is true;} \\
    0 & \text{if } H_{0k} \text{ is true.} 
  \end{cases}
\]

Let \( G_k \) be the set of hypotheses (including hypothesis \( k \)) where the parameters are dependent on the \( k \)-th hypothesis. In the new procedure, the decision of each hypothesis is penalized by incorrect decisions regarding other dependent parameters. Thus a compound criterion where all the decisions in \( G_k \) deterministically depends upon each other. Define the following quantity

\[
  z_k = \begin{cases} 
    1 & \text{if } H_{d_{j,k}} \text{ is true for all } j \in G_k \setminus \{k\}; \\
    0 & \text{otherwise.} 
  \end{cases}
\] (3.8)

If, for any \( k \in \{1, \ldots, K\} \), \( G_k = \{k\} \), a singleton, then we define \( z_k = 1 \). The notion of true positives (TP) are modified as the following

\[
  TP = \sum_{k=1}^{K} d_k r_k z_k, \tag{3.9}
\]

The posterior expectation of \( TP \) is maximized subject to controlling the posterior expectation
of the error term

\[ E = \sum_{k=1}^{K} d_k (1 - r_k z_k). \]  

(3.10)

It follows that the decision configuration can be obtained by minimizing the function

\[ \xi(d) = -\sum_{k=1}^{K} d_k E(r_k z_k | X_n, Y_{nm}) + \lambda_{nm} \sum_{k=1}^{K} d_k E[(1 - r_k z_k) | X_n, Y_{nm}] \]

\[ = -(1 + \lambda_{nm}) \sum_{k=1}^{K} d_k \left( w_{knm}(d) - \frac{\lambda_{nm}}{1 + \lambda_{nm}} \right), \]

with respect to all possible decision configurations of the form \( d = \{d_1, \ldots, d_K\} \), where \( \lambda_{nm} > 0 \), and

\[ w_{knm}(d) = E(r_k z_k | X_n, Y_{nm}) = \pi(H_{1,k} \cap \{ \cap_{j \neq k, j \in G_k} H_{d,j} \} | X_n, Y_{nm}) \]

is the posterior probability of the decision configuration \( \{d_1, \ldots, d_{k-1}, 1, d_{k+1}, \ldots, d_K\} \) being correct. Letting \( \beta_{nm} = \lambda_{nm}/(1 + \lambda_{nm}) \), one can equivalently maximize

\[ f_{\beta_{nm}}(d) = \sum_{k=1}^{K} d_k (w_{knm}(d) - \beta_{nm}) \]  

(3.11)

with respect to \( d \) and obtain the optimal decision configuration.

**Definition 1.** Let \( \mathbb{D} \) be the set of all \( m \)-dimensional binary vectors denoting all possible decision configurations. Define

\[ \hat{d} = \arg \max_{d \in \mathbb{D}} f_{\beta}(d) \]

where \( 0 < \beta < 1 \). Then \( \hat{d} \) is the optimal decision configuration obtained as the solution of the non-marginal multiple testing method.

Note that in the definitions of both \( TP \) and \( E_n \), \( d_i \) is penalized by incorrect decisions in the same group. This forces the decisions to be jointly taken also adjudging other dependent parameters.

### 3.3 Specialization of the general multiple testing procedure to inverse model selection problems

In our inverse model selection problem note that since the models \( M_k; k = 1, \ldots, K \), are independent, so are \( \hat{X}_n \) associated with the different models. Thus, the hypotheses are dependent only through the relation \( \sum_{k=1}^{K} I(\zeta = k) = 1 \). As we shall show, the posterior probability of the event \( \{\zeta = \bar{k}\} \) converges to one \textit{a posteriori} as the sample size tends to infinity, irrespective of any other dependence among \( (I(\zeta = 1), \ldots, I(\zeta = K)) \) induced through \( (p_1, \ldots, p_K) \). Hence, there is not enough reason to consider the hypotheses as dependent. Thus, for our purpose, we simply set \( G_k = \{k\} \). Consequently, (3.11) in our case reduces to

\[ f_{\beta_{nm}}(d) = \sum_{k=1}^{K} d_k (v_{knm} - \beta_{nm}), \]

(3.12)

where

\[ v_{knm} = E(r_k | X_n, Y_{nm}) = \pi(H_{1,k} | X_n, Y_{nm}). \]
In this case, the optimal decision configuration \( \hat{d} \) is given by the following: for \( k = 1, \ldots, K \),

\[
\hat{d}_k = \begin{cases} 
1 & \text{if } v_{knm} > \beta_{nm}; \\
0 & \text{otherwise}.
\end{cases}
\]  

(3.13)

Hence, although our formulation of the multiple hypothesis test for inverse model selection is novel, the Bayesian procedure for testing parallels that of Müller et al. (2004) (see also Guindani et al. (2009)), which is a special case of the general procedure proposed in Chandra and Bhattacharya (2019).

### 3.4 Error measures in multiple testing

Storey (2003) advocated positive False Discovery Rate (pFDR) as a measure of Type-I error in multiple testing. Let \( \delta(d|X_n, Y_{nm}) \) be the probability of choosing \( d \) as the optimal decision configuration given data \((X_n, Y_{nm})\) when a given multiple testing method is employed. Then pFDR is defined as:

\[
pFDR_{nm} = E_{Y_{nm}|X_n} \left[ \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} d_k (1 - r_k)}{\sum_{k=1}^{K} d_k} \delta(d|X_n, Y_{nm}) \right] \delta(d = 0|X_n, Y_{nm}) = 0. 
\]  

(3.14)

Analogous to Type-II error, the positive False Non-discovery Rate (pFNR) is defined as

\[
pFNR_{nm} = E_{Y_{nm}|X_n} \left[ \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} (1 - d_k) r_k}{\sum_{k=1}^{K} (1 - d_k)} \delta(d|X_n, Y_{nm}) \right] \delta(d = 1|X_n, Y_{nm}) = 0. 
\]  

(3.15)

Under prior \( \pi(\cdot) \), Sarkar et al. (2008) defined posterior FDR and FNR. The measures are given as following:

\[
\text{posterior FDR}_{nm} = E \left[ \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} d_k (1 - r_k)}{\sum_{k=1}^{K} d_k} \delta(d|X_n, Y_{nm}) \right| X_n, Y_{nm} 
\]  

(3.16)

\[
= \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} d_k (1 - v_{knm})}{\sum_{k=1}^{K} d_k} \delta(d|X_n, Y_{nm}); 
\]  

(3.17)

\[
\text{posterior FNR}_{nm} = E \left[ \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} (1 - d_k) r_k}{\sum_{k=1}^{K} (1 - d_k)} \delta(d|X_n, Y_{nm}) \right| X_n, Y_{nm} 
\]  

(3.18)

\[
= \sum_{d \in \mathbb{D}} \frac{\sum_{k=1}^{K} (1 - d_k)^2 v_{knm}}{\sum_{k=1}^{K} (1 - d_k)^2} \delta(d|X_n, Y_{nm}). 
\]  

(3.19)

Also under any non-randomized decision rule, \( \delta(d|X_n, Y_{nm}) \) is either 1 or 0 depending on data \((X_n, Y_{nm})\). Given \((X_n, Y_{nm})\), we denote these error measures conditional on the data by conditional FDR \( (cFDR_{nm}) \) and conditional FNR \( (cFNR_{nm}) \) respectively.

The positive Bayesian FDR \( (pBFDR_{nm}) \) and FNR \( (pBFNR_{nm}) \) are the expectations of conditional FDR \( (cFDR_{nm}) \) and conditional FNR \( (cFNR_{nm}) \) respectively, with respect to the distribution of \( Y_{nm} \) given \( X_n \).

For our Bayesian purpose, we shall consider the Bayesian measures \( cFDR_{nm}, pBFDR_{nm}, cFNR_{nm} \) and \( pBFNR_{nm} \), and investigate their asymptotic properties. Chandra and Bhattacharya (2019) and Chandra and Bhattacharya (2020) particularly recommend \( cFDR_{nm} \) and \( cFNR_{nm} \), since they are conditioned on the observed data \((X_n, Y_{nm})\) and hence qualify as \( \text{bona fide} \) Bayesian measures.

Let us now proceed towards development of the asymptotic theory for our proposed multiple testing strategy. The issue of misspecification will play a crucial role in this context.
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 asymptotic theory. Indeed, we shall build a general asymptotic framework that allows for possibly infinite-dimensional parameters, dependent data as well as 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.

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

Let $Y_n = \{Y_1, \ldots, Y_n\}$, 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

$$ \lim_{n \to \infty} \frac{1}{n} \log R_n(\theta) = -h(\theta), \quad (4.1) $$

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

$$ h(\theta) = \lim_{n \to \infty} \frac{1}{n} E_{\theta_0} \left( \log \frac{f_{\theta_0}(Y_n)}{f_\theta(Y_n)} \right), \quad (4.2) $$

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

$$ h(A) = \operatorname{ess\ inf}_{\theta \in A} h(\theta); \quad (4.3) $$

$$ J(\theta) = h(\theta) - h(\Theta); \quad (4.4) $$

$$ J(A) = \operatorname{ess\ inf}_{\theta \in A} J(\theta). \quad (4.5) $$

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 $G_n$ such that $G_n \to \Theta$ and $\pi(G_n') \leq \alpha \exp(-\beta n)$, for some $\alpha > 0$.

With the above notions, verification of (4.1) along with several other technical conditions ensure that for any $A \subseteq \Theta$ such that $\pi(A) > 0$,

$$ \lim_{n \to \infty} \pi(A|Y_n) = 0, \quad (4.6) $$

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 and in probability convergence by “$a.s.$” and “$P$”, respectively, almost sure equality by “$a.s.$” and weak convergence by “$w$.”
5 Asymptotic properties of the posterior probabilities of the alternative hypotheses

5.1 Posterior convergence to the best model

Theorem 1. Assume that for $k = 1, \ldots, K$, $\mathcal{M}_k$ satisfies conditions (S1)–(S6) of Shalizi, and that the competing models as well as the true model have densities with respect to some common $\sigma$-finite measure. Also assume that the posterior associated with $\mathcal{M}_k$ is dominated by the prior, which is again absolutely continuous with respect to some appropriate $\sigma$-finite measure, and that the priors satisfy $\pi(\theta_k|\mathcal{M}_k) > 0$ for all $\theta_k \in \Theta_k$. Let $h_k(\Theta_k) = \min\{h_k(\Theta_k) : k = 1, \ldots, K\}$. Then for any $m \geq 1$,

$$\lim_{n \to \infty} \pi(\zeta = k|X_n, Y_{nm}) = \begin{cases} 1 & \text{if } k = \tilde{k} \\ 0 & \text{if } k \neq \tilde{k}. \end{cases}$$

(5.1)

Proof. For any $k_1, k_2 \in \{1, \ldots, K\}$, let $BF^{(nm)}(\mathcal{M}_{k_1}, \mathcal{M}_{k_2})$ denote the Bayes factor of model $\mathcal{M}_{k_1}$ against model $\mathcal{M}_{k_2}$. Then as a direct consequence of Theorem 2 of Chatterjee et al. (2018), the following holds for any $m \geq 1$:

$$\frac{1}{n} \log BF^{(nm)}(\mathcal{M}_k, \mathcal{M}_0) \to -h_k(\Theta_k), \text{ as } n \to \infty,$$

(5.2)

almost surely with respect to the true model $\mathcal{M}_0$. In the above, $h_k(\Theta_k)$ corresponds to (4.1), (4.2) and (4.3) for model $\mathcal{M}_k$ with parameter space $\Theta_k$.

