

Scalable Empirical Bayes Inference and Bayesian Sensitivity Analysis

Hani Doss and Antonio Linero

Abstract. Consider a Bayesian setup in which we observe Y , whose distribution depends on a parameter θ , that is, $Y | \theta \sim \pi_{Y|\theta}$. The parameter θ is unknown and treated as random, and a prior distribution chosen from some parametric family $\{\pi_{\theta}(\cdot; h), h \in \mathcal{H}\}$, is to be placed on it. For the subjective Bayesian there is a single prior in the family which represents his or her beliefs about θ , but determination of this prior is very often extremely difficult. In the empirical Bayes approach, the latent distribution on θ is estimated from the data. This is usually done by choosing the value of the hyperparameter h that maximizes some criterion. Arguably the most common way of doing this is to let $m(h)$ be the marginal likelihood of h , that is, $m(h) = \int \pi_{Y|\theta} v_h(\theta) d\theta$, and choose the value of h that maximizes $m(\cdot)$. Unfortunately, except for a handful of textbook examples, analytic evaluation of $\arg \max_h m(h)$ is not feasible. The purpose of this paper is two-fold. First, we review the literature on estimating it and find that the most commonly used procedures are either potentially highly inaccurate or don't scale well with the dimension of h , the dimension of θ , or both. Second, we present a method for estimating $\arg \max_h m(h)$, based on Markov chain Monte Carlo, that applies very generally and scales well with dimension. Let g be a real-valued function of θ , and let $I(h)$ be the posterior expectation of $g(\theta)$ when the prior is v_h . As a byproduct of our approach, we show how to obtain point estimates and globally-valid confidence bands for the family $I(h), h \in \mathcal{H}$. To illustrate the scope of our methodology we provide three detailed examples, having different characters.

Key words and phrases: Bayesian model selection, Donsker class, geometric ergodicity, hyperparameter selection, Markov chain Monte Carlo, regenerative simulation.

1. INTRODUCTION

This paper deals with the situation where there is an observable Y whose distribution depends on a parameter θ , that is, $Y | \theta \sim \pi_{Y|\theta}$, where θ is unknown and treated as random. A prior distribution, π_{θ} , is placed on θ , and having observed Y , inference on θ is made through the posterior distribution $\pi_{\theta|Y}$. It is common that the prior is chosen from some parametric family $\{\pi_{\theta}(\cdot; h), h \in \mathcal{H}\}$. As is well known and we discuss later, inference can depend heavily on the hyperparameter value h that specifies the prior. For the subjective Bayesian there is a sin-

gle value of h which represents his or her beliefs about θ . However, for several reasons, including the possibility that $\dim(\theta)$ is large and the fact that understanding distributions on a high-dimensional space is very difficult, it is often the case that determination of this value of h is essentially impossible. In the empirical Bayes approach, the latent distribution on θ is estimated from the data (this is sometimes referred to as “frequentist estimation of the prior.” This is done by setting up some criterion function of h (we review two such below) and maximizing it. Unfortunately, maximizing a suitable criterion is very difficult in all but very simple situations. The following two examples illustrate the points above.

Shrinkage Estimation in the Normal Means Problem. The empirical Bayes approach to the normal means problem was initiated in a series of papers by Efron and Morris in the 1970s (see, e.g., [Efron and Morris, 1973](#)). The setup

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is the hierarchical model

$$(1.1) \quad \begin{aligned} Y_i | \theta_i &\stackrel{\text{indep}}{\sim} \mathcal{N}(\theta_i, 1), \quad i = 1, \dots, p, \\ \theta_i | (\mu, \lambda) &\stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \lambda), \quad i = 1, \dots, p, \end{aligned}$$

in which μ and λ are unknown. We observe $Y := (Y_1, \dots, Y_p)$ and we wish to estimate $\theta := (\theta_1, \dots, \theta_p)$. The posterior mean of θ_i is

$$(1.2) \quad \hat{\theta}_i^{\lambda, \mu} = \frac{\lambda}{\lambda + 1} Y_i + \frac{1}{\lambda + 1} \mu.$$

This gives a class of estimators of θ , indexed by (λ, μ) . The hyperparameter is $h = (\lambda, \mu)$, and plays an important role: μ is the point toward which there is shrinkage; and λ controls the amount of shrinkage—when it is large there is little shrinkage, and when it is small there is a lot of shrinkage. The goal is to find the “optimal” value of (λ, μ) . Let $R(\hat{\theta}^{\lambda, \mu}, \theta)$ denote the risk (under sum of squared errors as loss) of the estimate $\hat{\theta}^{\lambda, \mu} = (\hat{\theta}_1^{\lambda, \mu}, \dots, \hat{\theta}_p^{\lambda, \mu})$. Note that $R(\hat{\theta}^{\lambda, \mu}, \theta)$ depends on (λ, μ) and also on θ , which is unknown. The optimal value of (λ, μ) is taken to be the value that minimizes $R(\hat{\theta}^{\lambda, \mu}, \theta)$, and this can’t be obtained since we don’t know θ . Stein’s unbiased risk estimate (SURE, Stein, 1981), denoted $\text{SURE}(\lambda, \mu)$, is a statistic with the property that $E_\theta[\text{SURE}(\lambda, \mu)] = R(\hat{\theta}^{\lambda, \mu}, \theta)$, where the notation E_θ signifies that the expectation is taken under the assumption that $Y_i \stackrel{\text{indep}}{\sim} \mathcal{N}(\theta_i, 1)$. Since we can’t obtain $\arg \min_{\lambda, \mu} R(\hat{\theta}^{\lambda, \mu}, \theta)$, we compute $(\hat{\lambda}^{\text{opt}}, \hat{\mu}^{\text{opt}}) = \arg \min_{\lambda, \mu} \text{SURE}(\lambda, \mu)$ and use $(\hat{\lambda}^{\text{opt}}, \hat{\mu}^{\text{opt}})$ in place of (λ, μ) in (1.2). The result is an estimator of θ which is very similar to the James–Stein estimate (James and Stein, 1960). In this example, the θ_i ’s can be thought of as coming from some true but unknown latent distribution.

Variable Selection in Linear Regression. Bayesian approaches to variable selection provide a natural way of simultaneously treating both model and parameter uncertainty. In a linear regression situation, we have a response variable Y and a set of predictors X_1, \dots, X_p , each a vector of length m . For each $\gamma \subseteq \{1, \dots, p\}$ we have a potential model given by $Y = 1_m \beta_0 + X_\gamma \beta_\gamma + \epsilon$, where 1_m is the vector of m 1’s, X_γ is the design matrix whose columns consist of the predictor vectors corresponding to the subset γ , β_γ is the vector of coefficients for that subset, and $\epsilon \sim \mathcal{N}_m(0, \sigma^2 I)$. We view γ as a binary vector of length p , whose j th component, γ_j , is 1 if variable j is in the model, and is 0 otherwise. The unknown parameter is $\theta = (\gamma, \sigma, \beta_0, \beta_\gamma)$, which includes the indicator of the subset of variables that go into the linear model. In a common formulation of the Bayesian approach, the prior on θ is given by a hierarchy in which we first choose the indicator γ from some distribution, a “noninformative prior” is given to (σ^2, β_0) , and given γ and σ , we choose β_γ from some proper distribution. The distribution

for γ is the so-called independence Bernoulli prior—each variable goes into the model with a certain probability w , independently of all the other variables. The distribution for β_γ is taken to be Zellner’s g -prior (see (1.3b) below), which depends on a hyperparameter g . Let $p_\gamma = \sum_{j=1}^p \gamma_j$ denote the number of variables in the model indexed by γ . In detail, this common formulation is described as follows:

$$(1.3a) \quad Y \sim \mathcal{N}_m(1_m \beta_0 + X_\gamma \beta_\gamma, \sigma^2 I),$$

$$(1.3b) \quad \beta_\gamma \sim \mathcal{N}_{p_\gamma}(0, g \sigma^2 (X_\gamma^\top X_\gamma)^{-1}),$$

$$(1.3c) \quad (\sigma^2, \beta_0) \sim p(\beta_0, \sigma^2) \propto 1/\sigma^2,$$

$$(1.3d) \quad \gamma \sim w^{p_\gamma} (1 - w)^{p - p_\gamma}.$$

In (1.3), each line is understood to be a distributional statement conditional on all the variables specified in the lines below it. Here, the hyperparameter is $h = (g, w)$, and its effect is roughly as follows. When g is large the posterior is concentrated on models with few variables and large regression coefficients, and when g is small the posterior is concentrated on large models with small coefficients; and w in (1.3d) has the opposite effect, with small w favoring models with only a few variables, and large w favoring models with many variables (the interplay between w and g is not well understood). Therefore, the hyperparameter $h = (w, g)$ plays a very important role, and in effect determines the model that will be used to carry out variable selection. We return to this variable selection problem in Section 3. Here, obtaining an equivalent to the SURE does not appear to be feasible—this is the case for most models of current interest—and another objective function must be used. In this example, it is not appropriate to think of the latent variables (the γ_j ’s and the β_j ’s) as coming from some true but unknown latent distribution. However, empirical Bayes methodology can be applied to both the normal means problem and the variable selection problem.

Another objective function, one which is much more commonly used, is the marginal likelihood $m(h) = \int \ell_y(\theta) \pi_\theta(\theta; h) d\theta$, where $\ell_y(\theta) = \pi_{Y|\theta}(y)$ is the likelihood function, which we maximize; so with the marginal likelihood as the objective function, the empirical Bayes estimate of h is $\arg \max_h m(h)$. Unfortunately, except for a handful of textbook examples, analytic evaluation of $m(h)$ or its argmax is not feasible, and numerical approximations must be used.

The purpose of this paper is twofold. First we review the literature on deterministic and stochastic methods for the numerical approximation of $\arg \max_h m(h)$. An important component of our review is a discussion of scalability, and we find that the most commonly used procedures are either potentially highly inaccurate or don’t scale well with the dimension of h , the dimension of θ ,

or both. Our second purpose is to present an approach, based on Markov chain Monte Carlo (MCMC) and empirical process theory, for estimating $\arg \max_h m(h)$ which scales well with the dimensions of h and θ . The approach has the following advantages. (i) It provides provable $n^{1/2}$ convergence rates to the argmax, where n is the Markov chain length. (ii) It enables theoretically valid quantification of the Monte Carlo error. (iii) It can be used in a standard Bayesian analysis for simultaneous estimation of a posterior expectation as the hyperparameter varies. More specifically, let g be some function of θ . In Bayesian sensitivity analysis, we are interested in $I(h) := \int g(\theta) \pi_{\theta|Y}(\theta; h) d\theta$ as h varies continuously. We show that from the single Markov chain run, we can estimate the entire function $I(h)$ as h varies, and also to construct simultaneous confidence intervals for $I(h)$, as h varies continuously over \mathcal{H} .

The literature we review and our results pertain strictly to estimation of $\arg \max_h m(h)$. They say nothing about the quality of the empirical Bayes procedure, and it is natural to ask what are the consequences of using an empirical Bayes approach as opposed to a subjective Bayes approach, should such be feasible. The literature does address this question. Suppose a Bayesian has prior $\pi_{\theta}(\cdot; h_0)$ for some $h_0 \in \mathcal{H}$, but uses $\pi_{\theta}(\cdot; h_{EB})$ instead, where $h_{EB} = \arg \max_h m(h)$. What is the connection between $\pi_{\theta|Y}(\cdot; h_{EB})$ and $\pi_{\theta|Y}(\cdot; h_0)$? Suppose that Y is $Y_{(n)} = (Y_1, \dots, Y_n)$, and that $Y_1, Y_2, \dots \stackrel{\text{iid}}{\sim} p_{\theta_0}$ for some $\theta_0 \in \Theta$. [Petrone, Rousseau and Scricciolo \(2014\)](#) have shown that, under certain regularity conditions, $\|\pi_{\theta|Y}(\cdot; h_{EB}) - \pi_{\theta|Y}(\cdot; h_0)\|_1 \rightarrow 0$ as $n \rightarrow \infty$, where $\|\cdot\|_1$ denotes the L_1 norm, and the convergence is in the sense of almost sure with respect to $p_{\theta_0}^{(\infty)}$, the joint distribution of Y_1, Y_2, \dots . The significance of this result is that a Bayesian having prior $\pi_{\theta}(\cdot; h_0)$ but because of difficulty specifying h_0 uses h_{EB} instead, asymptotically will reach the same conclusion had h_0 been used.

Much contemporary Bayesian work deals with settings where the model is very complex and $\dim(\theta)$ is large. Determination of a class of priors to choose from is then very difficult. In these situations, the class is typically chosen on the basis of convenience; for example, one may work with some standard or familiar family $\{\pi_{\theta}(\cdot; h), h \in \mathcal{H}\}$, for instance one possessing some conjugacy properties, and in a setting where there is a true latent distribution on θ , call it G , underlying the model, this is done with the understanding that G is not a member of the family. Determination of $\arg \max_h m(h)$ is then still of practical interest, as $\pi_{\theta}(\cdot; \arg \max_h m(h))$ typically converges to the member of the family that is closest, in the Kullback–Leibler sense, to G .

The results of this paper are nonasymptotic: the data point Y does not need to correspond to i.i.d. points Y_1, \dots, Y_n where n is large, indeed it does not even need

to correspond to independent observations, and in the previous paragraphs n refers to the Markov chain length, not the data sample size. The rest of the paper is organized as follows. Section 2 contains our review of the literature on numerical approximation of $\arg \max_h m(h)$, and a description of our proposal for a scalable method for estimation of $\arg \max_h m(h)$ together with its theoretical underpinnings. Section 3 provides two of three illustrations which are chosen to have very different characters in order to demonstrate the scope of our methodology. The first illustration involves an empirical Bayes approach to variable selection in regression, in an extension of the second of the two examples discussed above. We consider an additive regression model in which each variable is fit using a regression spline. We show how our methodology can be used to select the significant knots for each predictor variable and, interestingly, also to eliminate variables which are not useful in the regression. The second illustration involves a Bayesian tree model for regression with many predictors. The model features a hyperparameter that controls sparsity. We show how our methodology can be used to select the sparsity parameter, and also show that with this adaptive choice, the model acts appropriately in sparse and nonsparse situations. The third illustration is in the supplement. In Section S-2 of the Supplementary Material ([Doss and Linero, 2024](#)), we discuss an example which involves a robust binary regression model. In this example, we use our methodology to select the “robustness” parameter, which is a parameter in the model, as opposed to the hyperparameter of the prior distribution. In Section 3 we also discuss the question of whether one should do a fully Bayes analysis instead of an empirical Bayes analysis. The proofs of our theoretical results are in Section S-3 of the Supplementary Material ([Doss and Linero, 2024](#)).

2. ESTIMATION OF THE MARGINAL LIKELIHOOD FUNCTION AND ITS ARGMAX

This section consists of three parts. In the first, we review current methods for hyperparameter selection, discussing strengths and weaknesses; in the second, we present our approach for obtaining the maximizer of the marginal likelihood function $m(h)$, and provide two theorems that give it theoretical support; and in the third, we show how the ideas underlying our approach can be used to construct simultaneous confidence bands for the posterior expectation of a function of θ as the hyperparameter of the prior varies continuously.