Now, since $h_k(\Theta_k) = \min\{h_k(\Theta_k) : k = 1, \ldots, K\}$, it follows from (5.2) that as $n \to \infty$, for any $m \geq 1$,

$$\frac{1}{n} \log BF^{(nm)}(\mathcal{M}_k, \mathcal{M}_{\tilde{k}}) \to [-h_k(\Theta_k) - h_{\tilde{k}}(\Theta_k)],$$

so that as $n \to \infty$, for any $m \geq 1$,

$$BF^{(nm)}(\mathcal{M}_k, \mathcal{M}_{\tilde{k}}) = \begin{cases} 1 & \text{if } k = \tilde{k} \\ \frac{a.s.}{\to 0} & \text{if } k \neq \tilde{k}. \end{cases}$$

(5.3)

Now note that (see, for example, Liang et al. (2008))

$$\pi(\zeta = k|X_n, Y_{nm}, p_1, \ldots, p_K) = \frac{p_k BF^{(nm)}(\mathcal{M}_k, \mathcal{M}_{\tilde{k}})}{\sum_{\ell=1}^K p_{\ell} BF^{(nm)}(\mathcal{M}_\ell, \mathcal{M}_{\tilde{k}})}.$$  

(5.4)

Hence it follows by applying (5.3) to (5.4) that the following holds:

$$\lim_{n \to \infty} \pi(\zeta = k|X_n, Y_{nm}, p_1, \ldots, p_K) \overset{a.s.}{\to} \begin{cases} 1 & \text{if } k = \tilde{k} \\ 0 & \text{if } k \neq \tilde{k}. \end{cases}$$

(5.5)

Now note that $\pi(\zeta = k|X_n, Y_{nm}) = E[\pi(\zeta = k|X_n, Y_{nm}, p_1, \ldots, p_K)]$, the expectation being over the posterior distribution of $(p_1, \ldots, p_K)$ given $X_n$ and $Y_{nm}$. Since $\pi(\zeta = k|X_n, Y_{nm}, p_1, \ldots, p_K) \leq 1$ almost surely, it follows by uniform integrability and (5.5), that

$$\lim_{n \to \infty} \pi(\zeta = k|X_n, Y_{nm}) = E[\pi(\zeta = k|X_n, Y_{nm}, p_1, \ldots, p_K)] \overset{a.s.}{\to} \begin{cases} 1 & \text{if } k = \tilde{k} \\ 0 & \text{if } k \neq \tilde{k}. \end{cases}$$

□

13
5.2 Convergence of the cross-validation posteriors of $\tilde{x}_i$

**Theorem 2.** For model $\mathcal{M}_k$ assume conditions (S1)--(S7) of Shalizi, and let the infimum of $h_k(\theta_k)$ over $\Theta_k$ be attained at $\theta_k \in \hat{\Theta}_k$, where $\hat{\theta}_k \neq \theta_0$. Also assume that $\Theta_k$ and $\Theta_0$ are complete separable metric spaces. Then, with the prior $(2.4)$, under further assumptions that $\pi(\tilde{x}_i|\theta_k, y, \mathcal{M}_k)$ is continuous in $\theta_k$, $f(y|\tilde{\theta}_k, \tilde{x}_i, \mathcal{M}_k)$ is continuous in $\tilde{x}_i$, for $i \geq 1$ and $\eta_k$ is a one-to-one function, the following holds:

$$\lim_{m \to \infty} \lim_{n \to \infty} \pi(\tilde{x}_i \in V_{ik}^c| X_{n,-i}, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k) = 0, \text{ almost surely,}$$

(5.6)

for any neighborhood $V_{ik}$ of $x_{ik}^*$. 

**Proof.** By the hypotheses, (4.6) holds, from which it follows that for any $\epsilon > 0$, and for any $m \geq 1$,

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

(5.7)

where $N_{k,\epsilon} = \{ \theta_k : h_k(\theta_k) \leq h_k(\Theta_k) + \epsilon \}$.

Now, by hypothesis, the infimum of $h_k(\theta_k)$ over $\Theta_k$ is attained at $\theta_k \in \hat{\Theta}_k$, where $\hat{\theta}_k \neq \theta_0$. Then by (5.7), the posterior of $\theta_k$ given $X_{n,-i}$ and $Y_{nm}$, concentrates around $\hat{\theta}_k$, the minimizer of the limiting KL-divergence rate from the true distribution. Formally, given any neighborhood $U_k$ of $\hat{\theta}_k$, the set $N_{k,\epsilon}$ is contained in $U_k$ for sufficiently small $\epsilon$. It follows that for any neighborhood $U_k$ of $\hat{\theta}_k$, $\pi(U_k| X_{n,-i}, Y_{nm}, \mathcal{M}_k) \to 1$, almost surely, as $n \to \infty$. Since $\Theta_k$ is a complete, separable metric space, it follows that (see, for example, Ghosh and Ramamoorthi (2003), Ghosal and van der Vaart (2017))

$$\pi(\cdot| X_{n,-i}, Y_{nm}, \mathcal{M}_k) \overset{w}{\to} \delta_{\hat{\theta}_k} (\cdot), \text{ almost surely, as } n \to \infty, \text{ for any } m \geq 1.$$  

(5.8)

In the above, $\delta_{\hat{\theta}_k} (\cdot)$ denotes point mass at $\hat{\theta}_k$.

Now since $\hat{\Theta}_k \subset \Theta_k$, $h_k(\hat{\Theta}_k) > h_k(\Theta_k)$. Hence, from (4.6) it follows that for any $m \geq 1$,

$$\pi(\theta_k \in \hat{\Theta}_k| X_n, Y_{nm}, \mathcal{M}_k) \overset{a.s.}{\to} 0, \text{ as } n \to \infty.$$  

(5.9)

Also note that since $\pi(\tilde{x}_i|\theta_k, y, \mathcal{M}_k)$ is continuous in $\theta_k$ by assumption, it follows by Scheffe’s theorem that any probability associated with $\pi(\tilde{x}_i|\theta_k, y, \mathcal{M}_k)$ is continuous in $\theta_k$ (see Lemma 4.3 of Chatterjee and Bhattacharya (2020b)). Hence, for any neighborhood $V_{ik}$ of $x_{ik}^*$, the probability $\pi(\tilde{x}_i \in V_{ik}^c|\theta_k, y, \mathcal{M}_k)$ is continuous in $\theta_k$. Moreover, since it is a probability, it is bounded. Hence, by the Portmanteau theorem, weak convergence of $\pi(\theta_k| X_{n,-i}, Y_{nm}, \mathcal{M}_k)$, and (5.9) it holds almost surely that

$$\pi(\tilde{x}_i \in V_{ik}^c| X_{n,-i}, Y_{nm}, \mathcal{M}_k) = \int_{\hat{\Theta}_k} \pi(\tilde{x}_i \in V_{ik}^c| \theta_k, y, \mathcal{M}_k) d\pi(\theta_k| X_{n,-i}, Y_{nm}, \mathcal{M}_k)$$

$$\pi(\hat{\Theta}_k| X_{n,-i}, Y_{nm}, \mathcal{M}_k) \overset{a.s.}{\to} \pi(\tilde{x}_i \in V_{ik}^c|\hat{\theta}_k, y, \mathcal{M}_k), \text{ as } n \to \infty, \text{ for any } m \geq 1.$$  

That $\pi(\tilde{x}_i \in V_{ik}^c|\hat{\theta}_k, y, \mathcal{M}_k) \overset{a.s.}{\to} 0$, as $m \to \infty$, follows in the same way as the proof of Theorem 2 of Chatterjee and Bhattacharya (2020b) by replacing $\theta_0$ with $\theta_k$. 

**5.3 Posterior convergence of the discrepancy measures**

**Theorem 3.** Under the conditions of Theorem 2, the following holds for any $\epsilon > 0$:

$$\pi(T^{(k)}(\tilde{X}_n) > \epsilon| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k) \overset{a.s.}{\to} 0, \text{ as } m \to \infty, n \to \infty,$$  

(5.10)
where \( T^{(k)} = T^{(1)}_k \) or \( T^{(2)}_k \).

**Proof.** For \( i \geq 1 \), Theorem 2 implies almost sure weak convergence of the \( i \)-th cross-validation posterior of \( \tilde{x}_i \) for model \( M_k \) to \( \delta_{x^*_ik} \), as \( m \to \infty \) and \( n \to \infty \). This is equivalent to convergence in (cross-validation posterior) distribution of \( \tilde{x}_i \) to the degenerate quantity \( x^*_ik \), almost surely. Degeneracy guarantees that this is equivalent to convergence in probability, almost surely. In other words, with respect to the cross-validation posterior distribution of \( \tilde{x}_i \) for model \( M_k \), almost surely, as \( m \to \infty \), \( n \to \infty \),

\[
\tilde{x}_i \overset{P}{\to} x^*_ik. \tag{5.11}
\]

Now note that \( T^{(k)}(\bar{X}_n) \) is an average of \( n \) terms, the \( i \)-th term being

\[
\frac{1}{\sqrt{\text{Var}(\tilde{x}_i|X_n, Y_{mn}, M_k, \hat{\Theta}_k)}} \to 0, \\
\text{for all } i \geq 1.
\]

This is equivalent to convergence of \( \tilde{x}_i \) to \( x^*_ik \) in the cross-validation posterior distribution of \( \tilde{x}_i \) for model \( M_k \), almost surely, as \( m \to \infty \), \( n \to \infty \),

\[
\tilde{x}_i \overset{P}{\to} x^*_ik. \tag{5.11}
\]

It follows from (5.12) and (5.13) that with respect to the cross-validation posterior distribution of \( \tilde{x}_i \) for model \( M_k \), almost surely, as \( m \to \infty \), \( n \to \infty \),

\[
\frac{1}{\sqrt{\text{Var}(\tilde{x}_i|X_n, Y_{mn}, M_k, \hat{\Theta}_k)}} \overset{P}{\to} 0, \text{ for all } i \geq 1. \tag{5.14}
\]

Hence, by Theorem 7.15 of Schervish (1995) (page 398), it follows that with respect to the cross-validation posterior distribution of \( \{\tilde{x}_i; i \geq 1\} \), for model \( M_k \), almost surely, as \( m \to \infty \), \( n \to \infty \),

\[
T^{(k)}(\bar{X}_n) \overset{P}{\to} 0, \tag{5.10}
\]

which is equivalent to (5.10).