2.1 Review of Methods for Estimation of the Marginal Likelihood or Its Maximizer

The literature on estimation of $\arg \max_h m(h)$ is very large, and we limit our review to the methods that are the most competitive, and also to those that are frequently

used in the machine learning literature, whether or not these are competitive. Our discussion spans three groups.

Direct Monte Carlo Estimation of the Marginal Likelihood Function. In approaches from this group, for each h over a fine grid in \mathcal{H} , we run a Monte Carlo experiment to form an estimate $\hat{m}(h)$ of $m(h)$; we do this separately for each h , and we estimate $\arg \max_h m(h)$ via $\arg \max_h \hat{m}(h)$. Papers that proceed in this way include Chib (1995), Chib and Jeliazkov (2001), and Newton and Raftery (1994) which introduced the “harmonic mean estimator.” These approaches do not scale well with $\dim(h)$, because the size of the grid needed to cover \mathcal{H} grows exponentially with $\dim(h)$. We mention them here simply because the machine learning literature frequently uses them, and this includes the harmonic mean estimator even though typically, for each h , the harmonic mean estimator of $m(h)$ converges at a rate that is much slower than $n^{1/2}$, where n is the Monte Carlo sample size (Wolpert and Schmidler, 2012).

Methods Based on Variants of Importance Sampling. A basic fact regarding estimation of the marginal likelihood is that, for given h and h_* , estimation of $m(h)$ and $m(h_*)$ individually is hard, but estimation of the ratio $m(h)/m(h_*)$ is easy (as we show momentarily). Consequently, if we fix h_* and let h vary, it is easy to estimate the function $m(\cdot)/m(h_*)$. For the purpose of estimating $\arg \max_h m(h)$, the information in the two functions $m(\cdot)$ and $m(\cdot)/m(h_*)$ is identical: the two functions have the same $\arg \max$, and the second derivative matrices of the logarithm of these two functions are identical. Therefore, the standard point estimates and confidence regions based on $m(\cdot)$ and $m(\cdot)/m(h_*)$ are identical.

There are several ways to use variants of importance sampling to estimate $m(h)/m(h_*)$ (see, e.g., Meng and Wong, 1996 and Gelman and Meng, 1998), and arguably the simplest one is as follows. Assume that all the priors in the family $\{\pi_\theta(\cdot; h), h \in \mathcal{H}\}$ are mutually absolutely continuous, which entails that all the posteriors are also mutually absolutely continuous. Let $h_* \in \mathcal{H}$, and suppose we are able to generate an ergodic Markov chain with invariant distribution $\pi_{\theta|y}(\cdot; h_*)$. Starting with the equation $\int [\pi_{\theta|y}(\theta; h)/\pi_{\theta|y}(\theta; h_*)] \pi_{\theta|y}(\theta; h_*) d\theta = 1$ and writing $\pi_{\theta|y}(\theta; h) = (1/m(h)) \ell_y(\theta) \pi_\theta(\theta; h)$, we trivially see that $\int [\pi_\theta(\theta; h)/\pi_\theta(\theta; h_*)] \pi_{\theta|y}(\theta; h_*) d\theta = m(h)/m(h_*)$. This is an interesting identity because it implies that if $\theta_1, \theta_2, \dots$ is an ergodic Markov chain with invariant distribution $\pi_{\theta|y}(\cdot; h_*)$, then

$$(2.1) \quad \frac{1}{n} \sum_{i=1}^n \frac{\pi_\theta(\theta_i; h)}{\pi_\theta(\theta_i; h_*)} \xrightarrow{\text{a.s.}} \frac{m(h)}{m(h_*)}.$$

The significance of the convergence statement (2.1) is that, in principle, with a single Markov chain run, we can estimate the entire function $m(\cdot)$ up to a multiplicative constant.

Unfortunately, some of what is said above is too good to be true, and in reality the estimate on the left side of (2.1) has a serious defect: unless h is close to h_* , $\pi_\theta(\cdot; h)$ can be nearly singular with respect to $\pi_\theta(\cdot; h_*)$ over the region where the θ_i 's are likely to be, resulting in a very unstable estimate. From a practical point of view, this means that there is effectively a “radius” around h_* within which one can safely move, and there may not exist a single value of h_* that gives rise to estimates that are stable for all $h \in \mathcal{H}$. One way of dealing with this problem is to select J fixed points $h_1, \dots, h_J \in \mathcal{H}$ that “cover” \mathcal{H} in the sense that for every $h \in \mathcal{H}$, $\pi_\theta(\cdot; h)$ is “close to” at least one of $\pi_\theta(\cdot; h_1), \dots, \pi_\theta(\cdot; h_J)$. The goal is to generate a Markov chain whose invariant distribution is a mixture of the $\pi_{\theta|y}(\cdot; h_j)$'s (whereas in the “simple importance sampling estimate” discussed above, we just generate a Markov chain whose invariant distribution is $\pi_{\theta|y}(\cdot; h_*)$). The updates sample different components of this mixture, with jumps from one component to another. This approach is called “serial tempering” and it is not trivial. It can give a great improvement over the simple importance sampling estimate, and Doss and Park (2018) developed theory for it. Roy and Evangelou (2024) give precise meaning to the notions of “close” and “cover,” and based on this develop effective ways to select the points h_1, \dots, h_J . We explain the approach in detail in Section S-1 of the Supplementary Material (Doss and Linero, 2024). Here, we mention only that it suffers from the curse of dimensionality: when $\dim(h)$ is large, it is necessary that J be huge in order for the points h_1, \dots, h_J to adequately cover \mathcal{H} , and in Section S-1 of the Supplementary Material (Doss and Linero, 2024) we explain why this can cause the approach to fail when $\dim(h) \geq 3$ or even when $\dim(h) = 2$.

EM-Based Approaches. To use the EM algorithm to find an approximation to $\arg \max_h m(h)$, we view Y as observed data and θ as missing data. Typically, the “complete data likelihood” $p_h(\theta, y)$ is available in closed form, so the algorithm can in principle be applied. In most complex problems, however, the E-step in the algorithm is infeasible, because it requires the calculation of an expectation with respect to the intractable distribution $\pi_{\theta|y}(\cdot; h)$. Several variants of the EM algorithm have been proposed to deal with this difficulty, and these include Monte Carlo EM (MCEM), originally proposed in Wei and Tanner (1990), in which the E-step is approximated by a Monte Carlo estimate; and variational EM (VEM) (see Beal and Ghahramani, 2003 and also Blei, Kucukelbir and McAuliffe, 2017), in which the E-step is approximated by an estimate produced through variational inference. Unfortunately, the EM algorithm can converge slowly, and therefore so can its variants, and this problem gets worse with “increasing missingness” (Liu, 1994, van Dyk and Meng, 2001). Thus, when the dimension of θ is large the

rate of convergence can be very problematic, since here θ is what is missing. Also, if the marginal likelihood surface is multimodal, all EM-type algorithms can fail, with the user having no clue that the estimate of $\arg \max_h m(h)$ is only a local mode. Additionally, for both MCEM and VEM, because an approximation is used at every iteration of the EM algorithm, the theoretical basis for these two methods is weak.

In MCEM, because the E-step is replaced by a Monte Carlo estimate, an error is introduced at every iteration, so there is no reason to expect that the algorithm will converge at all, let alone to the true maximizer of the likelihood. In fact, [Wei and Tanner \(1990\)](#) recognized this problem and suggested that the Markov chain length be increased at every iteration of the EM algorithm. Let m_k denote the Markov chain length at the k th iteration. [Fort and Moulines \(2003\)](#) showed that a minimal condition for convergence is that $m_k \rightarrow \infty$ at the rate of k^a , for some $a > 1$ (they do not give guidelines for choosing a). MCEM has been shown to perform very poorly in some cases. For example, [George and Doss \(2017\)](#), who deal with latent Dirichlet allocation (which is used in topic modeling and where $\dim(\theta)$ is very high), showed poor performance of MCEM even when a is taken to be 2.

The estimate of $\arg \max_h m(h)$ produced by VEM is obtained as follows. If h_k is the current value of h , the E-step of the EM algorithm is calculation of $E_{h_k}(\log(p_h(\theta, y)))$, where $p_h(\theta, y)$ is the joint distribution of (θ, y) under the model indexed by h , and the subscript to the expectation indicates that the expectation is taken with respect to $\pi_{\theta|y}(\cdot; h_k)$. This step is infeasible because $\pi_{\theta|y}(\cdot; h_k)$ is analytically intractable. We consider $\{q_\psi, \psi \in \Psi\}$, a (finite-dimensional) parametric family of analytically tractable distributions on θ , and within this family, we find the distribution, say q_{ψ_k} , which is closest to $\pi_{\theta|y}(\cdot; h_k)$ in the sense of minimizing the Kullback–Leibler (KL) divergence: $\psi_k = \arg \min_{\psi} \text{KL}(q_\psi \| \pi_{\theta|y}(\cdot; h_k))$. Let $Q(h)$ be the expected value of $\log(p_h(\theta, y))$ with respect to q_{ψ_k} . We view $Q(h)$ as a surrogate for $E_{h_k}(\log(p_h(\theta, y)))$, and the M-step is then to maximize $Q(h)$ with respect to h , to produce h_{k+1} . The maximization is done analytically. Suppose that $\theta = (\theta_1, \dots, \theta_p)$ for some p . In mean-field variational inference, the version of variational inference that is most commonly used, the distributions q_ψ are all products of marginal densities, that is, under q_ψ , $\theta_1, \dots, \theta_p$ are independent. At each iteration of VEM, the minimization step is carried out through an iterative scheme. At convergence of this scheme, what is obtained is a member, q_{ψ_k} , of the parametric family. Let \mathcal{P}_Θ be the space of distributions on Θ (endowed with some topology, which will not concern us here), let ρ be any given metric on \mathcal{P}_Θ , and let $h_{\text{EB}} = \arg \max_h m(h)$ denote the target of the EM scheme. Also, let $\delta = \inf_{\psi \in \Psi} \rho(\pi_{\theta|y}(\cdot; h_{\text{EB}}), q_\psi)$. Unless $\pi_{\theta|y}(\cdot; h_{\text{EB}})$

corresponds to a product measure, we necessarily have $\delta > 0$. Variational inference is very useful because it is fast and can handle very large datasets (and stochastic variational inference ([Hoffman et al., 2013](#)) can scale variational inference to massive data). On the other hand, even if at each outer iteration of VEM the inner iterative scheme was run long enough for convergence to take place, we would still have $\rho(\pi_{\theta|y}(\cdot; h_{\text{EB}}), q_{\psi_k}) \geq \delta > 0$, and therefore, there is no reason to think that the sequence h_1, h_2, \dots will converge to h_{EB} . [George and Doss \(2017\)](#) have documented cases (in the latent Dirichlet allocation model) where the sequence produced by VEM converges, but to a value that is far from h_{EB} , and the predictive accuracy of the model that results from VEM is worse than that of umbrella sampling.

We also mention [Atchadé \(2011\)](#). He uses an adaptive Monte Carlo scheme in which one creates a sequence (h_n, θ_n) , where θ_n is a draw from a Markov transition function that uses the current value of h , and h_n is an improved estimate of h_{EB} based on the sequence $(\theta_1, \dots, \theta_n)$. A brief summary of the algorithm is as follows: starting with $h_0 \in \mathcal{H}$ and $\theta_0 \in \Theta$, we repeat the following updates:

1. Sample $\theta_{n+1} \sim K_{h_n}(\theta_n, \cdot)$ where $K_h(\theta, \cdot)$ is a Markov transition function that leaves $\pi_{\theta|y}(\theta; h)$ invariant.
2. Set $h_{n+1} = h_n + a_n \nabla_h \log(\pi_\theta(\theta_{n+1}; h_n))$.

Here, a_n is a nonincreasing sequence of positive numbers such that $\sum_{n=1}^{\infty} a_n = \infty$ and $\sum_{n=1}^{\infty} a_n^2 < \infty$. [Atchadé \(2011\)](#) gives some guidelines on the choice of this sequence. He establishes almost sure convergence of the sequence h_n to h_{EB} , although this is under very strong regularity conditions. This approach has an obvious advantage over approaches which use importance sampling, in that it does not have the “small radius” limitation discussed earlier. On the other hand, because each new value of h depends on the entire sequence of previous θ ’s, the Markov property is lost; consequently, central limit theorems are not available, so there is no nice theory that gives rise to error margins to accompany point estimates of h_{EB} .

2.2 A Device for Implementation of the Empirical Bayes Method

Here we describe an MCMC-based approach for estimation of $\arg \max_h m(h)$ which gives estimates whose asymptotics can be studied through empirical process theory, and which have good rates of convergence. In the next two paragraphs we introduce the approach in a simple setting in order to enable a quick understanding of the basic ideas, and in the remainder of this subsection we develop the approach in a general setting, and provide all the details.

We consider a fully-Bayes model in which we put a prior distribution on the hyperparameter, which we

now denote by H . In this initial discussion we take the prior on H to be the uniform distribution, and later we remove this restriction. Let u denote the uniform distribution on H . This prior induces a joint distribution on (H, θ, Y) . We will use the letter π , with subscripts, to indicate distributions on the triple (H, θ, Y) , in a self-explanatory manner. Thus, π_H will indicate the prior on H , $\pi_{H|Y}$ will indicate the posterior distribution of H given $Y = y$, $\pi_{(H,\theta)|Y}$ the joint conditional distribution of (H, θ) given $Y = y$, etc. Regarding $\pi_{H|Y}$, we have $\pi_{H|Y}(h) \propto m(h)u(h)$. Since $u \propto 1$, this may be rewritten as $\pi_{H|Y}(h) \propto m(h)$, so the mode of $\pi_{H|Y}$ is $\arg \max_h m(h)$. Now, suppose that we can construct an ergodic Markov chain $(H_1, \theta_1), (H_2, \theta_2), \dots$ whose invariant distribution is $\pi_{(H,\theta)|Y}$. The marginal sequence H_1, H_2, \dots then has invariant distribution equal to $\pi_{H|Y}$. Any method for estimating the mode of $\pi_{H|Y}$ from the sequence H_1, H_2, \dots gives rise to an estimate of $\arg \max_h m(h)$.

Generally speaking, estimation of the mode is a hard problem, and the optimal rates of convergence are worse than $n^{1/2}$. The theory is technical but a typical result states that if f is a density on \mathbb{R}^k , then under some regularity conditions, the optimal convergence rate for estimation of the mode of f based on an i.i.d. sample is $n^{1/(4+k)}$ (Tsybakov, 1990; see also Donoho and Liu, 1991), so even in the simplest case where $k = 1$, this is the very slow rate of $n^{1/5}$. However, these pessimistic results pertain only to the case where the only information we have about f is the Monte Carlo information in the sample. In Bayesian problems, we typically also have some information concerning π . For example, the conditional density of H given θ and y may be available, and in this case, Rao–Blackwellization is possible: $\pi_{H|Y}$ may be estimated by $\hat{\pi}_{H|Y}(h) = (1/n) \sum_{i=1}^n \pi_{H|(\theta=\theta_i, Y=y)}(h)$. This is simply an average, and we will use tools from empirical process theory to show that $\hat{\pi}_{H|Y}(h)$ converges to $\pi_{H|Y}(h)$ uniformly in h , with $n^{1/2}$ asymptotics. From this uniform convergence, we will show that $\arg \max_h \hat{\pi}_{H|Y}$ converges to $\arg \max_h \pi_{H|Y}$, also with $n^{1/2}$ asymptotics, and this rate holds regardless of the dimension of h . Standard methods based on gradient-based approaches can be used to find $\arg \max_h \hat{\pi}_{H|Y}(h)$ rapidly, even when $\dim(h)$ is moderately large. We will also show how confidence sets for $\arg \max_h m(h)$ can be constructed.