**Theorem 4.** Assume the conditions of Theorem 3. Also assume that for \( i \geq 1 \), \( x^*_ik \) is a continuous function of \( \{x_1, x_2, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_{i+\ell}\} \), for some non-negative integer \( \ell \). Then there exist positive constants \( a_{1k} \) and \( a_{2k} \) such that

\[
\lim_{m \to \infty} \lim_{n \to \infty} T^{(k)}_1(X_n) = a_{1k}; \tag{5.15}
\]

\[
\lim_{m \to \infty} \lim_{n \to \infty} T^{(k)}_2(X_n) = a_{2k}. \tag{5.16}
\]

**Proof.** It follows from (5.12) and (5.13) that

\[
T^{(k)}_1(X_n) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} |x_i - x^*_ik|; \tag{5.17}
\]

\[
T^{(k)}_2(X_n) \xrightarrow{a.s.} \lim_{n \to \infty} \frac{1}{nc} \sum_{i=1}^{n} (x_i - x^*_ik)^2. \tag{5.18}
\]

Now, by our assumption, \( x^*_ik \) is a continuous function of \( \{x_1, x_2, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_{i+\ell}\} \), for some non-negative integer \( \ell \). Hence, letting \( u_{ik} = x_i - x^*_ik \), it follows by Riemann sum
convergence that

\[
\lim_{n \to \infty} \frac{1}{n \sqrt{c}} \sum_{i=1}^{n} |x_i - x_{ik}^*| = c^{-\frac{1}{2}} |\tilde{X}_k|^{-1} \int |u| \, du; \\
\lim_{n \to \infty} \frac{1}{n \sqrt{c}} \sum_{i=1}^{n} (x_i - x_{ik}^*)^2 = c^{-1} |\tilde{X}_k|^{-1} \int u^2 \, du,
\]

(5.19)

(5.20)

where \(\tilde{X}_k\) is the appropriate compact co-domain of \(u_{ik}\) induced by the transformation \(u_{ik} = x_i - x_{ik}^*\) and the original compact covariate space \(X\), and \(|\tilde{X}_k|\) stands for the Lebesgue measure of \(\tilde{X}_k\).

Since the right hand sides of (5.19) and (5.20) are well-defined positive quantities, the proof follows by combining (5.17) – (5.20).

**Theorem 5.** Assume the conditions of Theorem 4. Then the following holds for any \(\varepsilon > 0\), where \(T^{(k)} = T_1^{(k)}\) or \(T_2^{(k)}\) and respectively, \(a_k = a_{1k}\) or \(a_{2k}\):

\[
\lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in \left[ \ell_{kmn} - a_k - \varepsilon, \ell_{kmn} - a_k + \varepsilon \right] \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 0.
\]

(5.21)

**Proof.** First, observe that since for \(i = 1, \ldots, n\), \(\tilde{x}_i \in X\) almost surely, where \(X\) is compact, \(|\tilde{x}_i - E(\tilde{x}_i|X_n, Y_{nm}, M_k, \tilde{\Theta}_k)|\) are almost surely uniformly bounded. Hence, \(T_1^{(k)}(\tilde{X}_n)\) and \(T_2^{(k)}(\tilde{X}_n)\) are almost surely bounded. Consequently, using (5.10) of Theorem 3 and uniform integrability it follows that

\[
\lim_{m \to \infty} \lim_{n \to \infty} E \left( T_1^{(k)}(\tilde{X}_n) \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 0; \\
\lim_{m \to \infty} \lim_{n \to \infty} E \left( T_2^{(k)}(\tilde{X}_n) \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 0; \\
\lim_{m \to \infty} \lim_{n \to \infty} \text{Var} \left( T_1^{(k)}(\tilde{X}_n) \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 0; \\
\lim_{m \to \infty} \lim_{n \to \infty} \text{Var} \left( T_2^{(k)}(\tilde{X}_n) \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 0.
\]

(5.22)

(5.23)

(5.24)

(5.25)

The limits (5.22) – (5.25) imply that

\[
\lim_{m \to \infty} \lim_{n \to \infty} \tilde{\ell}_{kmn}^{\text{a.s.}} = 0; \\
\lim_{m \to \infty} \lim_{n \to \infty} \tilde{u}_{kmn}^{\text{a.s.}} = 0.
\]

(5.26)

(5.27)

Due to (5.26) and Theorem 4, given any \(\varepsilon > 0\), for sufficiently large \(m\) and \(n\), \(\ell_{kmn} - a_k + T^{(k)}(X_n) - \varepsilon < 0\). Since \(T^{(k)}(\tilde{X}_n) > 0\) with probability one, we thus have

\[
\lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) > \ell_{kmn} - a_k + T^{(k)}(X_n) - \varepsilon \mid X_n, Y_{nm}, M_k, \tilde{\Theta}_k \right)^{\text{a.s.}} = 1.
\]

(5.28)

Also, due to (5.27) and Theorem 4, given any \(\varepsilon > 0\), for sufficiently large \(m\) and \(n\), \(\tilde{u}_{kmn} - a_k + T^{(k)}(X_n) + \varepsilon > 0\). Hence, given any \(\varepsilon > 0\), for sufficiently large \(m\) and \(n\), we have by Markov’s
Proof. First, let $k \neq \tilde{k}$. Then

\[
\pi \left( T^{(k)}(\tilde{X}_n) > \bar{u}_{knm} - a_k + T^{(k)}(X_n) + \varepsilon \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right)
< \left( \bar{u}_{knm} - a_k + T^{(k)}(X_n) + \varepsilon \right)^{-2}
\times \left[ \text{Var} \left( T^{(k)}(\tilde{X}_n) \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right) + \left\{ E \left( T^{(k)}(\tilde{X}_n) \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right) \right\}^2 \right].
\]

Taking limits of both sides of (5.29) and using (5.22) – (5.25) we obtain

\[
\lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) > \bar{u}_{knm} - a_k + T^{(k)}(X_n) + \varepsilon \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right) \xrightarrow{a.s.} 0.
\]

Combining (5.28) and (5.30) yields

\[
\lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\hat{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right)
= \lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) > \hat{\ell}_{knm} - a_k + T^{(k)}(X_n) - \varepsilon \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right)
- \lim_{m \to \infty} \lim_{n \to \infty} \pi \left( T^{(k)}(\tilde{X}_n) > \bar{u}_{knm} - a_k + T^{(k)}(X_n) + \varepsilon \big| X_n, Y_{nm}, \mathcal{M}_k, \hat{\Theta}_k \right)
\xrightarrow{a.s.} 1,
\]

thus proving (5.21). \qed

**Remark 6.** In all the examples provided in Chatterjee and Bhattacharya (2020a), it has been shown that the conditions of Theorem 4 are satisfied. Hence, Theorem 5 holds for all the examples presented in Chatterjee and Bhattacharya (2020a).

### 5.4 Convergence of the posterior probabilities of $H_{1k}$

**Theorem 7.** Assume that for $k = 1, \ldots, K$, $\mathcal{M}_k$ satisfies conditions (S1)–(S7) of Shalizi, and that the competing models as well as the true model have densities with respect to some common $\sigma$-finite measure. Also assume that the posterior associated with $\mathcal{M}_k$ is dominated by the prior, which is again absolutely continuous with respect to some appropriate $\sigma$-finite measure, and that the priors satisfy $\pi(\theta_k | \mathcal{M}_k) > 0$ for all $\theta_k \in \Theta_k$. Let $h_k(\Theta_k) = \min\{h_k(\Theta_k) : k = 1, \ldots, K\}$. Then

\[
\lim_{m \to \infty} \lim_{n \to \infty} v_{knm} \xrightarrow{a.s.} \begin{cases} 1 & \text{if } k \neq \tilde{k} \\ 0 & \text{if } k = \tilde{k}, \end{cases}
\]

**Proof.** First, let $k \neq \tilde{k}$. Then

\[
v_{knm} = \pi \left( \zeta \neq \tilde{k} \big| X_n, Y_{nm} \right) + \pi \left( \zeta = k, \theta_k \in \hat{\Theta}_{\tilde{k}} \big| X_n, Y_{nm} \right)
+ \pi \left( \zeta = k, \theta_k \in \hat{\Theta}_{\tilde{k}}, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\hat{\ell}_{knm} - a_k - \varepsilon, \bar{u}_{knm} - a_k + \varepsilon] \big| X_n, Y_{nm} \right).
\]

Since $k \neq \tilde{k}$, it follows due to (5.1) that for any $m \geq 1$, as $n \to \infty$,

\[
\pi \left( \zeta \neq k \big| X_n, Y_{nm} \right) = \pi \left( \zeta = \tilde{k} \big| X_n, Y_{nm} \right) + \sum_{j \neq \tilde{k}, k} \pi \left( \zeta \neq k \big| X_n, Y_{nm} \right) \xrightarrow{a.s.} 1.
\]
Using (5.1) again it follows that for any \( m \geq 1 \),
\[
\pi \left( \zeta = k, \theta_k \in \Theta_k \mid X_n, Y_{nm} \right) \leq \pi \left( \zeta = k \mid X_n, Y_{nm} \right) \xrightarrow{a.s.} 0, \text{ as } n \to \infty
\] (5.34)

and
\[
\pi \left( \zeta = k, \theta_k \in \Theta_k, T^{(k)}(X_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{kmn} - a_k - \varepsilon, \tilde{u}_{kmn} - a_k + \varepsilon] \mid X_n, Y_{nm} \right)
\leq \pi \left( \zeta = k \mid X_n, Y_{nm} \right) \xrightarrow{a.s.} 0, \text{ as } n \to \infty.
\] (5.35)

Results (5.33), (5.34) and (5.35) imply that if \( k \neq \hat{k} \), then for any \( m \geq 1 \),
\[
v_{kmn} \xrightarrow{a.s.} 1, \text{ as } n \to \infty.
\] (5.36)

Now let us obtain the limit of \( v_{kmn} \) when \( k = \hat{k} \). By (5.1),
\[
\pi \left( \zeta \neq \hat{k} \mid X_n, Y_{nm} \right) \xrightarrow{a.s.} 0, \text{ as } n \to \infty.
\] (5.37)

For any \( m \geq 1 \), using (5.9) we obtain
\[
\pi \left( \zeta = \hat{k}, \theta_k \in \Theta_k \mid X_n, Y_{nm} \right) \leq \pi \left( \theta_k \in \Theta_k \mid X_n, Y_{nm} \right) \xrightarrow{a.s.} 0, \text{ as } n \to \infty.
\] (5.38)

Now note that
\[
\pi \left( \zeta = \hat{k}, \theta_k \in \Theta_k, T^{(k)}(X_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{kmn} - a_k - \varepsilon, \tilde{u}_{kmn} - a_k + \varepsilon] \mid X_n, Y_{nm} \right)
\leq \pi \left( T^{(k)}(X_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{kmn} - a_k - \varepsilon, \tilde{u}_{kmn} - a_k + \varepsilon] \mid X_n, Y_{nm}, \zeta = \hat{k} \right)
\xrightarrow{a.s.} 0, \text{ as } m \to \infty, n \to \infty, \text{ due to (5.21)}.
\] (5.39)

From (5.37), (5.38) and (5.39) it follows that
\[
v_{kmn} \xrightarrow{a.s.} 0, \text{ as } m \to \infty, n \to \infty.
\] (5.40)

The limits (5.36) and (5.40) show that (5.31) holds. \( \square \)

6 Asymptotic optimality theory for our multiple testing procedure

Let \( h_{\hat{k}}(\Theta_k) = \min \{ h_k(\Theta_k) : k = 1, \ldots, K \} \). Also let us define \( \tilde{d} = (\tilde{d}_1, \ldots, \tilde{d}_K) \), where
\[
\tilde{d}_k = \begin{cases} 
1 & \text{if } k \neq \hat{k} \\
0 & \text{if } k = \hat{k}.
\end{cases}
\] (6.1)

**Definition 2.** A multiple testing method for the inverse model selection is said to be asymptotically optimal for which
\[
\lim_{m \to \infty} \lim_{n \to \infty} \delta(\tilde{d} \mid X_n, Y_{nm}) \xrightarrow{a.s.} 1.
\]
Recall the constant $\beta_{nm}$ in (3.11), which is the penalizing constant between the error $E$ and true positives $TP$. For consistency of the non-marginal procedure, we need certain conditions on $\beta_n$, which we state below. These conditions will also play important roles in the asymptotic studies of the different versions of $FDR$ and $FNR$ that we consider.

(A1) We assume that the sequence $\beta_{nm}$ is neither too small nor too large, that is,

$$\beta = \liminf_{m \geq 1, n \geq 1} \beta_{nm} > 0;$$

$$\bar{\beta} = \limsup_{m \geq 1, n \geq 1} \beta_{nm} < 1.$$ (6.2)

With this conditions we propose and prove the following results.

**Theorem 8.** Let $\delta(\cdot | X_n, Y_{nm})$ denote the decision rule given data $X_n$ and $Y_{nm}$. Assume the conditions of Theorem 7 and condition (A1) on $\beta_{nm}$. Then the decision procedure is asymptotically optimal.

**Proof.** Due to (A1), given $\epsilon_1 > 0$, there exist $m_0 \geq 1$ and $n_0 \geq 1$ such that for $m \geq m_0$ and $n \geq n_0$,

$$0 < \beta - \epsilon_1 < \beta_{nm} < \bar{\beta} + \epsilon_1 < 1.$$ (6.4)

By (5.31), for any $0 < \epsilon_2 < 1 - \bar{\beta} - \epsilon_1$, for $k \neq \bar{k}$, there exist $m_k \geq 1$ and $n_k \geq 1$ such that for $m \geq m_k$ and $n \geq n_k$,

$$v_{km} > 1 - \epsilon_2 > \bar{\beta} + \epsilon_1.$$ (6.5)

Also, for $0 < \epsilon_3 < \beta - \epsilon_1$, there exist $m_{\bar{k}} \geq 1$ and $n_{\bar{k}} \geq 1$ such that for $m \geq m_{\bar{k}}$ and $n \geq n_{\bar{k}}$,

$$v_{km} < \epsilon_3 < \beta - \epsilon_1.$$ (6.6)

Let $\bar{m} = \max\{m_0, m_1, \ldots, m_K\}$ and $\bar{n} = \max\{n_0, n_1, \ldots, n_K\}$. Then it can be seen from (6.4), (6.5) and (6.6) that for $m \geq \bar{m}$ and $n \geq \bar{n}$ the following hold almost surely:

$$v_{km} > \beta_{nm}, \text{ if } k \neq \bar{k};$$

$$v_{km} < \beta_{nm}, \text{ if } k = \bar{k}. $$ (6.7)

(6.8)

Using (6.7) and (6.8) in (3.13) shows that for $m \geq \bar{m}$ and $n \geq \bar{n}$,

$$\hat{d}_k = \begin{cases} 1 & \text{if } k \neq \bar{k}; \\ 0 & \text{if } k = \bar{k}. \end{cases}$$ (6.9)

In other words, almost surely, $\hat{d} = \hat{d}$ for $m \geq \bar{m}$ and $n \geq \bar{n}$. This completes the proof.

**Remark 9.** Since $\delta(\cdot | X_n, Y_{nm})$ is an indicator function, the following also holds:

$$\lim_{m \to \infty} \lim_{n \to \infty} E_{Y_{nm} | X_n} \left[ \delta(d | X_n, Y_{nm}) \right] = 1.$$
7 Asymptotic theory of the error measures

7.1 Convergence of versions of FDR and FNR

**Theorem 10.** Assume the conditions of Theorem 7 and condition (A1) on \( \beta_{nm} \). Then

\[
\lim_{m \to \infty} \lim_{n \to \infty} cFDR_{nm} \overset{a.s.}{=} 0; \quad (7.1)
\]

\[
\lim_{m \to \infty} \lim_{n \to \infty} pBFDR_{nm} = 0. \quad (7.2)
\]

**Proof.** From (3.17) observe that

\[
cFDR_{nm} = \frac{\sum_{k=1}^{K} \tilde{d}_k(1 - v_{knm})}{\sum_{k=1}^{K} d_k \vee 1} \delta(d|X_n, Y_{nm}) + \sum_{d \neq \tilde{d} \in D} \frac{\sum_{k=1}^{K} d_k(1 - v_{knm})}{\sum_{k=1}^{K} d_k \vee 1} \delta(d|X_n, Y_{nm}) \quad (7.3)
\]

The proof of Theorem 8 shows that there exist \( \tilde{m} \geq 1 \) and \( \tilde{n} \geq 1 \) such that \( \delta(d|X_n, Y_{nm}) = 1 \) almost surely for \( m \geq \tilde{m} \) and \( n \geq \tilde{n} \). This, combined with (7.3) shows that for \( m \geq \tilde{m} \) and \( n \geq \tilde{n} \), almost surely,

\[
cFDR_{nm} = \frac{\sum_{k=1}^{K} \tilde{d}_k(1 - v_{knm})}{\sum_{k=1}^{K} \tilde{d}_k \vee 1} = \left( \sum_{k=1}^{K} d_k \vee 1 \right)^{-1} \quad (7.4)
\]

Applying (5.31) to the right most side of (7.4) shows that

\[
cFDR_{nm} \overset{a.s.}{\to} 0, \text{ as } m \to \infty, n \to \infty,
\]

establishing (7.1).

Since \( cFDR_{nm} < 1 \) almost surely, (7.2) follows from (7.1) by uniform integrability.

**Theorem 11.** Assume the conditions of Theorem 7 and condition (A1) on \( \beta_{nm} \). Then

\[
\lim_{m \to \infty} \lim_{n \to \infty} cFNR_{nm} \overset{a.s.}{=} 0; \quad (7.5)
\]

\[
\lim_{m \to \infty} \lim_{n \to \infty} pBFNR_{nm} = 0. \quad (7.6)
\]

**Proof.** It follows from (3.19) and the proof of Theorem 8 that there exist \( \tilde{m} \geq 1 \) and \( \tilde{n} \geq 1 \) such that for \( m \geq \tilde{m} \) and \( n \geq \tilde{n} \), almost surely,

\[
cFNR_{nm} = \frac{\sum_{k=1}^{K} (1 - \tilde{d}_k)v_{knm}}{\sum_{k=1}^{K} (1 - d_k) \vee 1} \delta(d|X_n, Y_{nm}) + \sum_{d \neq \tilde{d} \in D} \frac{\sum_{k=1}^{K} (1 - d_k)v_{knm}}{\sum_{k=1}^{K} (1 - d_k) \vee 1} \delta(d|X_n, Y_{nm})
\]

\[
= \frac{\sum_{k=1}^{K} (1 - \tilde{d}_k)v_{knm}}{\sum_{k=1}^{K} (1 - \tilde{d}_k) \vee 1} = v_{knm}. \quad (7.7)
\]

Application of (5.31) to the right most side of (7.7) yields

\[
cFNR_{nm} \overset{a.s.}{\to} 0, \text{ as } m \to \infty, n \to \infty,
\]

establishing (7.5).

Again, (7.6) follows from (7.5) by uniform integrability, since \( cFNR_{nm} \) is almost surely bounded above by one.

\[\square\]
7.2 Convergence of versions of FNR when versions of FDR are \( \alpha \)-controlled

**Theorem 12.** Assume the conditions of Theorem 7. Then \( \alpha = K^{-1} \) is the only asymptotic FDR control possible in the sense that there exist sequences \( \beta_{nm} \to 0 \) as \( m \to \infty \) and \( n \to \infty \) such that the following hold:

\[
\lim_{m \to \infty} \lim_{n \to \infty} cFDR_{nm} \overset{a.s.}{=} K^{-1}; \quad \text{(7.8)}
\]

\[
\lim_{m \to \infty} \lim_{n \to \infty} pBFDR_{nm} = K^{-1}. \quad \text{(7.9)}
\]

**Proof.** It follows from Chandra and Bhattacharya (2019) (see also Chandra and Bhattacharya (2020)) that \( pBFDR_{nm} \) is continuous and decreasing in \( \beta_{nm} \), for any given \( m \geq 1 \) and \( n \geq 1 \).