The Method in a More General Setting. The prior π_H may be something other than the uniform for several reasons. For example, the uniform prior may be improper, and may lead to an improper posterior. Also, even if the uniform leads to a proper posterior, this posterior may have a form that does not lend itself well to MCMC, whereas certain other forms for π_H may induce a partial conjugacy structure and thus enable the construction of MCMC algorithms in which the component updates exploit this conjugacy. Another reason for considering a prior other than the uniform is that it is useful

for the prior to concentrate near $\arg \max_h m(h)$, as the more time the chain spends near $\arg \max_h m(h)$, the more precisely this quantity will be estimated. Using such a prior is particularly helpful when the likelihood is flat around $\arg \max_h m(h)$. Of course, specifying a prior on H that concentrates near the argmax requires some additional input about where the argmax is, creating a circular problem, so the observation above should be taken simply as a guide regarding how to select the prior. In what follows, the prior π_H is completely arbitrary, and we may choose it strictly on the basis of convenience; in particular, it does not need to reflect any beliefs we have about θ . The posterior distribution of H is $\pi_{H|Y}(h) \propto m(h)\pi_H(h)$, which we may rewrite as $\pi_{H|Y}(h)/\pi_H(h) = cm(h)$, where c is a constant. Thus, $\arg \max_h m(h) = \arg \max_h \pi_{H|Y}(h)/\pi_H(h)$, so if we can estimate the right side of this equation then we can estimate the left side, and this is true regardless of our choice of π_H . We now discuss how we can estimate $\arg \max_h \pi_{H|Y}(h)/\pi_H(h)$. As in the previous paragraph, suppose that $(H_1, \theta_1), (H_2, \theta_2), \dots$ is a Markov chain with invariant distribution equal to $\pi_{(H,\theta)|Y}$, and also suppose that the conditional density of H given θ and y is available. Then from the chain we may form the Rao–Blackwellized estimate of $\pi_{H|Y}$ given by

$$(2.2) \quad \hat{\pi}_{H|Y}(h) = \frac{1}{n} \sum_{i=1}^n \pi_{H|(\theta=\theta_i, Y=y)}(h),$$

which, for fixed h , is an average. Now suppose temporarily that $(H_1, \theta_1), (H_2, \theta_2), \dots$ is a sequence of independently and identically distributed draws from $\pi_{(H,\theta)|Y}$. If

$$(2.3) \quad E(\pi_{H|(\theta=\theta_1, Y=y)}(h)) = \pi_{H|Y}(h)$$

and $E([\pi_{H|(\theta=\theta_1, Y=y)}(h)]^2) < \infty$, then the estimate in (2.2) would be consistent, and also satisfy a central limit theorem. The second moment assumption is, of course, standard, but statement (2.3) actually requires an argument, which is given in Section S-3 of the Supplementary Material (Doss and Linero, 2024).

We now return to the Markov chain case. Consistency of $\hat{\pi}_{H|Y}(h)$ is guaranteed under the minimal and easily checkable condition that the chain is Harris ergodic (i.e., it is irreducible, aperiodic, and Harris recurrent; see Chapter 17 of Meyn and Tweedie, 1993, for definitions). We get a central limit theorem under the condition that the chain is geometrically ergodic and that for some $\epsilon > 0$, $\pi_{H|(\theta=\theta_1, Y=y)}(h)$ has a moment of order $2 + \epsilon$ (corollary to Theorem 18.5.3 of Ibragimov and Linnik, 1971). (The definition of geometric ergodicity of a Markov chain X_1, X_2, \dots on the measurable space (X, \mathcal{B}) and having Π as an invariant probability measure is as follows. Let $K^n(x, A)$ be the n -step Markov transition function. The chain is *geometrically ergodic* if there exist a constant $\rho \in [0, 1)$ and a function $M: X \rightarrow [0, \infty)$ such that for $n = 1, 2, \dots$, $\sup_{A \in \mathcal{B}} |K^n(x, A) - \Pi(A)| \leq M(x)\rho^n$ for

all $x \in \mathbf{X}$.) Thus, under Harris and geometric ergodicity and the moment condition stated above, for each $h \in \mathcal{H}$,

$$(2.4) \quad \hat{\pi}_{H|Y}(h) \xrightarrow{\text{a.s.}} \pi_{H|Y}(h) \quad \text{as } n \rightarrow \infty$$

and

$$n^{1/2}(\hat{\pi}_{H|Y}(h) - \pi_{H|Y}(h)) \xrightarrow{d} \mathcal{N}(0, \sigma^2(h)) \quad \text{as } n \rightarrow \infty$$

for some $\sigma^2(h) < \infty$, and consequently, for each $h \in \mathcal{H}$, we have

$$(2.5) \quad \hat{\pi}_{H|Y}(h)/\pi_H(h) \xrightarrow{\text{a.s.}} cm(h)$$

and

$$(2.6) \quad n^{1/2} \left(\frac{\hat{\pi}_{H|Y}(h)}{\pi_H(h)} - cm(h) \right) \xrightarrow{d} \mathcal{N} \left(0, \frac{\sigma^2(h)}{\pi_H^2(h)} \right),$$

where c is the constant defined right above (2.2).

Our principal objectives are to show that

$$(2.7) \quad \arg \max_h [\hat{\pi}_{H|Y}(h)/\pi_H(h)] \xrightarrow{\text{a.s.}} \arg \max_h m(h)$$

and, more importantly,

$$(2.8) \quad n^{1/2} \left(\frac{\arg \max_h \hat{\pi}_{H|Y}(h)}{\pi_H(h)} - \arg \max_h m(h) \right) \xrightarrow{d} \mathcal{N}_{\dim(h)}(0, \Sigma),$$

where Σ can be estimated consistently, as this would enable us to construct confidence sets for $\arg \max_h m(h)$. A succinct summary of our methodology, including what to do if Rao–Blackwellization is not feasible, is given at the end of Section 2.2.

Note that the pointwise convergence statement that $\hat{\pi}_{H|Y}(h)/\pi_H(h) \xrightarrow{\text{a.s.}} cm(h)$ for every h does not imply convergence of $\arg \max_h [\hat{\pi}_{H|Y}(h)/\pi_H(h)]$ to $\arg \max_h m(h)$ in any sense at all. In fact, even in the very simple case where $\{f_n\}_{n=1}^\infty$ and f are deterministic functions defined on $[0, 1]$, the statement $f_n(x) \rightarrow f(x)$ for every $x \in [0, 1]$ does not imply that $\arg \max_x f_n(x)$ converges to $\arg \max_x f(x)$. (To get a counterexample, with $\phi_{\mu,v}$ denoting the density of the normal distribution with mean μ and variance v , consider $f_n(x) = \phi_{1/n, 1/n}(x) + (x - 0.9)^2$, and $f(x) = (x - 0.9)^2$.) To obtain convergence of the argmax, it is necessary to have uniformity in the convergence of f_n to f . Theorem 1 below has two parts. The first gives a version of (2.4) that is uniform in h . Thus, the first part is a nontrivial generalization of what one gets from the usual strong law of large numbers in two directions: (i) it gives a convergence statement that is uniform in h , and (ii) it does this for the Markov chain case. (The first part also gives a version of (2.5) that is uniform in h , which is an immediate consequence of the version of (2.4) that is uniform in h .) The second part, which is really a simple consequence of the first part, is assertion (2.7). Theorem 2, which is the result

of principal interest, uses the uniformity in Theorem 1 to arrive at (2.8), and the theorem is followed by the description of a method for obtaining confidence regions for $\arg \max_h m(h)$.

Before stating the theorems, we briefly review some basic facts regarding empirical process theory and regeneration sequences that form the underpinnings of the theorems. Suppose (Ω, \mathcal{A}, P) is a probability space, let $L_1(P) = L_1(\Omega, \mathcal{A}, P)$ be the usual space of measurable functions $f: \Omega \rightarrow \mathbb{R}$ satisfying $\int |f| dP < \infty$, and let $L_2(P)$ be the usual space of square-integrable functions. Assume that $X_1, X_2, \dots \stackrel{\text{iid}}{\sim} P$. If $f \in L_1(P)$, then the strong law of large numbers (SLLN) states that $(1/n) \sum_{i=1}^n f(X_i) \xrightarrow{\text{a.s.}} E(f(X))$, and if $f \in L_2(P)$, the central limit theorem (CLT) states that $n^{1/2} \times ((1/n) \sum_{i=1}^n f(X_i) - E(f(X))) \xrightarrow{d} \mathcal{N}(0, \sigma^2(f))$, where $\sigma^2(f)$ is the variance of $f(X)$ under P . For example, if $\Omega = \mathbb{R}$ and $f_t(X) = I(X \leq t)$, where I is the indicator function, then the SLLN states that

$$(2.9) \quad \left| \frac{1}{n} \sum_{i=1}^n f_t(X_i) - E(f_t(X)) \right| \xrightarrow{\text{a.s.}} 0,$$

and the CLT states that

$$(2.10) \quad n^{1/2} \left(\frac{1}{n} \sum_{i=1}^n f_t(X_i) - E(f_t(X)) \right) \xrightarrow{d} \mathcal{N}(0, \sigma^2(t)).$$

The classical Glivenko–Cantelli theorem asserts that convergence in (2.9) is uniform, that is, $\sup_{t \in \mathbb{R}} |(1/n) \sum_{i=1}^n f_t(X_i) - E(f_t(X))| \xrightarrow{\text{a.s.}} 0$, and the classical Donsker theorem gives a version of (2.10) that is uniform, namely $n^{1/2} ((1/n) \sum_{i=1}^n f_t(X_i) - E(f_t(X))) \xrightarrow{d} W_0(F(\cdot))$, where $W_0(\cdot)$ is the Brownian bridge on $[0, 1]$, and $F(t) = P(X \leq t)$. In empirical process theory, the one-parameter class of functions $\{f_t, t \in \mathbb{R}\}$ is replaced with far more general classes (and Ω is not necessarily \mathbb{R} , but can be a more general space). There are two kinds of results. Glivenko–Cantelli results pertain to classes of functions $\mathcal{F} \subset L_1(P)$ and these assert statements of the form

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^n f(X_i) - E(f(X)) \right| \xrightarrow{\text{a.s.}} 0.$$

Donsker results pertain to classes of functions $\mathcal{F} \subset L_2(P)$ and these assert statements of the form

$$n^{1/2} \left(\frac{1}{n} \sum_{i=1}^n f(X_i) - E(f(X)) \right) \xrightarrow{d} W(f),$$

where W is a mean-zero Gaussian process indexed by $f \in \mathcal{F}$. A good review of empirical process theory is given in [Kosorok \(2008\)](#).

We will be interested in the case where $X = (H, \theta)$, P is the conditional distribution of (H, θ) given $Y = y$, and our class of functions is $\{\pi_{H|(\theta, y)}(h), h \in \mathcal{H}\}$. (Recall

that these are the core functions of θ used to construct the Rao–Blackwellized estimate $\hat{\pi}_{H|y}(h)$ in (2.2), which is an average, and $\hat{\pi}_{H|y}(h)/\pi_H(h)$ is what features in (2.5) and (2.6.) Note that for fixed h , $\pi_{H|(\theta,y)}(h)$ is a function of (H, θ) which happens to use only the θ -component, and we emphasize this in our notation by writing

$$(2.11) \quad f_h(\theta) = \pi_{H|(\theta,y)}(h).$$

Of course, f_h also depends on y , but we have conditioned on y , and this dependence is suppressed in the notation. Throughout, we make the benign (and checkable) assumption that $f(\cdot): \mathcal{H} \times \Theta \rightarrow \mathbb{R}$ is continuous in h for $[\pi_{\theta|y}]$ -almost all θ . Glivenko–Cantelli results will give statements of the sort $\sup_{h \in \mathcal{H}} |(1/n) \sum_{i=1}^n f_h(\theta_i) - \pi_{H|y}(h)| \xrightarrow{\text{a.s.}} 0$, and hence

$$\sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^n f_h(\theta_i) / \pi_H(h) - cm(h) \right| \xrightarrow{\text{a.s.}} 0,$$

which is precisely the uniformity that we need in order to establish convergence of the estimator of the argmax; see (2.7). And Donsker theorems ultimately will give results of the sort (2.8).

Empirical process theory is fundamentally based on an i.i.d. assumption, whereas in our setting, typically the sequence $(H_1, \theta_1), (H_2, \theta_2), \dots$ will be a Markov chain. The best way to deal with the family of averages $(1/n) \sum_{i=1}^n f_h(\theta_i)$, $h \in \mathcal{H}$, is through the use of “regenerative simulation.” A *regeneration* is a random time at which a stochastic process probabilistically restarts itself; therefore, the tours made by the process in between such random times are i.i.d. Regeneration sequences are easy to construct and understand in the setting of Markov chains on a discrete state space. Suppose that α is a point to which the chain returns infinitely often with probability one. Assume we start the chain at α , and let $1 = \tau_0 < \tau_1 < \tau_2 < \dots$ be the times of return to α . For each $h \in \mathcal{H}$ and $r = 1, 2, \dots$, let

$$(2.12) \quad S_{h,r} = \sum_{i=\tau_{r-1}}^{\tau_r-1} f_h(\theta_i) \quad \text{and} \quad N_r = \tau_r - \tau_{r-1}.$$

These are the sum of f_h over the r th tour and the length of the r th tour, respectively. By the Markov property, the pairs $\{(S_{h,r}, N_r)\}_{r=1}^\infty$ are i.i.d., and we will show how the i.i.d. structure will enable us to convert Glivenko–Cantelli and Donsker theorems for the i.i.d. case to Glivenko–Cantelli and Donsker theorems for the case of Markov chains satisfying some regularity conditions.

Before we do this, we remark that in virtually all cases that arise in Bayesian statistics, the state space is continuous, and there does not exist a point to which the chain returns infinitely often with probability one. The technique

in Athreya and Ney (1978) allows us to construct a sequence of regeneration times $1 = \tau_0 < \tau_1 < \tau_2 < \dots$ satisfying $E(\tau_r - \tau_{r-1}) < \infty$ in a very general setting that includes Markov chains on a continuous state spaces where the probability of visiting any particular point is always 0. Markov chains for which there exist such regeneration sequences are called regenerative. We discuss the regularity conditions needed for the Athreya and Ney (1978) construction to be feasible after the statements of the theorems.

Suppose now that our Markov chain is regenerative. If we run the chain for R regenerations, then the total number of cycles is given by $n = \sum_{r=1}^R N_r$. Also, $\sum_{i=1}^n f_h(\theta_i) = \sum_{r=1}^R S_{h,r}$. These two facts, which are true by definition, give rise to the key equation

$$(2.13) \quad \frac{\sum_{i=1}^n f_h(\theta_i)}{n} = \frac{\sum_{r=1}^R S_{h,r}}{\sum_{r=1}^R N_r} = \frac{(\sum_{r=1}^R S_{h,r})/R}{(\sum_{r=1}^R N_r)/R}.$$

On the left are the averages of interest, but the θ_i 's are not independent. On the right, the numerator is a class of averages of independent quantities, indexed by h , to which we can apply empirical process results. We have Glivenko–Cantelli theorems for the class of averages $(\sum_{r=1}^R S_{h,r})/R$ and hence for the class of ratios on the right side of (2.13) (the denominator does not depend on h). And to obtain Donsker theorems for the class of ratios $[(\sum_{r=1}^R S_{h,r})/R]/[(\sum_{r=1}^R N_r)/R]$, we apply the delta method to the function $t(x, y) = x/y$. There are, of course, many details that we have not discussed, but the present paragraph gives the big picture, and the details are dealt with in the proofs of the theorems.

Recall that f_h is defined by (2.11), and $S_{h,1}$ is defined by (2.12). Let $M(h) = cm(h)$ and let $\hat{M}_n(h) = \hat{\pi}_{H|y}(h)/\pi_H(h)$ (see (2.5)). For a function $g: \mathcal{H} \rightarrow \mathbb{R}$, $\nabla_h g(h)$ denotes the gradient vector and $\nabla_h^2 g(h)$ denotes the Hessian matrix. We will refer to the regularity conditions below. They are discussed after the statements of Theorems 1 and 2.

C1 The hyperparameter space \mathcal{H} is a convex compact subset of \mathbb{R}^k .

C2 The prior π_H is twice continuously differentiable on \mathcal{H} , and is positive on \mathcal{H} .

C3 For every θ , $\nabla_h f_h(\theta)$ and $\nabla_h^2 f_h(\theta)$ exist and are continuous for all h .

C4 The family $\{f_h, h \in \mathcal{H}\}$ is such that the interchange of the order of integration and either first or second order differentiation is permissible, that is, $\nabla_h \int f_h(\theta) \pi_{\theta|y}(\theta) d\theta = \int \nabla_h f_h(\theta) \pi_{\theta|y}(\theta) d\theta$ and $\nabla_h^2 \int f_h(\theta) \pi_{\theta|y}(\theta) d\theta = \int \nabla_h^2 f_h(\theta) \pi_{\theta|y}(\theta) d\theta$.

C5 The marginal likelihood $m(\cdot)$ is twice continuously differentiable in \mathcal{H} , and the $k \times k$ Hessian matrix $\nabla_h^2 m(\arg \max_h m(h))$ is nonsingular.

C6 Each of $\widehat{M}_n(\cdot)$, $n = 1, 2, \dots$ and $m(\cdot)$ has a unique maximizer (thus it makes sense to talk about $\arg \max_h \widehat{M}_n(h)$ and $\arg \max_h m(h)$).

C7 The sequence $\{(H_i, \theta_i)\}_{i=1}^\infty$ is a geometrically ergodic Markov chain with invariant distribution equal to $\pi_{(H, \theta) | y}$.

C8 For every $h \in \mathcal{H}$, there exists $\epsilon > 0$ such that $E(\|\nabla_h f_h(\theta)\|^{2+\epsilon}) < \infty$, where the expectation is with respect to $\pi_{\theta | y}$, and $\|\cdot\|$ is Euclidean norm.

C9 $E(\sup_h S_{h,1}) < \infty$.

C10 $E(\sup_h |\nabla_h^2 S_{h,1}|) < \infty$.

The condition in C10 is of the form $E(|A|) < \infty$ where A is a $k \times k$ matrix, and the statement $E(|A|) < \infty$ should be taken to mean that the expected value is finite for every component of A .

THEOREM 1. *Suppose that $\{H_i, \theta_i\}_{i=0}^\infty$ is a regenerative Harris ergodic Markov chain.*

1. *Under C2 and C9, (2.4) holds uniformly in h ; consequently, (2.5) holds uniformly in h , that is,*

$$\sup_{h \in \mathcal{H}} |\widehat{M}_n(h) - M(h)| \xrightarrow{a.s.} 0.$$

2. *Under C1, C2, C6, and C9, $\arg \max_h \widehat{M}_n(h) \xrightarrow{a.s.} \arg \max_h M(h)$ (which is equivalent to (2.7)).*

THEOREM 2. *Suppose that $\{H_i, \theta_i\}_{i=0}^\infty$ is a regenerative Harris ergodic Markov chain. Under C1–C10,*

$$n^{1/2}(\arg \max_h \widehat{M}_n(h) - \arg \max_h m(h)) \xrightarrow{d} \mathcal{N}_k(0, \Sigma),$$

where Σ is a positive definite $k \times k$ matrix.

Batch-based estimation of Σ and confidence regions for $\arg \max_h m(h)$. The variance matrix Σ may be estimated in several ways. One way is to exploit the representation of $\widehat{M}_n(h)$ as the ratio of two averages, in which the numerator is an average of the i.i.d. quantities $S_{h,r}$, $r = 1, \dots, R$ (see (2.13) and the proof of Theorem 1). We then produce an argument showing that $\arg \max_h \widehat{M}_n(h)$ inherits the representation in terms of averages, and apply standard methods for estimating the variance of an average.

Another way, which is much easier and is the one we recommend and we have implemented, is to use the method of batching, which is described as follows. The sequence $\theta_1, \dots, \theta_n$ is broken up into B_n consecutive pieces of equal lengths called batches. Let $A_n^{[b]}$ denote the estimate of the argmax based on batch b , let A_n^{full} be the estimate based on the full sequence, and let A be short for $\arg \max_h m(h)$. Suppose that the number of batches and the batch length both go to infinity, that is, $B_n \rightarrow \infty$ and $n/B_n \rightarrow \infty$ as $n \rightarrow \infty$. We note the following.

1. By Theorem 2, for $b = 1, \dots, B_n$, the distribution of $(n/B_n)^{1/2}(A_n^{[b]} - A)$ is approximately $\mathcal{N}_k(0, \Sigma)$.

2. Under geometric ergodicity, for large n the variables $(n/B_n)^{1/2}A_n^{[1]}, \dots, (n/B_n)^{1/2}A_n^{[B_n]}$ are nearly independent.

If statements 1 and 2 above were exact, as opposed to approximations, then the batch-based estimate defined by

$$\widehat{\Sigma}_n = \frac{\sum_{b=1}^{B_n} (n/B_n)(A_n^{[b]} - A_n^{\text{full}})(A_n^{[b]} - A_n^{\text{full}})^\top}{B_n - 1}$$

would be a consistent estimator of Σ , since $\widehat{\Sigma}_n$ is (essentially) the sample variance based on the sequence $(n/B_n)^{1/2}A_n^{[1]}, \dots, (n/B_n)^{1/2}A_n^{[B_n]}$.

In general terms, the literature shows that batch-based estimates are consistent under certain regularity assumptions. Jones et al. (2006) and Flegel and Jones (2010) establish strong consistency under the condition that $\{H_i, \theta_i\}_{i=1}^\infty$ is geometrically ergodic, some moment conditions, and stipulations regarding the rate at which $B_n \rightarrow \infty$ (Jones et al., 2006 recommend taking $B_n = n^{1/2}$, which is within the range of rates that Jones et al., 2006 and Flegel and Jones, 2010 allow); see also Flegel, Haran and Jones (2008). Their results pertain to the case where the statistic whose variance we need to estimate is an average, whereas our statistic is an argmax. However, in view of the fact that $\arg \max_h \widehat{M}_n(h)$ may be represented as an average plus a term that is asymptotically negligible (this fact is the crux of the proof of Theorem 2), we expect the batch-based estimate to be consistent in our situation also. An additional difference is that in our definition of $\widehat{\Sigma}_n$ we have used A_n^{full} as the centering value, instead of the traditional $A_n^{[1]} := (1/B_n) \sum_{b=1}^{B_n} A_n^{[b]}$; but we do not think that making this change affects the theory.

If $\widehat{\Sigma}_n \xrightarrow{a.s.} \Sigma$, then $\widehat{\Sigma}_n$ is invertible for large n . Hence the ellipse \mathcal{E} given by $\mathcal{E} = \{h : (\arg \max_h \widehat{M}_n(h) - h)^\top \widehat{\Sigma}_n^{-1} (\arg \max_h \widehat{M}_n(h) - h) \leq \chi_{k, .95}^2/n\}$ is an asymptotic 95% confidence set for $\arg \max_h m(h)$. Here, $\chi_{k, .95}^2$ denotes the 0.95 quantile of the chi-square distribution with k degrees of freedom.

We now remark on the existence of regeneration sequences. First, we note that, at the theoretical level, it is a fact that for any chain satisfying our minimal regularity condition of Harris ergodicity, letting $K(x, A)$ denote its Markov transition function, there exists a $j \geq 1$ such that for the Markov chain driven by the j -step Markov transition function K^j , there is a regeneration sequence satisfying $E(\tau_r - \tau_{r-1}) < \infty$; see Meyn and Tweedie (1993), Theorem 5.2.2. At a more practical level, Mykland, Tierney and Yu (1995) have provided a very general method, the so-called distinguished point technique, for constructing regeneration sequences. When the method produces regeneration times that are reasonably short, estimation of standard errors of $(1/n) \sum_{i=1}^n f_h(\theta_i)$ becomes trivial, since by (2.13), the problem is reduced to estimating the standard error of ratios of averages of i.i.d. quantities. An

often-heard criticism of the method is that it is very hard to tune, especially in high-dimensional problems. This criticism is irrelevant for us: for our theoretical development, we need only the *existence* of the construction, not a construction that is useful in the practical sense.

Conditions C1–C10. Conditions C1 and C3–C6 are standard. C2 is fairly benign and is likely to be satisfied by most priors in common use, possibly after a redefinition of \mathcal{H} . The geometric ergodicity condition C7 and the moment condition C8 are typical of the sort needed for proving CLTs for averages, and we recall that in the fixed h regime, the Rao–Blackwell estimate (2.2) is just that, a (single) average.

We now discuss C9 and C10. Given a family of functions $g_h: \Theta \rightarrow \mathbb{R}$, Glivenko–Cantelli theorems are uniform SLLNs, and Donsker theorems are “uniform CLTs,” that is, theorems that assert convergence to Gaussian processes indexed by $h \in \mathcal{H}$, as opposed to convergence to a multivariate normal random variable. The regularity conditions of substance are $E(\sup_h |g_h(\theta)|) < \infty$ and $E(\sup_h |g_h(\theta)|^2) < \infty$, for Glivenko–Cantelli and Donsker theorems, respectively (there are other conditions, but they are very easily checked in Bayesian problems, where the prior is indexed by a finite-dimensional parameter). The conditions that these expectations are finite are *far* more stringent than the conditions $\sup_h E(|g_h(\theta)|) < \infty$ and $\sup_h E(|g_h(\theta)|^2) < \infty$. The difficulty is even more severe because in our situation, the functions we are dealing with are $\{S_{h,1}, h \in \mathcal{H}\}$. For any h , $S_{h,1}$ is a sum of the functions $f_h(\theta_i)$ over a random number of indices i (see (2.12)), so verification of a condition of the form $E(\sup_h |S_{h,1}|) < \infty$ could potentially be extremely problematic, and we now address this issue. Consider the conditions below:

CC1 $\int f_h(\theta) \pi_{\theta|y}(\theta) d\theta < \infty$ for all $h \in \mathcal{H}$, and for some $d \geq 1$, there exist $h_1, \dots, h_d \in \mathcal{H}$ and constants c_1, \dots, c_d such that $\sup_h f_h(\theta) \leq \sum_{j=1}^d c_j f_{h_j}(\theta)$ for all $\theta \in \Theta$.

CC2 $\int |\nabla_h f_h(\theta)| \pi_{\theta|y}(\theta) d\theta < \infty$ for all $h \in \mathcal{H}$, and for some $d \geq 1$, there exist $h_1, \dots, h_d \in \mathcal{H}$ and constants c_1, \dots, c_d such that $\sup_h |\nabla_h f_h(\theta)| \leq \sum_{j=1}^d c_j |\nabla_h f_{h_j}(\theta)|$ for all $\theta \in \Theta$.

CC3 $\int |\nabla_h^2 f_h(\theta)| \pi_{\theta|y}(\theta) d\theta < \infty$ for all $h \in \mathcal{H}$, and for some $d \geq 1$, there exist $h_1, \dots, h_d \in \mathcal{H}$ and constants c_1, \dots, c_d such that $\sup_h |\nabla_h^2 f_h(\theta)| \leq \sum_{j=1}^d c_j |\nabla_h^2 f_{h_j}(\theta)|$ for all $\theta \in \Theta$.

(In CC2 and CC3, the inequality signs are taken to mean componentwise inequalities.) CC2 is not relevant for Theorems 1 and 2, but we mention it because it will be needed later for Theorem 3.

Obviously, CC1 implies $E(\sup_h f_h(\theta)) < \infty$, CC2 implies $E(\sup_h |\nabla_h f_h(\theta)|) < \infty$, and CC3 implies $E(\sup_h |\nabla_h^2 f_h(\theta)|) < \infty$. But, as we will see, much more can be said: CC1 implies $E(\sup_h S_{h,1}) < \infty$, CC2

implies $E(\sup_h |\nabla_h S_{h,1}|) < \infty$, and CC3 implies $E(\sup_h |\nabla_h^2 S_{h,1}|) < \infty$. We will prove the first of these assertions. Let \mathcal{T}_1 denote the set of indices that comprise the first tour. We have

$$\begin{aligned} S_{h,1} &= \sum_{i \in \mathcal{T}_1} f_h(\theta_i) \leq \sum_{i \in \mathcal{T}_1} \sum_{j=1}^d c_j f_{h_j}(\theta_i) \\ (2.14) \quad &= \sum_{j=1}^d c_j \sum_{i \in \mathcal{T}_1} f_{h_j}(\theta_i) \quad \text{for all } h \in \mathcal{H}. \end{aligned}$$

We may replace $S_{h,1}$ with $\sup_h S_{h,1}$ on the left side of (2.14), and then taking expectations, we obtain

$$\begin{aligned} E_P\left(\sup_h S_{h,1}\right) &= \sum_{j=1}^d c_j E_P\left(\sum_{i \in \mathcal{T}_1} f_{h_j}(\theta_i)\right) \\ &= \sum_{j=1}^d c_j E_{\pi_{\theta|y}}(f_{h_j}(\theta)) E_P(N_1) < \infty, \end{aligned}$$

where E_P denotes expectation with respect to the Markov chain. The other two assertions are proved in essentially the same way. To summarize: establishing C9–C10 reduces to checking CC1 and CC3, and these are typically not difficult to check using the compactness of \mathcal{H} . (And we will see later one of the principal regularity conditions required for Theorem 3 reduces to checking CC2.)