Hence, the maximum error given any \( m \geq 1 \) and \( n \geq 1 \) occurs when \( \beta_{nm} = 0 \). Hence, in this case, for any given \( m \geq 1 \) and \( n \geq 1 \), for our multiple testing procedure we must maximize \( \sum_{k=1}^{K} d_k v_{km} \) with respect to \( d \). This of course yields \( d_k = 1 \), for \( k = 1, \ldots, K \). For this decision \( d \), we obtain using (5.31):

\[
cFDR_{nm} = \frac{\sum_{k=1}^{K} d_k (1 - v_{km})}{\sum_{k=1}^{K} d_k \vee 1} = \frac{\sum_{k=1}^{K} (1 - v_{km})}{K} \overset{a.s.}{\to} K^{-1}, \quad \text{as } m \to \infty, \ n \to \infty. \quad \text{(7.10)}
\]

Uniform integrability and (7.10) shows that when \( \beta_{nm} = 0 \) for any \( m \geq 1 \) and \( n \geq 1 \),

\[
pBFDR_{nm} \to K^{-1}, \quad \text{as } m \to \infty, \ n \to \infty. \quad \text{(7.11)}
\]

Now consider any sequence \( \beta_{nm} \) that yields any decision \( d \) such that \( d_k = 1 \) almost surely, for sufficiently large \( m \) and \( n \). Note that \( d_k = 1 \) can occur only if \( v_{km} > \beta_{nm} \). Since \( v_{km} \overset{a.s.}{\to} 0 \) by (5.31), we must have \( \beta_{nm} \to 0 \) as \( m \to \infty \) and \( n \to \infty \) in such cases. Also since \( v_{km} \overset{a.s.}{\to} 1 \) for \( k \neq k \) due to (5.31), it follows that \( d_k = 1 \) almost surely for large enough \( m \) and \( n \), for \( k \neq k \).

Hence, the limits (7.10) and (7.11) continue to hold in all cases such that \( d_k = 1 \), for sufficiently large \( m \) and \( n \).

On the other hand, for any sequence \( \beta_{nm} \) that yields any decision \( d \) such that \( d_k = 0 \) almost surely for sufficiently large \( m \) and \( n \), it is easily seen that \( cFDR_{nm} \overset{a.s.}{\to} 0 \) and \( pBFDR_{nm} \to 0 \), as \( m \to \infty \) and \( n \to \infty \).

In other words, asymptotic control of \( cFDR_{nm} \) and \( pBFDR_{nm} \) is possible only at \( \alpha = K^{-1} \). \( \square \)

**Theorem 13.** Assume that either of \( cFDR_{nm} \) or \( pBFDR_{nm} \) is asymptotically controlled at \( \alpha = K^{-1} \). Then for sufficiently large \( m \) and \( n \),

\[
cBFNR_{nm} \overset{a.s.}{=} 0; \quad \text{(7.12)}
\]

\[
pBFNR_{nm} = 0. \quad \text{(7.13)}
\]

**Proof.** From the proof of Theorem 12, recall that for asymptotic control of \( cFDR_{nm} \) or \( pBFDR_{nm} \) at \( \alpha = K^{-1} \), we must obtain decision \( d \) where \( d_k = 1 \), for \( k = 1, \ldots, K \), for large enough \( m \) and \( n \). Hence, (7.12) and (7.13) follow simply from the definitions of \( cBFNR_{nm} \) and \( pBFNR_{nm} \) with \( d = d \) for sufficiently large \( m \) and \( n \). \( \square \)

**Remark 14.** Theorem 13 shows that \( cBFNR_{nm} \) and \( pBFNR_{nm} \) are exactly zero for large enough \( m \) and \( n \). Needless to mention, these are far stronger results than convergence to zero in the limit. In other words, essentially in keeping with the classical hypothesis testing paradigm, \( \alpha \)-control of the Type-I error actually minimizes the Type-II error for sufficiently large \( m \) and \( n \).

21
8 Modification of the multiple testing procedure for practical implementation

Note that the constants $a_k$ in (3.5) and (3.6), which depend upon the true parameter(s) $\theta_0$, are unknown, since $\theta_0$ is unknown. The constants $a_k$ also depend upon $\hat{\theta}_k$, the minimizer of the KL-divergence of model $\mathcal{M}_k$ from the true model. Since the true model itself is generally unknown, $\hat{\theta}_k$ is usually unknown. Estimation of these parameters need not be reliable unless assumptions regarding the true model is accurate enough.

In practice, the considered models $\mathcal{M}_k; k = 1, \ldots, K$, are expected to be carefully chosen for final model selection so that misspecifications, if any, are not expected to be severe. Hence, for finite samples, where the variability of $T^{(k)}(X_n)$, and hence the desired credible intervals, are reasonably large, $a_k$ is not expected to play significant role. In such cases, it makes sense to set $a_k = 0$. Similarly, setting $\varepsilon = 0$ also makes sense.

Also in practice, one might set $\tilde{\Theta}_k = \Theta_k$ since accurate specification of a small set containing $\tilde{\theta}_k$ is not possible without knowledge of $\tilde{\theta}_k$. With these, for practical purposes we re-formulate (3.5) and (3.6) as follows:

$$H_{0k} : \zeta = k, T^{(k)}(\hat{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm}, \tilde{u}_{knm}]$$

versus

$$H_{1k} : \{\zeta \neq k\} \cup \{\zeta = k, T^{(k)}(\hat{X}_n) - T^{(k)}(X_n) \in [\tilde{\ell}_{knm}, \tilde{u}_{knm}]\}.$$  

We shall consider the above hypotheses for our applications.

9 First simulation study: selection among Poisson and geometric parametric and nonparametric inverse regression models

For our simulation experiments we consider the same data and models considered in Chatterjee and Bhattacharya (2020a) for their forward and inverse pseudo-Bayes factor illustration. 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 regression 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.

Here we demonstrate that the forward and inverse pseudo-Bayes factor results obtained by Chatterjee and Bhattacharya (2020a) for both the experiments involving model selection and variable selection can be significantly improved with our inverse multiple testing framework. Let us begin with the model selection framework. The true, data-generating distribution and the competing inverse regression models are of course detailed in Chatterjee and Bhattacharya (2020a) but to make this article as self-contained as possible, we briefly describe these next.

9.1 True and competing inverse regression models

9.1.1 True distribution

The true data-generating distribution for this experiment is $y_{ij} \sim \text{Poisson}(\lambda(x_i))$, with $\lambda(x) = \exp(\alpha_0 + \beta_0 x)$. 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 $y_{ij} \sim \text{Poisson}(\lambda(x_i)); j = 1, \ldots, m, i = 1, \ldots, n$. We shall also consider the true model as one of the competing models when no misspecification is assumed.


9.1.2 Inverse 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 $-\infty < \alpha, \beta < \infty$. The prior for $\bar{x}_i$ is given by $\pi(\bar{x}_i | \alpha, \beta) \equiv U(a, b)$, where

$$a = \min \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha \right) , \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha \right) \right\} \quad (9.1)$$

and

$$b = \max \left\{ \beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha \right) , \beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha \right) \right\}. \quad (9.2)$$

We set $c_1 = 1$ and $c_2 = 100$, for ensuring positive value of $\bar{y}_i - \frac{c_1 s_i}{\sqrt{m}}$ (so that logarithm of this quantity is well-defined) and a reasonably large support of the prior for $\bar{x}_i$.

9.1.3 Inverse 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 $\text{Cov}(\eta(x_1), \eta(x_2)) = \sigma^2 \exp \left\{ -(x_1 - x_2)^2 \right\}$, where $\sigma$ is unknown. 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 $-\infty < \alpha, \beta, \omega < \infty$. Note that the prior for $\bar{x}_i$, which is uniform on $B_{im}(\eta) = \{ x : \eta(x) \in \log \left\{ \left[ \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}}, \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right] \right\} \}$, does not have a closed form, since the form of $\eta(x)$ is unknown. However, if $m$ is large, the interval $\log \left\{ \left[ \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}}, \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right] \right\}$ 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 $\pi(\bar{x}_i | \eta) \equiv U(a, b)$, where $a$ and $b$ are given by (9.1) and (9.2), respectively. As before we set $c_1 = 1$ and $c_2 = 100$.

9.1.4 Inverse geometric logit and probit linear and Gaussian process regression models

We also model the data by geometric models of the form

$$f(y_{ij}|\theta, x_i) = (1 - p(x_i))^y_{ij} p(x_i), \quad (9.3)$$

where $p(x_i)$ is modeled as logit or probit linear or nonparametric regression having the following forms:

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

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

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

We assign prior on $\bar{x}_i$ such that the mean of the geometric distribution, namely, $\frac{1 - p(x)}{p(x)}$, lies 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 principles as before shows that for the logit link, either for linear or Gaussian process regression, the prior for $\bar{x}_i$ is $U(a_1, b_1)$, where

$$a_1 = \min \left\{ -\beta^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha \right) , -\beta^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha \right) \right\} \quad (9.4)$$

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


and
\[ b_1 = \max \left\{ -\beta^{-1} \left( \log \left( \frac{y_i - c_1 s_i}{\sqrt{m}} \right) + \alpha \right), -\beta^{-1} \left( \log \left( \frac{y_i + c_2 s_i}{\sqrt{m}} \right) + \alpha \right) \right\}. \quad (9.5) \]

We set \( c_1 = 1 \) and \( c_2 = 100 \), as before.

In the case of geometric probit regression, let us first define \( \ell_{im} = y_i - \frac{c_1 u_{im}}{\sqrt{m}} \) and \( u_{im} = y_i + \frac{c_2 u_{im}}{\sqrt{m}} \). Then with
\[ a_2 = \min \left\{ \frac{\Phi^{-1} \left( \frac{1}{\ell_{im} + 1} \right) - \alpha}{\beta}, \frac{\Phi^{-1} \left( \frac{1}{\ell_{im} + 1} \right) - \alpha}{\beta} \right\}; \quad (9.6) \]
\[ b_2 = \max \left\{ \frac{\Phi^{-1} \left( \frac{1}{\ell_{im} + 1} \right) - \alpha}{\beta}, \frac{\Phi^{-1} \left( \frac{1}{\ell_{im} + 1} \right) - \alpha}{\beta} \right\}. \quad (9.7) \]

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

**9.2 Implementation of our multiple testing procedure for inverse model selection**

We now briefly discuss our strategy for implementing our multiple testing procedure for hypotheses (8.1) and (8.2). We set \( \Theta_k \) to \( \Theta_k \), so we shall denote \( \pi(\tilde{x}_i|X_{n-i}, Y_{nm}, M_k, \Theta_k) \) by \( \pi(\tilde{x}_i|X_{n-i}, Y_{nm}, M_k) \).

**9.2.1 Obtaining the posterior distributions of the discrepancy measures using IRMCMC and TMCMC**

For each competing model \( M_k; k = 1, \ldots, K \), we obtain samples from the cross-validation posterior distribution \( \pi(\tilde{x}_i|X_{n-i}, Y_{nm}, M_k) \), for \( i = 1, \ldots, n \), using fast and efficient IRMCMC. The key idea is to first generate realizations of size \( N \) from some appropriate “importance sampling density” of the form \( \pi(\tilde{x}_i, \theta_k|X_{n-i}, Y_{nm}, M_k) \), for some \( i^* \in \{1, \ldots, n\} \) using TMCMC. Note that a major advantage of TMCMC over regular MCMC is that it effectively reduces the dimensionality of the parameters to a single dimension, thus drastically improving the acceptance rate and computational speed, while ensuring good mixing properties at the same time. Appropriate choice of \( i^* \), which is equivalent to appropriate choice of the importance sampling density, has been proposed in Bhattacharya and Haslett (2007). For \( i \in \{1, \ldots, n\} \), a sub-sample of the realizations of \( \theta_k \) (but not of \( \tilde{x}_i \)) of size \( M (< N) \) is selected without replacement with importance weights proportional to the ratio of \( \pi(\tilde{x}_i, \theta_k|X_{n-i}, Y_{nm}, M_k) \) and \( \pi(\tilde{x}_{i^*}, \theta_k|X_{n-i^*}, Y_{nm}, M_k) \). For each member \( \theta_k \) of the sub-sampled realizations, \( R \) realizations of \( \tilde{x}_i \) are generated using TMCMC from \( \pi(\tilde{x}_i|\theta_k, X_{n-i}, Y_{nm}, M_k) \), to yield a total of \( R \times M \) realizations from \( \pi(\tilde{x}_i|X_{n-i}, Y_{nm}, M_k) \).

In our examples, we generate 30,000 TMCMC samples from \( \pi(\tilde{x}_{i^*}, \theta_k|X_{n-i^*}, Y_{nm}, M_k) \) of which we discard the first 10,000 as burn-in, and re-sample 1000 \( \theta_k \)-realizations without replacement from the remaining 20,000 realizations with importance weights proportional to the ratio of \( \pi(\tilde{x}_i, \theta_k|X_{n-i}, Y_{nm}, M_k) \) and \( \pi(\tilde{x}_{i^*}, \theta_k|X_{n-i^*}, Y_{nm}, M_k) \). For each re-sampled \( \theta_k \)-value, we generate 100 TMCMC realizations of \( \tilde{x}_j \). We discard the first 10,000 realizations of \( \tilde{x}_j \) as burn-in for the first re-sampled \( \theta_k \)-realization, and for the subsequent \( \theta_k \)-realizations, we set the final value of \( \tilde{x}_i \) of the previous value of \( \theta_k \) as the initial value for \( \tilde{x}_i \) given the current \( \theta_k \)-value, and continue TMCMC without any further burn-in. We thus obtain \( 1000 \times 100 = 100,000 \) realizations of \( \tilde{x}_i \) for each \( i = 1, \ldots, n \). In all our examples, the above IRMCMC strategy, in conjunction with efficient implementation of additive TMCMC, has led to excellent mixing properties.
Using the 100,000 IRMCMC samples, we obtain the posterior distribution of any given discrepancy measure \( T^{(k)}(X_n) \).

### 9.2.2 Obtaining the posterior model probabilities using Gibbs sampling

To obtain the posterior distribution of \( \zeta, p \), we first need to specify a prior for \((p_1, \ldots, p_K)\). We consider the Dirichlet prior with parameters \((\alpha_1, \ldots, \alpha_K)\), where \(\alpha_k > 0\), for \(k = 1, \ldots, K\). Given \( \zeta \), the posterior distribution of \((p_1, \ldots, p_K)\) is again a Dirichlet distribution with parameters \((\alpha_1 + I(\zeta = 1), \ldots, \alpha_K + I(\zeta = K))\). In other words,

\[
\pi(p_1, \ldots, p_K | X_n, Y_{nm}, \zeta) \equiv \text{Dirichlet}(\alpha_1 + I(\zeta = 1), \ldots, \alpha_K + I(\zeta = K)).
\] (9.8)

Given \((p_1, \ldots, p_K)\), the posterior distribution of \( \zeta \) is given by (5.4), which is a function of the Bayes factors \( BF^{(nm)}(M_k, M_{\tilde{k}}) \); \(k = 1, \ldots, K\). Chatterjee and Bhattacharya (2020a) have shown that the corresponding pseudo-Bayes factors \( PBF^{(nm)}(M_k, M_{\tilde{k}}) \); \(k = 1, \ldots, K\), have the same asymptotic properties as the Bayes factors and are computationally far more efficient. Moreover, unlike Bayes factors, pseudo-Bayes factors do not suffer from Lindley’s paradox. Thus, it seems reasonable to replace \( BF^{(nm)}(M_k, M_{\tilde{k}}) \) in (5.4) with the corresponding \( PBF^{(nm)}(M_k, M_{\tilde{k}}) \). In other words, we approximate the posterior probability \( \pi(\zeta = k | X_n, Y_{nm}, p_1, \ldots, p_K) \) as

\[
\pi(\zeta = k | X_n, Y_{nm}, p_1, \ldots, p_K) \approx \frac{p_k PBF^{(nm)}(M_k, M_{\tilde{k}})}{\sum_{\ell=1}^K p_\ell PBF^{(nm)}(M_{\ell}, M_{\tilde{k}})}; \ k = 1, \ldots, K.
\] (9.9)

Since the model probabilities are associated with the forward part, that is, where all the covariate values are treated as fixed, we consider the forward, or the traditional pseudo-Bayes factor in (9.9). In our examples, the values of \( PBF^{(nm)}(M_k, M_{\tilde{k}}) \); \(k = 1, \ldots, K\), are already available from Chatterjee and Bhattacharya (2020a) who provide estimates of \( \frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, M_k) \) in the second last column of Table 9.1. Note that

\[
\frac{1}{n} \log PBF^{(nm)}(M_k, M_{\tilde{k}}) = \frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, M_k) \approx \frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, M_k).
\]

Here \( \tilde{k} = \arg \max_{k=1, \ldots, K} \frac{1}{n} \sum_{i=1}^n \log \pi(y_{i1} | Y_{nm,-i}, X_n, M_k) \).

Using the full conditional distributions (9.8) and (9.9), we obtain 100,000 realizations from the posterior distribution of \((\zeta, p_1, \ldots, p_K)\) using Gibbs sampling, after discarding the first 10,000 iterations as burn-in.

### 9.2.3 Obtaining the posterior probabilities of the alternative hypotheses \( H_{1k} \)

Note that for \( k = 1, \ldots, K \), the posterior probability of \( H_{1k} \) is given by

\[
v_{kmn} = 1 - \pi \left( \zeta = k, T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\epsilon}_{knm}, \tilde{u}_{knm}] | X_n, Y_{nm} \right)
= 1 - \pi \left( \zeta = k | X_n, Y_{nm} \right) \pi \left( T^{(k)}(\tilde{X}_n) - T^{(k)}(X_n) \in [\tilde{\epsilon}_{knm}, \tilde{u}_{knm}] | \zeta = k, X_n, Y_{nm} \right).
\] (9.10)

Once we obtain realizations from the posteriors of \( T^{(k)}(\tilde{X}_n) \) for \( k = 1, \ldots, K \), and \((\zeta, p_1, \ldots, p_K)\), evaluation of the posterior probabilities of \( H_{1k} \), denoted by \( v_{kmn} \); \( k = 1, \ldots, K \), follows simply by Monte Carlo averaging associated with the two factors of (9.10).
9.3 Results of the simulation experiment for model selection

9.3.1 Non-misspecified situation

Section 9.1 shows that for this experiment, $K = 6$, when no misspecification is considered. We set $\alpha_k = 1$; $k = 1, \ldots, K$, for the parameters of the Dirichlet prior for $(p_1, \ldots, p_K)$. That is, we assume a uniform prior distribution for $(p_1, \ldots, p_K)$ on the simplex. We report our results with respect to this prior, but our experiments with other values of $(\alpha_1, \ldots, \alpha_K)$ did not yield different results.

For $n = m = 10$, the $cFDR_{nm}$ and $cFNR_{nm}$, for $\beta_{nm} \in [0.01, 0.99]$ are provided in Figure 9.1. The red and green colours correspond to $T_1^{(k)}(\hat{X}_n) - T_1^{(k)}(X_n)$ and $T_2^{(k)}(\hat{X}_n) - T_2^{(k)}(X_n)$, respectively. In the plots we denote these red and green coloured $cFDR$s as $cFDR_1$ and $cFDR_2$, respectively. Similarly, $cFNR_1$ and $cFNR_2$ denote the red and green coloured $cFNR$s. When $T_1^{(k)}(\hat{X}_n) - T_1^{(k)}(X_n)$ is considered, $cFDR_{nm} = 0.024$ for $\beta_{nm} < 0.86$ and equals $9.023 \times 10^{-6}$ for $\beta_{nm} \geq 0.86$. On the other hand, for $T_2^{(k)}(\hat{X}_n) - T_2^{(k)}(X_n)$, $cFDR_{nm} = 0.087$ for $0.01 \leq \beta_{nm} < 0.48$ and falls to $5.444 \times 10^{-5}$ for $0.48 \leq \beta_{nm} \leq 0.99$. In the first case, the multiple testing procedure selects $H_{ik}$ for $k = 1, \ldots, K$ when $0.01 \leq \beta_{nm} < 0.86$. When $0.86 < \beta_{nm} \leq 0.99$, the method selects $H_{i\bar{k}}$, and $H_{ik}$ for $k \neq \bar{k}$. Here $\bar{k}$ corresponds to the true data-generating model, namely, the Poisson log-linear regression model. In the second case, all the alternative hypotheses are selected when $0.01 \leq \beta_{nm} < 0.48$; the true null and remaining alternative hypotheses are chosen for $0.48 \leq \beta_{nm} \leq 0.99$. Thus, for both the discrepancy measures, the correct model is selected for appropriate values of $\beta_{nm}$. However, $cFDR_2$ falls close to zero much faster than $cFDR_1$, and from the point onwards where the true decision occurs, $cFNR_2$ is much lesser than $cFNR_1$. These demonstrate that $T_2^{(k)}(\hat{X}_n) - T_2^{(k)}(X_n)$ is a more efficient choice compared to $T_1^{(k)}(\hat{X}_n) - T_1^{(k)}(X_n)$.