An Alternative to Rao–Blackwellization. Suppose that $(U_1, V_1), (U_2, V_2), \dots$ is a Markov chain with invariant density $f_{U,V}$ on a space $U \times V$ where V is Euclidean. For the purpose of estimating the marginal density f_V , Chen (1994) introduced the so-called Importance Weighted Marginal Density Estimation (IWMDE) method, a very general procedure which can be applied in cases where Rao–Blackwellization is not feasible. In our context, in which θ corresponds to U , H corresponds to V , and our Markov chain is $(H_1, \theta_1), (H_2, \theta_2), \dots$, the method is described as follows. Let $\{w_\theta(\cdot), \theta \in \Theta\}$ be a family of densities on \mathcal{H} . To estimate $\pi_{H|y}$ we use the estimator

$$(2.15) \quad \hat{\pi}_{H|y}^{\text{iwmde}}(h) = \frac{1}{n} \sum_{i=1}^n w_{\theta_i}(H_i) \frac{\pi_{(\theta,H)|y}(\theta_i, h)}{\pi_{(\theta,H)|y}(\theta_i, H_i)}.$$

Note that to calculate (2.15), we need only that $\pi_{(\theta,H)|y}$ is known up to a normalizing constant, and this is typically the case in Bayesian problems, where the posterior is proportional to the likelihood times the prior. Chen (1994) required that the family $\{w_\theta(\cdot), \theta \in \Theta\}$ correspond to a joint distribution on (θ, H) ; more precisely, he required that there exist a joint density $W_{\theta,H}$ on (θ, H) , and that $w_\theta(h) = W_{H|\theta}(h)$, in self-explanatory notation. Actually, no such stipulation is needed, and in Section S-3 of the Supplementary Material (Doss and Linero, 2024) we show that under the minimal condition that for each θ , w_θ is a density on \mathcal{H} , $\hat{\pi}_{H|y}^{\text{iwmde}}(\cdot)$ is an unbiased estimate of $\pi_{H|y}(\cdot)$.

In principle, any family $\{w_\theta(\cdot), \theta \in \Theta\}$ of densities can be used in (2.15), but Chen (1994) showed that the choice $w_\theta(\cdot) = \pi_{H|(\theta,y)}(\cdot)$ is optimal in the sense of minimizing the asymptotic variance and, moreover, for this choice the estimator reduces to the Rao–Blackwell estimate $\hat{\pi}_{H|y}^{\text{RB}}(h) = (1/n) \sum_{i=1}^n \pi_{H|(\theta_i,y)}(h)$. This leads to the heuristic that the family $\{w_\theta(\cdot), \theta \in \Theta\}$ should be taken to be as close to $\pi_{H|(\theta,y)}(\cdot)$ as possible.

For every fixed $h \in \mathcal{H}$, consider the function $f_h^{\text{iwmde}}: \Theta \times \mathcal{H} \rightarrow \mathbb{R}$ defined by

$$(2.16) \quad f_h^{\text{iwmde}}(\theta, h_*) = w_\theta(h_*) \frac{\pi_{(\theta,H)|y}(\theta, h)}{\pi_{(\theta,H)|y}(\theta, h_*)}.$$

The IWMDE is $\hat{\pi}_{H|y}^{\text{iwmde}}(h) = (1/n) \sum_{i=1}^n f_h^{\text{iwmde}}(\theta_i, H_i)$. Our statement that $\hat{\pi}_{H|y}^{\text{iwmde}}(\cdot)$ is an unbiased estimate of $\pi_{H|y}(\cdot)$ may be written as $E_{\pi_{(\theta,H)|y}}(f_h^{\text{iwmde}}(\theta, H)) = \pi_{H|y}(h)$, and Theorems 1, 2 and 3 hold for the IWMDE: we simply replace $f_h(\theta) = \pi_{H|(\theta,y)}(h)$ (see (2.11)) with $f_h^{\text{iwmde}}(\theta, h_*)$ defined by (2.16), and definitions and assumptions involving f_h are now taken to refer to the function f_h^{iwmde} .

Our methodology is summarized as follows.

1. Choose a prior for H . The methodology is invariant to this choice, and different priors give rise to the same answers in the limit, so the selection should be based on convenience, for example, exploiting any conjugacy or partial conjugacy in the problem.

2. Generate a suitably ergodic Markov chain on (H, θ) with invariant distribution equal to the posterior distribution of (H, θ) given $Y = y$.

3. If the conditional distributions needed for Rao–Blackwellization are available, then calculate the Rao–Blackwellized estimate (2.2). If the conditionals are not available, then use the IWMDE (which results in an estimator whose variance is greater than or equal to that of the Rao–Blackwellized estimate).

4. Adjust the Rao–Blackwellized estimate or the IWMDE via division by $\pi_H(\cdot)$, and find the argmax of this ratio, which is an estimate of $\arg \max_h m(h)$.

5. Form confidence sets for $\arg \max_h m(h)$ via the method of batching.

2.3 Simultaneous Estimation of a Family of Posterior Expectations

Let g be some function of θ , and let $I(h) = \int g(\theta) \times \pi_{\theta|Y}(\theta; h) d\theta$ be the posterior expectation of $g(\theta)$ when the prior on θ is $\pi_\theta(\theta; h)$. Suppose we are interested in the family $I(h)$ as h varies continuously. For any $h \in \mathcal{H}$, we have

$$(2.17a) \quad \int g(\theta) \pi_{\theta|(H=h,y)}(\theta) d\theta$$

$$(2.17b) \quad = \frac{\pi_{H|y}(h) \int g(\theta) \pi_{\theta|(H=h,y)}(\theta) d\theta}{\pi_{H|y}(h)}$$

$$(2.17c) \quad = \frac{\int g(\theta) \pi_{\theta|(H=h,y)}(\theta) \pi_{H|y}(h) d\theta}{\pi_{H|y}(h)}$$

$$(2.17d) \quad = \frac{\int g(\theta) \pi_{(\theta,H)|y}(\theta, h) d\theta}{\pi_{H|y}(h)}$$

$$(2.17e) \quad = \frac{\int [g(\theta) \pi_{H|(\theta,y)}(h)] \pi_{\theta|y}(\theta) d\theta}{\pi_{H|y}(h)}$$

$$(2.17f) \quad =: \frac{N(h)}{\pi_{H|y}(h)}.$$

Now suppose, as before, that we can construct a geometrically ergodic Markov chain $(H_1, \theta_1), (H_2, \theta_2), \dots$ whose invariant distribution is $\pi_{(H,\theta)|y}$; and also suppose, as before, that the conditional density of H given θ and y is available. The numerator, $N(h)$, and denominator, $\pi_{H|y}(h)$, of (2.17f) may be estimated (using only the θ -component of the chain) respectively by

$$(2.18) \quad \begin{aligned} \hat{N}_n(h) &:= \frac{1}{n} \sum_{i=1}^n g(\theta_i) \pi_{H|(\theta=\theta_i,y)}(h) \quad \text{and} \\ \hat{\pi}_{H|y}(h) &= \frac{1}{n} \sum_{i=1}^n \pi_{H|(\theta=\theta_i,y)}(h), \end{aligned}$$

where $\hat{\pi}_{H|y}(h)$ was defined earlier (see (2.2)). Therefore, we may estimate $I(h)$ by the ratio of $\hat{N}_n(h)$ and $\hat{\pi}_{H|y}(h)$, that is, estimate $I(h)$ via

$$(2.19) \quad \hat{I}_n(h) = \frac{\sum_{i=1}^n g(\theta_i) \pi_{H|(\theta=\theta_i,y)}(h)}{\sum_{i=1}^n \pi_{H|(\theta=\theta_i,y)}(h)}.$$

It is interesting to observe that if we define $w_{h,i} = [\pi_{H|(\theta=\theta_i,y)}(h) / \sum_{j=1}^n \pi_{H|(\theta=\theta_j,y)}(h)]$, then the $w_{h,i}$'s are weights, and $\hat{I}_n(h) = \sum_{i=1}^n g(\theta_i) w_{h,i}$, that is, $\hat{I}_n(h)$ has the interpretation as a weighted average of the $g(\theta_i)$'s, with weights given by the $w_{h,i}$'s.

For any fixed h , $\hat{I}_n(h) \xrightarrow{\text{a.s.}} I(h)$. To see this informally, note that $\hat{N}_n(h) \xrightarrow{\text{a.s.}} N(h)$ and $\hat{\pi}_{H|y}(h) \xrightarrow{\text{a.s.}} \pi_{H|y}(h)$, because $\hat{N}_n(h)$ and $\hat{\pi}_{H|y}(h)$ are averages over an ergodic Markov chain. Also, for fixed h , $n^{1/2}(\hat{I}_n(h) - I(h))$ is asymptotically normal. Informally, this is because under regularity conditions on the mixing rate of the Markov chain and some moment conditions, the bivariate vector $n^{1/2}(\hat{N}_n(h) - N(h), \hat{\pi}_{H|y}(h) - \pi_{H|y}(h))$ is asymptotically jointly bivariate normal, by the Markov chain CLT. Asymptotic normality of $n^{1/2}(\hat{I}_n(h) - I(h))$ follows from the delta method applied to the function $t(x, y) = x/y$. However, we will be interested in versions of these consistency and asymptotic normality statements that are uniform in h . For example, if $\dim(h) = 1$, in order to form simultaneous confidence bands for $I(h)$ (or regions, if $\dim(h) > 1$), we need the asymptotic distribution of $\hat{I}_n(h)$, viewed as a process in h . The uniform versions of these convergence statements are given by Theorem 3, whose proof uses results from empirical process theory.

Before stating the theorem, we give some definitions and state the assumptions we will need. Let $C(\mathcal{H})$ be the space of all continuous functions $x: \mathcal{H} \rightarrow \mathbb{R}$, with the topology induced by the sup norm metric ρ : for $x, y \in C(\mathcal{H})$, $\rho(x, y) = \|x - y\|_\infty = \sup_h |x(h) - y(h)|$. For a regenerative Markov chain $\theta_1, \theta_2, \dots$ with regeneration times $1 = \tau_0 < \tau_1 < \tau_2 < \dots$ satisfying $E(\tau_r - \tau_{r-1}) < \infty$, the sequence $S_{h,r}, r = 1, 2, \dots$ was defined by (2.12), and in analogy, we define

$$T_{h,r} = \sum_{i=\tau_{r-1}}^{\tau_r-1} g(\theta_i) f_h(\theta_i) \quad \text{for } h \in \mathcal{H}, r = 1, 2, \dots$$

We will refer to the following assumptions.

D1 $\pi_{H|Y}(\cdot)$ is continuous and positive on \mathcal{H} .

D2 For every θ , $\nabla_h f_h(\theta)$ exists and is continuous for all h .

D3 The families $\{g f_h, h \in \mathcal{H}\}$ and $\{f_h, h \in \mathcal{H}\}$ are such that the order of integration and differentiation can be interchanged: $\nabla_h \int g(\theta) f_h(\theta) \pi_{\theta|Y}(\theta) d\theta = \int \nabla_h [g(\theta) \times f_h(\theta)] \pi_{\theta|Y}(\theta) d\theta$, $\nabla_h \int f_h(\theta) \pi_{\theta|Y}(\theta) d\theta = \int \nabla_h f_h(\theta) \times \pi_{\theta|Y}(\theta) d\theta$.

D4 For every $h \in \mathcal{H}$, there exists an $\epsilon > 0$ such that $E(f_h^{2+\epsilon}(\theta)) < \infty$ and $E((g(\theta) f_h(\theta))^{2+\epsilon}) < \infty$, where the expectations are with respect to $\pi_{\theta|Y}$.

D5 For every $h \in \mathcal{H}$, there exists an $\epsilon > 0$ such that $E(\|\nabla_h [g(\theta) f_h(\theta)]\|^{2+\epsilon})$ and $E(\|\nabla_h f_h(\theta)\|^{2+\epsilon})$ are finite, where the two expectations are with respect to $\pi_{\theta|Y}$.

D6 $E(\sup_h \|\nabla_h S_{h,1}\|^2) < \infty$.

D7 $E(\sup_h \|\nabla_h T_{h,1}\|^2) < \infty$.

For Theorem 3, recall that $\hat{\pi}_{H|Y}(\cdot)$, $N(\cdot)$, and $\hat{N}_n(\cdot)$ are defined by (2.2), (2.17f), and (2.18), respectively, and that $\hat{I}_n(\cdot) = \hat{N}_n(\cdot) / \hat{\pi}_{H|Y}(\cdot)$.

THEOREM 3. Suppose that $\{H_i, \theta_i\}_{i=0}^\infty$ is a regenerative Harris ergodic Markov chain, and assume C1, C7, and D1–D7. Then:

1.

$$\sup_{h \in \mathcal{H}} |\hat{I}_n(h) - I(h)| \xrightarrow{a.s.} 0.$$

2.

$$(2.20) \quad n^{1/2}(\hat{\pi}_{H|Y}(h) - \pi_{H|Y}(h)) \xrightarrow{d} \mathbb{P}(\cdot),$$

$$(2.21) \quad n^{1/2}(\hat{N}_n(\cdot) - N(\cdot)) \xrightarrow{d} \mathbb{N}(\cdot),$$

$$(2.22) \quad n^{1/2}(\hat{I}_n(\cdot) - I(\cdot)) \xrightarrow{d} \mathbb{I}(\cdot),$$

where \mathbb{P} , \mathbb{N} , and \mathbb{I} are mean 0 Gaussian processes indexed by \mathcal{H} , and the convergence takes place in $C(\mathcal{H})$.

In Part 2 of the theorem, (2.20) and (2.21) may be viewed as lemmas that are needed to prove (2.22), which is the result of principal interest. As will emerge in the

proof of the theorem, it is possible to give explicit expressions for the covariance function of $\mathbb{I}(\cdot)$ in terms of first and second moments of certain random variables and, in principle, it is possible to estimate these moments and hence the covariance function of $\mathbb{I}(\cdot)$. However, to use this covariance function to form simultaneous confidence bands (or sets) for $I(h)$, we would also need the distribution of $\sup_{h \in \mathcal{H}} |\mathbb{I}(h)|$, which is extremely complicated, even for the simplest parametric models. A convenient alternative way to form simultaneous confidence bands for $I(h)$ is through the method of batching, which we describe in the paragraph below.