Here is an important point regarding comparison with our multiple testing result with that of inverse pseudo-Bayes factor reported in the last column of Table 9.1 of Chatterjee and Bhattacharya (2020a). The column shows that the inverse pseudo-Bayes factor identifies the true Poisson log-linear regression model as only the second best. However our multiple testing procedure correctly identifies the true model as the best one, for appropriate values of $\beta_{nm}$.

It is also important to remark in this context that the posterior probabilities of $T^{(k)}(\hat{X}_n) - T^{(k)}(X_n) \in [\ell_{knm}, \bar{u}_{knm}]$ when $k$ is the true model, is significantly smaller than several other models. That the true model still turns out to be the best is due to its much larger posterior model probability compared to the others. The point is that even the true data-generating model need not have large posterior probabilities associated with the inverse discrepancy measure, and if the corresponding posterior model probability is not significantly large, then any other model can turn out to be the best on the basis of its stronger inverse perspective.

9.3.2 Misspecified situation

Let us now consider the case of misspecification, that is, when the true Poisson log-linear model is left out from consideration among the competing models. Thus, $K = 5$ in this case. The remaining setup is the same as in the non-misspecified scenario. Figure 9.2 display the $cFDR$s and $cFNR$s for this situation, each associated with both $T_1^{(k)}(\hat{X}_n) - T_1^{(k)}(X_n)$ and $T_2^{(k)}(\hat{X}_n) - T_2^{(k)}(X_n)$. In this case, for both the discrepancy measures, the correct decision, namely, the null hypothesis for the Poisson log-Gaussian process and the alternative hypotheses for the remaining models, is reached for relatively large values of $\beta_{nm}$. Indeed, $cFDR_1 = 0.002$ for $0.01 \leq \beta_{nm} < 0.99$ and $0.0003$ for $\beta_{nm} = 0.99$ and $cFDR_2 = 0.020$ for $0.01 \leq \beta_{nm} < 0.91$ and $0.0003$ for $0.91 \leq \beta_{nm} < 0.99$. Again, $T_2^{(k)}(\hat{X}_n) - T_2^{(k)}(X_n)$ performs better than $T_1^{(k)}(\hat{X}_n) - T_1^{(k)}(X_n)$ in terms of faster decrease of $cFDR_{nm}$ towards zero and lesser value of $cFNR_{nm}$ once the right decision has been obtained.
Here the multiple testing procedure turns out to be consistent with both forward and inverse pseudo-Bayes factor, since the last two columns of Table 9.1 of Chatterjee and Bhattacharya (2020a) show that if the Poisson log-linear model is not considered among the competing models, then the Poisson log-Gaussian process model is the best. Here the corresponding posterior probability of $T^{(k)}(X_n) - T^{(k)}(X_n) \in [\hat{\ell}_{kmn}, \hat{u}_{kmn}]$ is higher than those of the other models, in addition to higher posterior model probability.

10 Second simulation study: variable selection in Poisson and geometric linear and nonparametric regression models when true model is Poisson linear regression

Again, for the purpose of making this article as self-contained as possible, we begin with brief descriptions of the true and competing inverse regression models in the variable selection context.

We now consider covariates $x$ and $z$, where the true data-generating distribution is $y_{ij} \sim \text{Poisson}(\lambda(x_i, z_i))$, with $\lambda(x, z) = \exp(\alpha_0 + \beta_0 x + \gamma_0 z)$. The data is generated as follows. We simulate $\alpha_0, \beta_0, \gamma_0 \sim U(-1, 1)$ independently and $x_i \sim U(-1, 1), z_i \sim U(0, 2)$; $i = 1, \ldots, n$, independently. Finally, we generate $y_{ij} \sim \text{Poisson}(\lambda(x_i, z_i)); j = 1, \ldots, m, i = 1, \ldots, n$, independently.

As in Chatterjee and Bhattacharya (2020a) we model the data $y_{ij}; i = 1, \ldots, n; j = 1, \ldots, m$ with both Poisson and geometric models letting the regression part consist 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 $(\alpha, \beta, \gamma, \omega)$ 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 $\text{Cov}(\eta(x_1, z_1), \eta(x_2, z_2)) = \exp(\omega)\exp[-\{(x_1 - x_2)^2 + (z_1 - z_2)^2\}]$, 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. Where the model consists of the single covariate $x$ or $z$, 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 $\tilde{z}_i$, and the same priors for $\tilde{x}_i$ and $\tilde{z}_i$ as the previous situations where the models

![Figure 9.1: cFDR and cFNR as functions of $\beta_{nm}$](image-url)
Figure 9.2: $cFDR_{nm}$ and $cFNR_{nm}$ as functions of $\beta_{nm}$ in the misspecified case.

consisted of single covariates, will not be consistent here. Letting $\alpha$ be the intercept, $\beta$ and $\gamma$ the coefficients of $x_i$ and $z_i$ respectively in the regression forms, we consider the same consistent priors for $\tilde{x}_i$ and $\tilde{z}_i$ as proposed in Chatterjee and Bhattacharya (2020a). In Sections 10.0.1, 10.0.2 and we provide the forms of the priors for $\tilde{x}_i$ and $\tilde{z}_i$ when the models consist of both the covariates $x$ and $z$.

10.0.1 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

$$b_z^{(1)} = \max \left\{ \gamma^{-1} \left( \log \left( \bar{y}_i - \frac{c_1 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right), \gamma^{-1} \left( \log \left( \bar{y}_i + \frac{c_2 s_i}{\sqrt{m}} \right) - \alpha - \beta x_i \right) \right\}.$$
10.0.2 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 $\tilde{x}_i \sim U\left(\tilde{a}_x^{(2)}, \tilde{b}_x^{(2)}\right)$ and $\tilde{z}_i \sim U\left(\tilde{a}_z^{(2)}, \tilde{b}_z^{(2)}\right)$, where

$$a_x^{(2)} = \min \left\{ -\beta^{-1} \left( \log \left( y_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) , -\beta^{-1} \left( \log \left( y_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) \right\} ,$$

$$b_x^{(2)} = \max \left\{ -\beta^{-1} \left( \log \left( y_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) , -\beta^{-1} \left( \log \left( y_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha + \gamma z_i \right) \right\} ,$$

$$a_z^{(2)} = \min \left\{ -\gamma^{-1} \left( \log \left( y_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) , -\gamma^{-1} \left( \log \left( y_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) \right\} ,$$

and

$$b_z^{(2)} = \max \left\{ -\gamma^{-1} \left( \log \left( y_i - \frac{c_1 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) , -\gamma^{-1} \left( \log \left( y_i + \frac{c_2 s_i}{\sqrt{m}} \right) + \alpha + \beta x_i \right) \right\} .$$

10.0.3 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 $\tilde{x}_i \sim U\left(\tilde{a}_x^{(3)}, \tilde{b}_x^{(3)}\right)$ and $\tilde{z}_i \sim U\left(\tilde{a}_z^{(3)}, \tilde{b}_z^{(3)}\right)$, where

$$a_x^{(3)} = \min \left\{ \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \gamma z_i , \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \gamma z_i \right\} ,$$

$$b_x^{(3)} = \max \left\{ \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \gamma z_i , \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \gamma z_i \right\} ,$$

$$a_z^{(3)} = \min \left\{ \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \beta x_i , \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \beta x_i \right\} ,$$

and

$$b_z^{(3)} = \max \left\{ \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \beta x_i , \Phi^{-1} \left( \frac{1}{\sqrt{m} + 1} \right) - \alpha - \beta x_i \right\} .$$

10.1 Discrepancy measure and Dirichlet prior parameters for more than one covariate

In models where both the covariates are considered, for any two $n$-dimensional vectors $v_{1n} = (v_{11}, \ldots, v_{1n})$ and $v_{2n} = (v_{21}, \ldots, v_{2n})$, letting $v_i = (v_{1i}, v_{2i})^T$, $V_n = (v_1, \ldots, v_n)$ and denoting the posterior mean vector and covariance matrix of $\tilde{u}_i = (\tilde{x}_i, \tilde{z}_i)^T$ by $E_k(\tilde{u}_i)$ and $Var_k(\tilde{u}_i)$ respectively, for $i = 1, \ldots, n$, we set

$$T_3^{(k)}(V_n) = \frac{1}{n} \sum_{i=1}^{n} (\tilde{v}_i - E_k(\tilde{u}_i))^T Var_k(\tilde{u}_i) + c \bar{c}^{-1} (\bar{v}_i - E_k(\tilde{u}_i)) ,$$

(10.1)
where $c > 0$ and $I$ is the identity matrix. Here $E_k(\mathbf{u}_i)$ and $Var_k(\mathbf{u}_i)$ correspond to the cross-validation posterior $\pi(\mathbf{u}_i|X_{n-i}, Y_{nm}, M_k)$.

In our experiment, as before we shall compare the results corresponding to $T_1^{(k)}(\mathbf{W}_n) - T_1^{(k)}(\mathbf{W}_n)$ and $T_2^{(k)}(\mathbf{W}_n) - T_2^{(k)}(\mathbf{W}_n)$, where $\mathbf{W}_n$ is either $\mathbf{X}_n$ or $\mathbf{Z}_n$ and $\mathbf{W}_n$ is either $\mathbf{X}_n$ or $\mathbf{Z}_n$. But for any inverse model that consists of both the covariates $x$ and $z$, we replace both $T_1^{(k)}(\mathbf{W}_n) - T_1^{(k)}(\mathbf{W}_n)$ and $T_2^{(k)}(\mathbf{W}_n) - T_2^{(k)}(\mathbf{W}_n)$ with $T_3^{(k)}(\mathbf{V}_n) - T_3^{(k)}(\mathbf{V}_n)$, where $\mathbf{v}_i = (\tilde{x}_i, \tilde{z}_i)^T$, $\mathbf{V}_n = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$.

For models having both $x$ and $z$ as covariates, the corresponding discrepancy measures $T_3^{(k)}(\mathbf{V}_n) - T_3^{(k)}(\mathbf{V}_n)$ are associated with joint cross-validation posterior distributions of $(\tilde{x}_i, \tilde{z}_i)$, and hence the corresponding posterior probabilities of the hypotheses are expected to be much smaller than posterior probabilities of the hypotheses of the models with single covariates. We make amends for this by setting the parameters $\alpha_k$ of the Dirichlet prior for $(p_1, \ldots, p_K)$ for any model $M_k$ with both covariates to be 5 times that of the remaining parameters. So, in our case, we set $\alpha_k = 5$ for those $k$ associated with both the covariates, and set the remaining parameters to 1.

Note that in this experiment, $K = 18$, including the true inverse Poisson log-linear regression model with both the covariates $x$ and $z$. The implementation details remain the same as described in Section 9.2.