Batch-based simultaneous confidence bands for the family $\{I(h), h \in \mathcal{H}\}$. The map $K: C(\mathcal{H}) \rightarrow [0, \infty)$ defined by $K(x) = \sup_{h \in \mathcal{H}} |x(h)|$ is continuous, so by (2.22) in Theorem 3, $\sup_h n^{1/2} |\hat{I}_n(h) - I(h)| \xrightarrow{d} \sup_h |\mathbb{I}(h)|$. Suppose the distribution of $\sup_h |\mathbb{I}(h)|$ is continuous. For $\alpha \in (0, 1)$, let q_α be such that $P(\sup_h |\mathbb{I}(h)| \leq q_\alpha) = 1 - \alpha$. If q_α was known, then

$$P\left(\sup_h n^{1/2} |\hat{I}_n(h) - I(h)| \leq q_\alpha\right) \rightarrow P\left(\sup_h |\mathbb{I}(h)| \leq q_\alpha\right) = 1 - \alpha,$$

that is,

$$P\left[\hat{I}_n(h) - \frac{q_\alpha}{n^{1/2}} \leq I(h) \leq \hat{I}_n(h) + \frac{q_\alpha}{n^{1/2}} \text{ for all } h \in \mathcal{H}\right] \rightarrow 1 - \alpha.$$

The difficulty is that the distribution of $\sup_h |\mathbb{I}(h)|$ is analytically intractable, so q_α is not known. The method of batching can be used to estimate it. As before, the sequence $\theta_1, \dots, \theta_n$ is broken up into B_n consecutive batches of equal lengths. Let $\hat{I}_b^{(m)}(h)$ be the estimate of $I(h)$ formed from the b th batch and, as before, suppose that as $n \rightarrow \infty$, $B_n \rightarrow \infty$ and $n/B_n \rightarrow \infty$. We will write B instead of B_n . For $b = 1, \dots, B$, let $S_b = \sup_h (n/B)^{1/2} |\hat{I}_b(h) - I(h)|$. Then, because the batch length is large, the distribution of S_b is approximately equal to that of $\sup_h |\mathbb{I}(h)|$. Therefore, we may estimate q_α by the $(1 - \alpha)$ -quantile of the sequence S_1, \dots, S_B . Unfortunately, the S_b 's are not available, because they involve $I(h)$, which is unknown. So instead we use $\mathcal{S}_b = \sup_h (n/B)^{1/2} |\hat{I}_b(h) - \hat{I}(h)|$, in which we have substituted $\hat{I}(h)$ for $I(h)$. To conclude, let $\mathcal{S}_{[1]} \leq \mathcal{S}_{[2]} \leq \dots \leq \mathcal{S}_{[B]}$ denote the ordered values of the sequence $\mathcal{S}_1, \dots, \mathcal{S}_B$. We estimate q_α via $\mathcal{S}_{[(1-\alpha)B]}$, and our simultaneous $(1 - \alpha)$ -level confidence band for $\{I(h), h \in \mathcal{H}\}$ is $\{\hat{I}(h) \pm \mathcal{S}_{[(1-\alpha)B]}/n^{1/2}, h \in \mathcal{H}\}$.

REMARK 1. There is a highly-developed theory on the consistency of estimates based on batching, including results on the optimal rate at which $B_n \rightarrow \infty$. However, this theory is focused primarily on the case where we are

estimating a variance, whereas in the present situation, we are estimating the quantile of the distribution of the supremum of a stochastic process. There are some differences; for example, theoretically we need to show that substitution of $\hat{I}(h)$ for $I(h)$ in going from S_m to S_m does not cause any difficulties, and on the practical side, the rate at which B_n goes to infinity may differ because here we are estimating a moderately large quantile. Establishing the theoretical validity of the batch-based simultaneous confidence bands and providing theoretical and empirical results on the optimal rate at which $B_n \rightarrow \infty$ are interesting open problems.

REMARK 2. Result (2.20) is of interest in its own right: together with the method of batching, it enables us to form simultaneous confidence bands for the marginal posterior density of H . Moreover, there is nothing intrinsic about H being a hyperparameter in the model. Result (2.20) and the construction of the batch-based confidence band apply in any situation where we have a multivariate parameter $\theta = (\theta_1, \dots, \theta_k)$ and we wish to form a simultaneous confidence band for the posterior density of θ_j for some j . The conditions needed are those stated in Theorem 3 (except for those that involve the function g), and we need a proof that the simultaneous confidence bands are asymptotically valid.

3. ILLUSTRATIONS

We provide three illustrations of our approach for implementing the empirical Bayes procedure, with three different purposes. The first involves many hyperparameters, and we show that because the approach can handle a high-dimensional hyperparameter, it actually gives rise to new statistical methodology, namely a new way to do variable selection in nonparametric regression. The second illustration deals with the Dirichlet additive trees model mentioned in Section 1. Although it involves only a single hyperparameter, none of the existing methods (see Section 2.1) can be used to estimate it, because of the inherent complexity of this model. In the third illustration, which is in Section S-2 of the Supplementary Material (Doss and Linero, 2024), we use our approach to select the likelihood function, as opposed to a hyperparameter of the prior, and this shows that in some cases our approach can be used, effectively, to do model selection.

Before proceeding, we mention two points regarding computational considerations.

Computation of the Argmax. When $\dim(h)$ is 1 or 2, we can simply evaluate our estimate of $\pi_{H|y}(\cdot)$ over a fine grid and find the maximizer via a grid search; and we can even plot the estimate and inspect it visually. When $\dim(h) > 2$, suppose first that Rao–Blackwellization is possible, in which case our estimate of $\pi_{H|y}(\cdot)$ is given by (2.2) (we are temporarily assuming that the prior on H is the uniform). Thus, we seek

$\arg \max_h (1/n) \sum_{i=1}^n \pi_{H|(\theta=\theta_i, y)}(h)$. Now, if the function $\pi_{H|(\theta, y)}(\cdot)$ is available in closed form, then so is its derivative, and therefore the derivative of $\hat{\pi}_{H|y}(\cdot)$ in (2.2) is available in closed form. This means that all gradient-based optimization methods are available to us. (If the prior on H is not the uniform, we make the obvious adjustment.) If Rao–Blackwellization is not feasible, then we need to use Chen’s (1994) method, but the comments above still apply.

Construction of a Markov Chain on (θ, H) . In many situations, for the model in which h is a fixed constant, there will already exist a Markov transition function $\Phi_h(\cdot, \cdot)$ on Θ -space with invariant density equal to $\pi_{\theta|Y}(\theta; h)$. In this case, we may be able to use Hamiltonian Monte Carlo (HMC; see, e.g., Neal, 2011 for a review) to construct a Markov transition function $\Psi_{\theta}(\cdot, \cdot)$ on \mathcal{H} -space with $\pi_{H|(\theta, y)}$ as invariant density. The only requirement we need in order to implement HMC is that we know $\nabla_h \log(\pi_{H|(\theta, y)}(h))$. Now typically, $\pi_{H|(\theta, y)}(h)$ is available in closed form, except for a normalizing constant that may involve θ and y , but does not involve h . So except for pathological models in which there are nondifferentiability issues, $\nabla_h \log(\pi_{H|(\theta, y)}(\cdot))$ exists and is available in closed form. The chain that alternates between Φ_h draws and Ψ_{θ} draws then has $\pi_{(\theta, H)|y}$ as invariant density.

3.1 Variable Selection in Bayesian Nonparametric Additive Regression

We return to the second example in Section 1. For the model in this example, the posterior distribution of θ given Y may be estimated by MCMC schemes which run on the variable $\gamma = (\gamma_1, \dots, \gamma_p)$, with $(\beta_0, \beta_{\gamma}, \sigma)$ integrated out. Because the state space for γ is finite, the Markov chains are uniformly ergodic. The original papers which develop such schemes are Madigan and York (1995), Smith and Kohn (1996), Clyde, DeSimone and Parmigiani (1996), and Raftery, Madigan and Hoeting (1997), and there have been many enhancements since. Model (1.3) was considered by Liang et al. (2008), who showed that g -priors with a fixed g give rise to posteriors with paradoxical (and highly undesirable) properties. They propose to use mixtures of g -priors; specifically, they advocate “hyper- g ” priors (which we discuss shortly), and show that if we use them, the paradoxes do not arise.

Smith and Kohn (1996) were interested in the case where some of the variables need to be treated nonlinearly, and so considered the additive model $Y_l = \beta_0 + \sum_{j=1}^p f_j(x_{lj}) + \epsilon_l$, $l = 1, \dots, m$, in which the f_j ’s are represented by regression splines: $f_j(x) = \sum_{k=1}^K \beta_{jk} B_{jk}(x)$, where B_{j1}, \dots, B_{jK} are cubic regression splines with evenly-spaced knots. The model is then expressed as

$$(3.1) \quad Y = 1_m \beta_0 + \sum_{j=1}^p f_j + \epsilon \quad \text{where } f_j = B_j \beta_j,$$

where B_j is an $m \times K$ matrix with (ℓ, k) th entry $B_{jk}(x_{j\ell})$ and $\beta_j = (\beta_{j1}, \dots, \beta_{jK})^\top$. Equivalently, we can write $Y = 1_m \beta_0 + B\beta + \epsilon$, where $B = [B_1, \dots, B_p]$, and $\beta = (\beta_1^\top, \dots, \beta_p^\top)^\top$, this last representation fitting in with the usual formulation of a linear model.

When estimating the parameters of the spline model given by (3.1), one option is to use a relatively small number of knots, positioned at evenly spaced points along the predictor axes, and to choose the number of knots via cross-validation (or some model selection criterion). A second option is to use a large number of knots but then apply ℓ_1 penalization on the regression coefficients. This has the advantage that it captures local curvature better. Using ℓ_1 penalization sets some of the knot coefficients to 0 and therefore leads to knot selection. The approach of Smith and Kohn (1996) is, effectively, a Bayesian version of the second option. If in model (1.3) we replace (1.3b) with the statement that β_γ is distributed according to a hyper- g prior, then the model is indexed by the hyperparameter w . Smith and Kohn (1996) use a fixed value for g ($g = 100$) and specify $w = 1/2$.

We will take the approach of Smith and Kohn (1996), modified so that for each $j = 1, \dots, p$, there is a separate inclusion probability w_j for the knots corresponding to variable j , and a hyper- g prior is used for g . The hyper- g prior is given by $\mu(g) \propto (1 + g)^{-a/2}$ for $g > 0$, and is indexed by the parameter $a > 2$. Following Liang et al. (2008), we take $a = 3$. The reason for having separate inclusion probabilities for the p variables is that this allows the different f_j 's to a priori have different curvatures but, as we will see, allowing separate inclusion probabilities has interesting ramifications for variable selection. Let $w = (w_1, \dots, w_p)$. Also, let $\gamma_{j1}, \dots, \gamma_{jK}$ be the knot-inclusion indicators for variable j , define $\gamma_j = \sum_{k=1}^K \gamma_{jk}$, and denote $\gamma_{[j]} = (\gamma_{j1}, \dots, \gamma_{jK})$ and $\gamma = (\gamma_{[1]}, \dots, \gamma_{[p]})$. Lines (1.3d) and (1.3b) of Model (1.3) now need to be changed to

$$\gamma_{[j]}^{\text{indep}} \sim w_j^{\gamma_j} (1 - w_j)^{K - \gamma_j}, \quad j = 1, \dots, p,$$

and

$$g \sim \mu, \text{ and given } g,$$

$$\beta_{\gamma_{[j]}}^{\text{indep}} \sim \mathcal{N}_{p_{\gamma_{[j]}}}(0, g\sigma^2(B_{j,\gamma_{[j]}}^\top B_{j,\gamma_{[j]}})^{-1}),$$

$$j = 1, \dots, p,$$

respectively. We then estimate the hyperparameter w using the methods of this paper.

None of the procedures described in Section 2.1 works here: the EM-based approaches give estimates which converge, but to incorrect values, and serial tempering MCMC gives estimates which are extremely unstable, as discussed earlier. We now describe how our approach may be implemented. We take $w_j \stackrel{\text{iid}}{\sim} \text{Unif}(0, 1)$. Our Markov

chain will run over (γ, w, g) , with $(\beta_0, \beta_\gamma, \sigma)$ integrated out. It will be driven by a Markov transition function (MTF) which consists of the composition of three MTFs, of which the first updates γ , the second updates w , and the third updates g . Our first MTF modifies the proposal of Yang, Wainwright and Jordan (2016) to take into account that $\gamma_{[1]}, \dots, \gamma_{[p]}$ constitute p groups; it applies one of the two changes below, each with probability $1/2$. (1) Flip a randomly selected γ_{jk} . (2) For each $j = 1, \dots, p$, randomly select two indicators from the set $\{\gamma_{j1}, \dots, \gamma_{jK}\}$, one of which is a 1 and the other a 0, and swap their values (if $\gamma_{j1}, \dots, \gamma_{jK}$ are all 1 or all 0, then we do nothing). In either case, the move is accepted or rejected based on the Metropolis–Hastings acceptance probability. This update leaves the conditional distribution of γ given (w, g, Y) invariant.

The second MTF generates w according to its conditional distribution given (γ, g, Y) . From the hierarchical nature of the model, it is easy to see that

$$\begin{aligned} \pi(w | \gamma, g, Y) \\ &= \pi(w | \gamma) \propto \prod_{j=1}^p \prod_{k=1}^K w_j^{\gamma_{jk}} (1 - w_j)^{1 - \gamma_{jk}} \\ &\propto \prod_{j=1}^p \text{beta}(w_j; 1 + \gamma_j, 1 + K - \gamma_j), \end{aligned}$$

where $\text{beta}(w; a, b)$ denotes the $\text{beta}(a, b)$ density evaluated at w . This update leaves the conditional distribution of w given γ, g , and Y invariant. The equation above gives rise to the Rao–Blackwellized estimate

$$(3.2) \quad M_n(w) = \frac{1}{n} \sum_{i=1}^n \prod_{j=1}^p \text{beta}(w_j; 1 + \gamma_j^{(i)}, 1 + K - \gamma_j^{(i)}),$$

of the marginal likelihood of w (up to a constant), where $i = 1, \dots, n$ indexes the iterations of the Markov chain. In our illustrations, the empirical Bayes estimate of w is obtained by maximizing (3.2) through the `optim` function in R using the L-BFGS-B algorithm (Byrd et al., 1995).

The final MTF updates g , and this is done through the slice sampler (Neal, 2011). We remark that Liang et al. (2008) show that we can actually modify the first two MTFs by marginalizing out g , thereby eliminating the need to construct an update for g ; we include an update for g to allow for the possibility of including g in our empirical Bayes analysis, if this is desired. The composition of the three updates leaves the conditional distribution of (γ, w, g) given Y invariant.

It is notable that some of the components of $\arg \max_w m(w)$ can be zero (and if $\gamma_j^{(i)} = 0$ for the n iterations of the Markov chain, then the j th component of

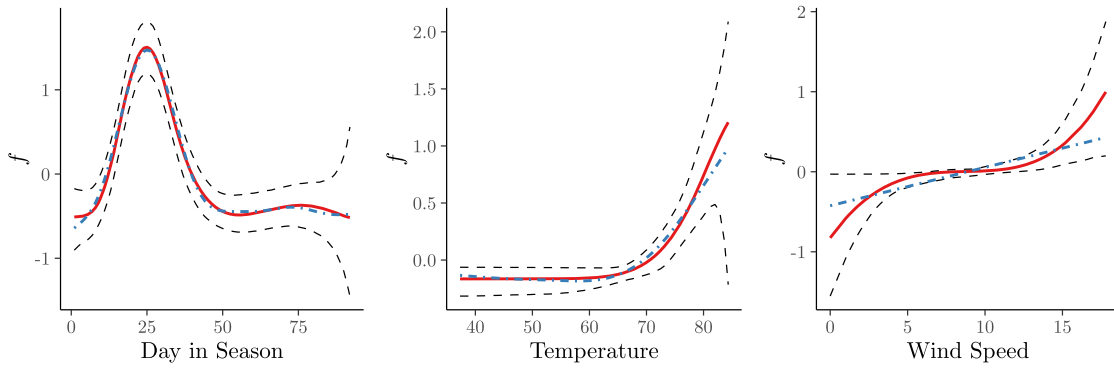


FIG. 1. Estimates of the f_j 's for the ragweed data. Solid line (—) gives the posterior mean, dashed lines (---) give 95% pointwise credible intervals, and dot-dashed line (-.-) gives the estimate obtained from the `gam` function in the R package `mgcv`.

the maximizer of $M_n(w)$ in (3.2) is zero, that is, w_j is estimated to be zero.) In this case, it is not just some knots that are excluded; rather variable j in its entirety is eliminated from the model. As is the case for many likelihood-based methods, some issues arise when the maximizing value is at the boundary of the parameter space, and this was noted in the context of Bayesian variable selection by Scott and Berger (2010). (The situation here is similar to that where we have $Y \sim \text{binomial}(m, p)$: if we observe $Y = 0$, then not only is the maximum likelihood estimate of p equal to 0, but the associated standard error estimate is also 0, and the naive Wald-type confidence interval for p is the singleton $\{0\}$.) As is the case for the simple binomial example, if uncertainty quantification regarding variable selection is required, a fully-Bayes approach can be used.

We apply our empirical Bayes approach to the ragweed dataset of Stark et al. (1997). This dataset consists of measurements of the ragweed pollen for 335 days in Kalamazoo, Michigan, along with several meteorological predictors: the day number of the ragweed pollen season, the temperature, the wind speed, and whether it rained. The first three predictors are numeric, and the fourth is binary, and the effect of the three numeric predictors is modeled using cubic regression splines with at most $K = 50$ knots for each predictor. The binary predictor contributes an additive effect $\gamma_j \beta_j$ where $\gamma_j \sim \text{Bernoulli}(w_j)$.

Before proceeding, we check that the empirical Bayes procedure gives reasonable results by comparing the fit it gives to an additive fit using the `gam` function in the R package `mgcv`. This experiment and all the others below are based on a Markov chain of length 55,000, with the first 5,000 cycles discarded as burn-in and the remaining cycles thinned by 10, giving 5,000 cycles. The results are displayed in Figure 1. We see that for the day in season and temperature variables the fit from `gam` is quite similar to the one using our empirical Bayes approach, although the fit for the wind speed variable is somewhat different due to the preference of `gam` to favor linear terms before

including nonlinear terms (our approach can be easily extended to also favor linear terms).

To evaluate the variable selection performance of our model, we added noise variables as follows. Let D_l , T_l , W_l , and R_l be the day, temperature, wind, and rain variables for observation l ($l = 1, \dots, 335$), and let π be a random permutation of the integers $1, \dots, 335$. With a single permutation, the augmented data set is $(Y_l, D_l, T_l, W_l, D_{\pi(l)}, T_{\pi(l)}, W_{\pi(l)}, R_l), l = 1, \dots, 335$. We then modeled each of the continuous predictors using our spline basis function expansion. The reason for creating noise variables in this way is that the correlation structure for the added variables is identical to that in the original variables.

Figure 2 shows the empirical Bayes estimate of w obtained from our procedure when we used two permutations to generate noise variables. We see that our approach correctly removes all the noise variables and includes all the original variables. Maximizing (3.2) numerically confirms that the empirical Bayes estimators of the w 's corresponding to the noise variables are all 0. To get more detail, we would like to plot the marginal likelihood function $m(\cdot)$, but it is not possible to do so because $m(\cdot)$ is a function of 10 variables. Instead, for each $j = 1, \dots, 10$, we can take $(w_1, \dots, w_{j-1}, w_{j+1}, \dots, w_{10}) \stackrel{\text{iid}}{\sim} \text{Unif}(0, 1)$ and plot the marginal likelihood function for w_j , with all the other w 's integrated out. Figure 3 presents the plots for variables $1, \dots, 9$. Here, w_1, w_2 , and w_3 are associated with the original continuous variables, and w_4, \dots, w_9 are associated with the noise variables. The figure additionally gives pointwise and uniform confidence bands for these marginal likelihoods. This marginal analysis also suggests that these predictors do not appear in the model selected by the empirical Bayes method.

We now make a brief comparison of our empirical Bayes approach to penalized regression using the commonly-used composite minimax concave penalty (cMCP) method proposed by Breheny and Huang (2009). The cMCP method carries out bi-level selection by performing both group-level (predictor) and within-group

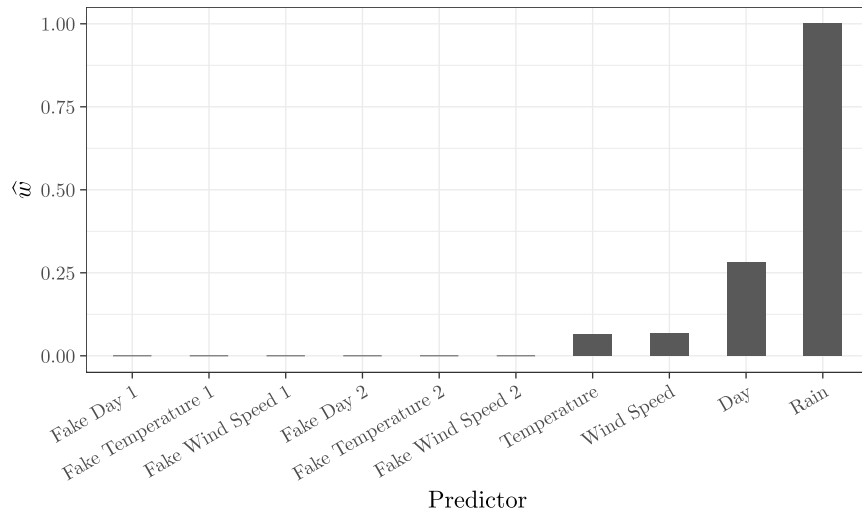


FIG. 2. Empirical Bayes estimates of the w_j 's for the ragweed data augmented with noise predictor variables.

level (basis function) selection, which is similar to what our method is doing. We fit the cMCP regression using the `grpreg` package in R and selected tuning parameters using cross-validation. In addition to the dataset augmented with two permutations, we considered a second dataset which used six permutations. The two methods were evaluated using the number of true positives (regarding the four original predictors as positives) and the number of false positives. Table 1 gives the results. From the table, we see that for both datasets, each method correctly identified all the original predictors; however, we also see that cMCP is prone to false positives when we increase the number of noise variables. Of course, there are several other procedures for doing bi-level variable selection, for example, group bridge (Huang et al., 2009) and `spikeSlabGAM` (Scheipl, Fahrmeir and Kneib, 2012). A thorough comparison of our empirical Bayes approach with all other methods is beyond the scope of this paper. Our goal in this first illustration is only to demonstrate the potential of our method for enabling the implementation of empirical Bayes approaches in models where these would be useful but no existing procedure for estimating $\arg \max_h m(h)$ works. (Note that there is a distinction between our method, which is a Monte Carlo procedure for obtaining an estimate of $\arg \max_h m(h)$, and the resulting empirical Bayes scheme, which is a statistical procedure.)

3.2 Choosing the Sparsity Parameter in the Dirichlet Additive Regression Trees Model

Consider the nonparametric regression model $Y_l = f(x_l) + \epsilon_l, l = 1, \dots, m$, where $\epsilon_l \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ and $x_l \in \mathbb{R}^p$. An increasingly popular strategy for estimating f is to take a Bayesian approach in which f is modeled as a sum of random decision trees (see Chipman et al., 2013 and Linero, 2017 for reviews). The most popular such approach is to use a Bayesian additive regression trees

(BART, Chipman, George and McCulloch, 2010) model, which sets $f(x) = \sum_{t=1}^T g(x; \mathcal{T}_t, \mathcal{M}_t)$, where the \mathcal{T}_t 's are regression trees and the \mathcal{M}_t 's are the corresponding vectors of terminal node parameters. Here, $g(x; \mathcal{T}_t, \mathcal{M}_t) = \mu_{t\ell}$ if x goes to terminal node ℓ of tree t .

In the generative tree-construction process, there is a variable, $s = (s_1, \dots, s_p)$, where s_j is the probability that the variable chosen for a split is variable j . Chipman, George and McCulloch (2010) take s to be deterministic: $s = (p^{-1}, \dots, p^{-1})$. Linero (2018) argues that when dealing with regression that is potentially sparse, it is better to allow s to be random. He specifies that s is drawn from the Dirichlet distribution $\text{Dir}_p(\alpha/p, \dots, \alpha/p)$, in which α is a hyperparameter; we refer to this model as “Dirichlet additive regression trees” (DART) for the purpose of comparison with BART. The hyperparameter α plays a key role related to sparsity. Suppose $U \sim \text{Dir}_p(a, \dots, a)$. As is well known, if a is small, there is a tendency for most of the components of U to be near zero, and in the limit where $a \rightarrow 0$, one component is 1, the rest are zero, and the position of the nonzero component is uniformly distributed on $\{1, \dots, p\}$. On the other hand, when a increases to infinity, U is nearly the vector (p^{-1}, \dots, p^{-1}) . In the generative tree-construction process, the variable s is chosen once, and then is applied to all T trees. As a consequence, when α is small, only a few of the predictor variables are chosen for splits in the entire ensemble; and when α is large, many predictors are involved, and DART reverts to BART. (See Linero, 2018 and the supplement to Linero, 2018 for a precise version of this statement.) This technique has also been used by Linero and Yang (2018).

In Linero (2018), α is given a prior of the form $\rho_\eta(\alpha) = \eta \cdot [2\alpha^{1/2}(\alpha + \eta)^{3/2}]^{-1}$, where the scale parameter η is taken to be p by default. This prior is unbounded near 0, which enables sparsity, and it has a Cauchy-like right tail, which allows DART to revert to BART. Unfortunately,

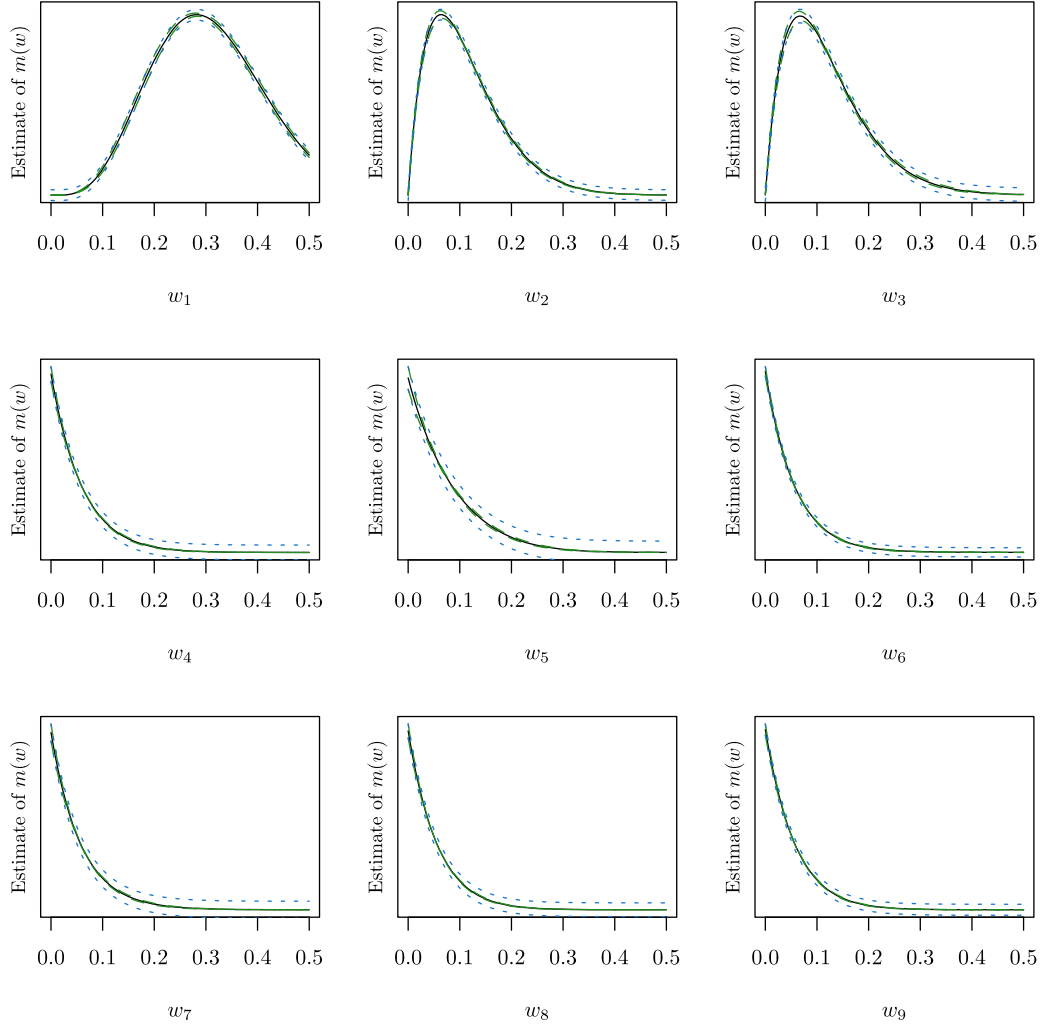


FIG. 3. Estimates of the marginal likelihood of w_j when treating all other w 's as $\text{Unif}(0, 1)$, for the synthetic ragweed dataset. Estimated marginal likelihood is given by solid lines (—), uniform 95% confidence bands are given by short-dashed lines (- - -), and pointwise 95% confidence bands are given by long-dashed lines (---).

these two features of the prior can result in poor mixing of the Markov chain used to estimate the posterior distribution. An alternative to putting a prior on α is to select α by maximum marginal likelihood, that is, via the empirical Bayes method, for which the methodology of the present paper is designed. In short, the empirical Bayes

method will enable us to determine whether to use BART ($\arg \max_{\alpha} m(\alpha)$ is large) or DART ($\arg \max_{\alpha} m(\alpha)$ is not large). In the rest of this section we will explain how our approach may be implemented (we will present our MCMC algorithm and discuss how the IWMDE method of [Chen \(1994\)](#) may be carried out), and then illustrate, on real and artificial data, how DART implemented through the empirical Bayes approach acts appropriately in both sparse and nonsparse situations. (The only hyperparameter we will allow to vary is α , all the others being set to the default values recommended by [Chipman, George and McCulloch, 2010](#).)

Our methodology provides an asymptotically exact estimate of $\arg \max_{\alpha} m(\alpha)$ regardless of our choice of prior on α , so we will take $\pi_{\alpha} = \text{gam}(a_0, b_0)$. This choice enables a very convenient data augmentation scheme that takes advantage of some conjugacy in the problem. Here, $\text{gam}(x; a, b)$ is the density proportional to $x^{a-1} \exp(-xb)$. We introduce the augmentation variable

TABLE 1

Comparison of performance of the empirical Bayes and cMCP methods, on the augmented ragweed data. TP denotes the number of true positives and FP denotes the number of false positives. Replications denotes the number of permutations used to construct the noise variables

Replications = 2			Replications = 6		
Method	TP	FP	Method	TP	FP
cMCP	4	1	cMCP	4	6
EB	4	0	EB	4	1

$\lambda \sim \text{gam}(\alpha, 1)$, where λ is independent of s , and define $Z = \lambda s$. Then $Z_j \stackrel{\text{iid}}{\sim} \text{gam}(\alpha/p, 1)$, $j = 1, \dots, p$ follows from routine distribution theory (see, e.g., Devroye, 1986, Chapter 11, Theorem 4.1).