10.2 Results of our multiple testing experiment for model and variable selection

10.2.1 Non-misspecified situation

For $n = m = 10$, when the true model is Poisson with log-linear regression on both the covariates $x$ and $z$, Figure 10.1 shows $cFDR_{nm}$ and $cFNR_{nm}$ as functions of $\beta_{nm}$. In this case $cFDR_1$ decreases towards zero slightly faster than $cFDR_2$. The numerical values of step functions $cFDR_1$ and $cFDR_2$ are provided as follows:

$$
cFDR_1 = \begin{cases} 
0.025 & \text{if } 0.01 \leq \beta_{nm} < 0.67; \\
0.007 & \text{if } 0.67 \leq \beta_{nm} < 0.91; \\
0.001 & \text{if } 0.91 \leq \beta_{nm} < 0.99; \\
6.214 \times 10^{-7} & \text{if } \beta_{nm} = 0.99 
\end{cases}
$$

and

$$
cFDR_2 = \begin{cases} 
0.032 & \text{if } 0.01 \leq \beta_{nm} < 0.67; \\
0.014 & \text{if } 0.67 \leq \beta_{nm} < 0.80; \\
0.002 & \text{if } 0.80 \leq \beta_{nm} < 0.98; \\
5.767 \times 10^{-6} & \text{if } 0.98 \leq \beta_{nm} \leq 0.99. 
\end{cases}
$$

Note that the first change point for both $cFDR_1$ and $cFDR_2$ occurs at $\beta_{nm} = 0.67$, and at this point, we obtain the decision configuration that selects the null hypothesis of the true, Poisson log-linear model with both covariates $x$ and $z$, and alternative hypotheses of all other models. For $\beta_{nm} < 0.67$, for all the models, the alternative hypotheses are selected. Thus, the first change point associated with both $cFDR_1$ and $cFDR_2$ yields the correct decision configuration. The next change points $\beta_{nm} = 0.91$ and $\beta_{nm} = 0.80$ for $cFDR_1$ and $cFDR_2$ are associated with selecting the null hypothesis for the model with the Poisson log-linear model with covariate $x$, in addition to the null hypothesis of the true, Poisson log-linear model with both covariates $x$ and $z$. The final change points $\beta_{nm} = 0.99$ and $\beta_{nm} = 0.98$ yield the decision configurations that select the null hypothesis for the model with the Poisson log-linear model with covariate $z$, in addition to the previous null hypotheses. Thus, $cFDR_1$ and $cFDR_2$ behave quite consistently in
this example and there seems to be no obvious reason for preferring one discrepancy measure to the other. Observe in Figure 10.1 that cFNR1 and cFNR2 are also quite consistently behaved.

Again the important observation is that our multiple testing procedure seems to easily identify the true inverse model, while neither forward nor inverse pseudo-Bayes factor successfully identified the true inverse model, as shown in the last two columns of Table 9.2 of Chatterjee and Bhattacharya (2020a). The second and third best models, namely, the Poisson log-linear model with covariate $x$ and the Poisson log-linear model with covariate $z$, respectively, are however, consistent with forward and inverse pseudo-Bayes factor results reported in Chatterjee and Bhattacharya (2020a).

Again we find that the posterior probabilities of $T(k)(\tilde{X}_n) - T(k)(X_n) \in [\tilde{l}_{knm}, \tilde{u}_{knm}]$ when $k$ is the true model, is significantly smaller than most of the other models, but its much higher posterior model probability compared to the others succeeds in making it the winner. The above inverse posterior probabilities for the second and third best models are also not higher than the remaining ones.

### 10.2.2 Misspecified situation

In the misspecified situation we leave out the true Poisson log-linear model with both covariates $x$ and $z$ from among the competing models and implement our multiple testing procedure to obtain the best possible inverse models among the remaining ones. Figure 10.2 summarizes the results of our implementation in this direction. Both cFDR1 and cFDR2 yield the Poisson log-linear model with covariate $x$ and the Poisson log-linear model with covariate $z$ as the best and the next best inverse models, corresponding to the two change points observed in the graphs of cFDR1 and cFDR2. Recall that these were the second and the third best models in the non-misspecified situation, showing that our results for this misspecified case is very much coherent.

Observe that the best model in this case is detected by cFDR2 much earlier than cFDR1, and its value falls close to zero much earlier than that of cFDR1 in the process. The graphs for cFNR1 and cFNR2 shows that at points where the best and the next best models are selected, cFNR2 is significantly smaller than cFNR1. Hence, in this misspecified situation, $T_2^{(k)}$ is again

---

**Figure 10.1:** $cFDR_{nm}$ and $cFNR_{nm}$ as functions of $\beta_{nm}$ in the non-misspecified situation of the model and variable selection problem.
11 Summary and discussion

Inverse regression problems have received little attention and Bayesian inverse regression problems occupy even lesser space in the statistical literature (see Chatterjee and Bhattacharya (2017) for an overview). In particular, model selection procedures that account for the inverse perspective has not even been touched upon so far, except the recent pseudo-Bayes factor undertaking by Chatterjee and Bhattacharya (2020a). In this article we propose and develop a novel Bayesian multiple testing formulation for the above purpose. Despite the relevance and elegance of the asymptotic theory, the real importance of our contribution lies in realistic, small sample situations where the inverse perspective of the competing models are expected to be most pronounced. The fast and efficient computational strategy that we employ for implementing our multiple testing procedure renders inverse model selection straightforward in the realistic finite sample context. Interestingly, the forward pseudo-Bayes factor also features in our computational methodology, lending efficiency once it is available for the competing models. Most importantly, our simulation experiments demonstrate that our Bayesian multiple testing procedure can improve upon the results of both forward and inverse pseudo-Bayes factors.

Although in this article we have exclusively considered the consistent prior for $\tilde{x}_1$ developed by Chatterjee and Bhattacharya (2020b), at least for applications there is no bar to specifying any other sensible prior for $\tilde{x}_1$. Even though such priors need not lead to consistency of the inverse cross-validation posteriors, acceptable finite-sample based Bayesian inference can be obtained as in any other situations, for any $n > 1$ and $m \geq 1$.

Although we shall consider applications of our multiple testing procedure to various real data problems, let us present here some of our previous results on assessment of some palaeoclimate reconstruction models using the inverse reference distribution approach of Bhattacharya (2013) in the light of our new multiple testing strategy.

Vasko et al. (2000) reported a regular MCMC based inverse cross-validation exercise for a data set comprising multivariate counts $y_i$ on $m = 52$ species of chironomid at $n = 62$ lakes.
(sites) in Finland. The unidimensional \( x_i \) denote mean July air temperature. As species respond differently to summer temperature, the variation in the composition provides the analyst with information on summer temperatures. This information is exploited to reconstruct past climates from count data derived from fossils in the lake sediment; see Korhola et al. (2002). The Bayesian model is a Multinomial-Dirichlet model for the species counts with a Gaussian response function of the species parameters. However, Bhattacharya (2013) showed that the posterior probabilities associated with the discrepancy measures \( T_1 \) and \( T_2 \) given by (1.1) and (1.2) were almost zero. Bhattacharya (2006) proposed an improved Bayesian model for the same dataset, by replacing the unimodal Gaussian response function with a Dirichlet process (Ferguson (1974)) based mixture of Gaussian functions, which very flexibly allows unknown number of climate preferences and tolerance levels for each species. Although this model brought about marked improvement over that of Vasko et al. (2000) in terms of including significantly more \( x_i \) in the associated 95% highest posterior density credible intervals of the cross-validation posteriors, the posterior probabilities associated with \( T_1 \) and \( T_2 \) were still almost zero. A much improved palaeoclimate model was finally postulated by Mukhopadhyay and Bhattacharya (2013) by replacing the multinomial model with zero-inflated multinomial to account for excess zero species counts typically present in the data. The other features of the model are similar to that of Bhattacharya (2006). Not only does this model far surpasses the previous models in terms of including the percentage of \( x_i \) in the corresponding 95% highest posterior density credible intervals of the cross-validation posteriors (indeed, about 97% \( x_i \) are included in the respective intervals), inverse reference distributions for various discrepancy measures, including \( T_1 \) and \( T_2 \), comfortably contain the observed discrepancy measures in their respective 95% highest posterior density credible intervals such that the relevant posterior probabilities associated with the discrepancy measures are significantly large. Recast in our multiple testing framework, the results show that irrespective of the posterior probabilities of the aforementioned three Bayesian models, the multiple testing method would select the model of Mukhopadhyay and Bhattacharya (2013) because of the overwhelming impact of its inverse regression part compared to the other two competing models.

In Haslett et al. (2006) pollen data was used, rather than chironomid data. The training data consisted of 7815 observations of two climate variables and 14 species of pollen. The model proposed by Haslett et al. (2006) is again a Multinomial-Dirichlet distribution, but the two-dimensional response surface is based on lattice Gaussian Markov Random Field (GMRF) (see, for example, Rue and Held (2005)) which is responsible for creation of a very large number of parameters. Indeed, their model consists of about 10,000 parameters. The other limitations of this model are summarized in Mukhopadhyay and Bhattacharya (2013). Applying the inverse reference distribution approach to this model and data Bhattacharya (2004) (Chapter 7) obtained almost zero posterior probability of the inverse part. In fact, he demonstrated that this model overfits the pollen data; see also Mukhopadhyay and Bhattacharya (2013) who point out that such overfit is the consequence of the very large number of parameters and the GMRF assumption. The general zero-inflated Multinomial-Dirichlet model along with the Dirichlet process based bivariate Gaussian mixture model for the response functions proposed by Mukhopadhyay and Bhattacharya (2013) again turned out to be very successful in handling this pollen based palaeoclimate data. While including more than 94% of the two observed climate variables in their respective 95% highest posterior density credible intervals, the inverse reference distributions well-captured the observed discrepancy measures, so that again the posterior probability of the inverse part turned out to be emphatically pronounced. Thus, recast in our multiple testing paradigm, one can easily see that the zero-inflated Multinomial-Dirichlet model with the Dirichlet process based response function would emerge the clear winner.
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

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

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:

\[
\begin{align*}
(1) & \quad \pi(G_n) \geq 1 - \zeta \exp(-\gamma n), \text{ for some } \zeta > 0, \gamma > 2h(\Theta); \\
(2) & \quad \text{The convergence in (S3) is uniform in } \theta \text{ over } G_n \setminus I; \\
(3) & \quad h(G_n) \to h(\Theta), \text{ as } n \to \infty.
\end{align*}
\]

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 \(\limsup_{n \to \infty} n^{-1} \log \pi(I_A R_n) < \infty\). 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 $\pi(A) > 0$,

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

(A.3)
as $n \rightarrow \infty$.

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