Denote $Y = (Y_1, \dots, Y_m)$, $y = (y_1, \dots, y_m)$, and let $\theta = (s, \sigma^2, \lambda, \{\mathcal{T}_t, \mathcal{M}_t, t = 1, \dots, T\})$. We will generate a Markov chain on (θ, α) whose invariant distribution is the distribution of (θ, α) given $Y = y$. The MTF for doing so will consist of the composition of four MTFs. The first updates $(\sigma^2, \{\mathcal{T}_t, \mathcal{M}_t, t = 1, \dots, T\})$ using the Bayesian backfitting algorithm of Chipman, George and McCulloch (2010). The second MTF is the update from Linero (2018), which updates s . The third MTF draws λ from its conditional distribution given all the other parameters and $Y = y$, which is $\text{gam}(\alpha, 1)$. The combination of these MTFs leaves the full-conditional distribution of θ invariant.

The final MTF updates α . The conditional distribution of α given θ and $Y = y$ is given by $\pi_{\alpha|(\theta, y)}(\alpha) \propto \Gamma(\alpha/p)^{-p} \exp\{(\alpha/p) \sum_{j=1}^p \log(Z_j)\} \alpha^{a_0-1} \exp(-b_0\alpha)$. This depends only on α and the Z_j 's because the only factors of the joint distribution of (θ, α, Y) in which α appears are π_α , $\pi_{s|\alpha}$, and $\pi_{\lambda|\alpha}$. It is easy to see that this distribution is also equal to the posterior distribution of α in the model where $\alpha \sim \text{gam}(a_0, b_0)$ and $Z_j \stackrel{\text{iid}}{\sim} \text{gam}(\alpha/p, 1)$ for $j = 1, \dots, p$. Unfortunately, there is no analytic expression for the posterior distribution. Miller (2019) considered a setup which includes precisely this situation. He showed that the posterior distribution of α is very well approximated by $\text{gam}(A(Z), B(Z))$, if $A(Z)$ and $B(Z)$ are chosen appropriately. Ideally, the parameters $A(Z)$ and $B(Z)$ are chosen by matching the first and second derivatives of $\log(p_{\alpha|Z})$ to those of $\log(\text{gam}(A(Z), B(Z)))$ at the mean of $\text{gam}(A(Z), B(Z))$. Unfortunately, the mean of $\text{gam}(A(Z), B(Z))$ is not known, because $A(Z)$ and $B(Z)$ are not known. So a trial value for the mean is initially used, leading to an improved estimate, and this scheme is iterated. Miller (2019) states that convergence occurs within four iterations in all the situations he has seen, and that the final approximation is excellent.

Our update of α will be a Metropolis–Hastings step that uses the Miller (2019) approximation as a proposal density (as suggested by Miller, 2019). This gives rise to an MTF for which the invariant density is $\pi_{\alpha|(\theta, y)}$. Because the approximation is excellent, the acceptance probability is nearly one, and we are essentially sampling from $\pi_{\alpha|(\theta, y)}$. For estimating $\pi_{\alpha|y}$, Rao–Blackwellization is not feasible, and we must use the IWMDE method of Chen (1994). The Miller (2019) approximation provides a very convenient family $\{w_\theta, \theta \in \Theta\}$ of densities on α : we take $w_\theta = \text{gam}(A(Z), B(Z))$. Because the approximation of $\pi_{\alpha|(\theta, y)}$ by $\text{gam}(A(Z), B(Z))$ is very good, the IWMDE method is essentially as good as Rao–Blackwellization.

We now illustrate our methodology on real and simulated data. Our goals are limited: recalling that small values of α encourage sparse models and that as $\alpha \rightarrow \infty$ DART reverts to BART, we establish that the empirical Bayes choice of α reflects the sparsity in the regression. A broad comparison of DART, with α chosen via the empirical Bayes method (DART-EB), to other regression methods is beyond our scope. We consider three datasets: (1) the Waste Isolation Pilot Plant (WIPP) data, described in Storlie and Helton (2008), for which there are $m = 300$ observations and $p = 31$ variables; (2) the Triazines data, available from the UCI Machine Learning repository, and for which $n = 186$ and $p = 60$; and (3) the Blood Brain Barrier data (BBB), available and described in the *caret* package in R, and for which $n = 208$ and $p = 134$.

We set $a_0 = 1$, $b_0 = 1/50$. We used our MTF to generate 120,000 samples of θ , and discarded the first 20,000 as burn-in. We then estimated the marginal likelihood (up to a constant) using the IWMDE procedure, and also estimated the posterior density of α , using $\hat{\pi}_{H|y}^{\text{iwmde}}$ (see (2.15)). We also formed pointwise and simultaneous confidence bands for both the marginal likelihood function and the posterior density. The pointwise bands were constructed via standard batching methodology, with the number of batches set using the values recommended by Jones et al. (2006). The simultaneous confidence bands were constructed using the procedure described after the statement of Theorem 3. The Markov chain lengths were chosen to make the simultaneous confidence bands acceptably narrow. Plots for all three data sets are given in Figure 4. The results are as follows.

WIPP It is a priori known that the regression for this data set is sparse; for example, Storlie et al., 2011 report that only 8 of the 31 variables are informative. The top-right panel of Figure 4 correctly reflects this sparsity, and indicates that the marginal likelihood of BART vs. DART with $\alpha = 5$ is essentially 0.

Triazines Linero (2018) noted that for this dataset, the performance of DART (with the default prior for α) was about the same as that of BART, under a criterion of predictive error. The top-middle panel of Figure 4 confirms this: the marginal likelihood of BART is higher than that of DART for all α .

BBB Linero (2018) noted that for this data set, BART and DART have similar performance in terms of prediction error, but that DART used fewer variables; hence DART obtained a more parsimonious fit to the data with the same predictive accuracy. The top-left panel of Figure 4 confirms this: the marginal likelihood of DART at its argmax is only slightly higher than the marginal likelihood of BART.

Next, we show that DART-EB behaves appropriately in a simple simulation study in which the true underlying

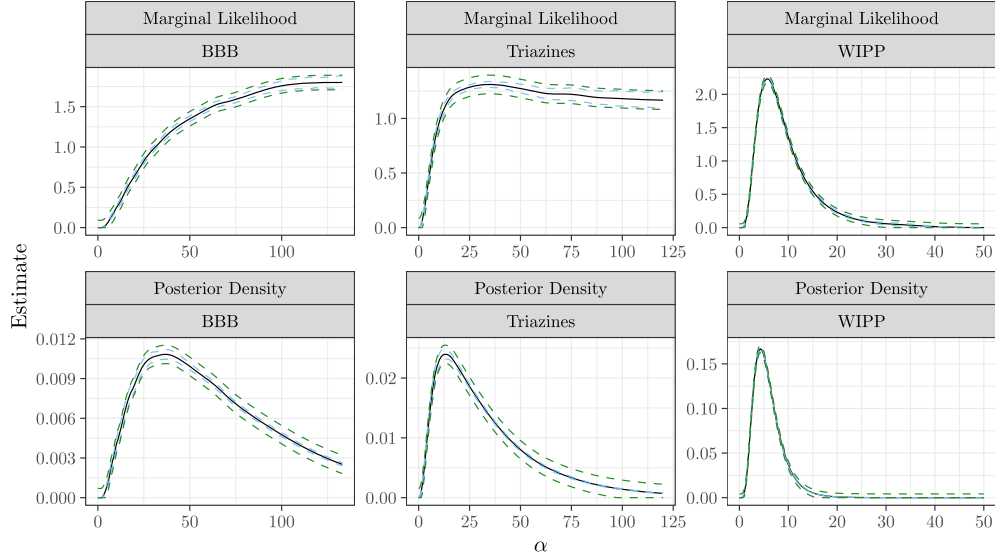


FIG. 4. Estimates of the marginal likelihood (top) and posterior distribution (bottom) of α for the DART model. Left: the BBB dataset; middle: the Triazines dataset; right: the WIPP dataset. The estimated marginal likelihood is given by solid lines (—), simultaneous 95% confidence bands are given by long-dashed lines (---), and pointwise 95% confidence bands are given by short-dashed lines (- - -).

regression function is $f_0(x) = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5$. This function was introduced by Friedman (1991) and has been used many times in the context of BART (see, e.g., Chipman, George and McCulloch, 2010 and Linero and Yang, 2018). Here, $f_0(x)$ depends on only the first five predictors, x_6, x_7, \dots, x_p being irrelevant noise variables. We consider 200 independent replicates of the following experiment. First, we sample $X_l \stackrel{\text{iid}}{\sim} \text{Unif}([0, 1]^p)$, $l = 1, \dots, 250$, and draw $Y_l \stackrel{\text{indep}}{\sim} \mathcal{N}(f_0(X_l), \sigma^2)$. Then, based on (X_l, Y_l) , $l = 1, \dots, 100$, we fit (i) the usual BART model and (ii) DART-EB, using $\text{gam}(1, 1/20)$ as the prior on α . For each replication and each method, we consider the median probability model, which is defined to be the model that includes all variables that occur in at least half of the samples from the posterior distribution (i.e., the variables for which the marginal inclusion probability is estimated to be at least $1/2$). The integrated root-mean-squared error is given by $\text{rmse} = \{\int (\hat{f}(x) - f_0(x))^2 dx\}^{1/2}$, where $\hat{f}(x)$ is the Bayes estimate of $f_0(x)$. For each method and replication we approximate this by simple Monte Carlo and we form RMSE, which is rmse averaged over the 200 replicates. Furthermore, for each method and replication we compute the *precision* and *recall*, defined by $\text{precision} = \text{TP}/(\text{TP} + \text{FP})$ and $\text{recall} = \text{TP}/(\text{TP} + \text{FN})$, where TP, FP, and FN denote the number of true positives, false positives, and false negatives in carrying out variable selection. The results are given in Table 2 for $p \in \{100, 500\}$ and $\sigma \in \{1, 5\}$. We report the F_1 score, which is the harmonic mean of the precision and recall, averaged over the replications, as well as RMSE relative to the RMSE of DART-EB. From the table we see that DART-EB significantly outperforms BART. It behaves appropriately as the

number of irrelevant predictors increases. Specifically, for both the $\sigma = 1$ and $\sigma = 5$ cases, as p increases, the estimated value of α remains roughly constant, so that in the statement $s \sim \text{Dir}_p(\alpha/p, \dots, \alpha/p)$, the shape parameter of the Dirichlet decreases roughly in proportion with p , correctly reflecting the increase in sparsity.

We note that importance sampling via serial tempering will not work here because it is difficult to obtain an analytic expression for the ratio of densities $\pi_{\alpha_1}/\pi_{\alpha_2}$ due to the complexity of the parameter θ , and even if such an expression was available, unless α_1 and α_2 are extremely close, π_{α_1} and π_{α_2} will be nearly singular because of the high dimension of θ . VEM is currently not an option either, as there are no variational algorithms for BART.

Concluding remarks. In the Bayesian approach to inference one has to select the hyperparameter h that specifies the prior, and this can be very difficult, especially when $\dim(\theta)$ is large. In this case there are two options: one is to put a prior on h , that is, use the fully-Bayes approach, and the other is to use the empirical Bayes approach.

The principal objection to the fully-Bayes approach is that it requires a choice of prior on h . A subjective choice must be justified, since different priors can give different conclusions, particularly in small sample situations. (Consider, e.g., the Triazines and BBB data sets in Section 3.2—see Figure 4. For these data sets, the marginal likelihood is not very informative, so a proper prior has a large influence on the posterior.) In some situations, for example, when the goal is to set public policy or in legal settings, the objection to subjective choices can be very strong. On the other hand, there is no good principle for

TABLE 2

DART simulation results. RMSE is relative to the RMSE of DART-EB so that DART-EB by definition has an RMSE of 1. $\text{Avg}(\hat{\alpha}_{\text{opt}})$ is the estimate of $\arg \max_{\alpha} m(\alpha)$, averaged over the 200 replications of the simulation study. The Monte Carlo standard error of $\text{Avg}(\hat{\alpha}_{\text{opt}})$ is less than 0.21 throughout

Method	$\sigma = 1, p = 100$		$\sigma = 1, p = 500$		$\sigma = 5, p = 100$		$\sigma = 5, p = 500$	
	RMSE	F_1	RMSE	F_1	RMSE	F_1	RMSE	F_1
DART-EB	1.00	1.00	1.00	1.00	1.00	0.903	1.00	0.877
BART	1.75	0.48	2.26	0.76	1.25	0.251	1.29	0.719
$\text{Avg}(\hat{\alpha}_{\text{opt}})$	1.31		1.27		4.52		5.06	

selecting a noninformative, or nonsubjective, prior, and in any case noninformative priors are usually improper, and these can lead to improper posteriors (e.g., if $m(\alpha)$ is bounded away from 0 as $\alpha \rightarrow \infty$, as is the case for the Triazines and BBB data sets, then any prior giving infinite mass to the interval $[1, \infty)$ necessarily results in an improper posterior).

The empirical Bayes approach avoids the prior specification issue—this is largely why it was invented. The principal objection against it is that it uses the data twice, once to select the prior, and again to calculate the posterior, acting as if the selected prior is the true prior. This is similar in spirit to what we do in variable selection in regression: we use the data to select the variables that go in the regression model, and use the data again to estimate the regression coefficients, acting as if the selected model is the true model.

The device discussed in this paper is not a method for statistical inference. It is a method for numerical implementation of the empirical Bayes approach. To carry it out we need the existence of a prior on H for which there is an MCMC implementation of the fully-Bayes method. Any prior leads to an asymptotically exact estimate of $\arg \max_h m(h)$, our empirical Bayes estimate of h . So the prior may be taken to be any convenient choice, for example, one that takes advantage of any conjugacy that exists in the model. If an MCMC implementation of a fully-Bayes approach based on a prior π_H has been carried out then we could of course stop there, if we are satisfied that π_H reflects our true beliefs. But because of the objections to a fully-Bayes approach discussed above, we can also opt to carry out an empirical Bayes analysis, based on our device. The question of whether in general one should use empirical Bayes or fully-Bayes methods has been around for decades and is unlikely to be settled soon. Our purpose here is not to advocate an empirical Bayes over a fully-Bayes approach at a philosophical level, but rather to provide a methodology that gives the user the option of using an empirical Bayes approach.

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SUPPLEMENTARY MATERIAL

Supplement to “Scalable Empirical Bayes Inference and Bayesian Sensitivity Analysis” (DOI: [10.1214/24-STS936SUP](https://doi.org/10.1214/24-STS936SUP); .pdf). The supplement provides a description of serial tempering Markov chain Monte Carlo, an additional illustration, proofs of Theorems 1–3, and a proof that the importance weighted marginal density estimator is an unbiased estimate of the true marginal density.

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