Black Box Variational Bayes Model Averaging

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Abstract

For many decades now, Bayesian Model Averaging (BMA) has been a popular framework to systematically account for model uncertainty that arises in situations when multiple competing models are available to describe the same or similar physical process. The implementation of this framework, however, comes with multitude of practical challenges including posterior approximation via Markov Chain Monte Carlo and numerical integration. We present a Variational Bayes Inference approach to BMA as a viable alternative to the standard solutions which avoids many of the aforementioned pitfalls. The proposed method is “black box” in the sense that it can be readily applied to many models with little to no model-specific derivation. We illustrate the utility of our variational approach on a suite of standard examples and discuss all the necessary implementation details. Fully documented Python code with all the examples is provided as well.

Keywords: Bayesian inference; Model uncertainty; Model selection; Markov Chain Monte Carlo; Model evidence; Variational Bayes

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1 Introduction

The existence of several competing models to solve the same or similar problem is a common scenario across scientific applications. One typically encounters a slew of candidate models during standard regression analysis with multiple covariates. Another widely familiar example is a numerical weather prediction with multitudes of forecasting models available. The routine practice in this situation is to select a single model and then make inference based on this model which ignores a major component of uncertainty - model uncertainty (Leamer, 1978). Bayesian model averaging (BMA) is the natural Bayesian framework to systematically account for uncertainty due to several competing models.

For any quantity of interest $\Delta$, such as a future observation or an effect size, the BMA posterior density $p(\Delta|d)$ corresponds to the mixture of posterior densities of the individual models $p(\Delta|d, M)$ weighted by their posterior model probabilities $p(M|d)$:

$$p(\Delta|d) = \sum_{M \in \mathcal{M}} p(\Delta|d, M)p(M|d),$$

(1)

where $\mathcal{M}$ denotes the space of all models, $d = (d_1, \ldots, d_n)$ are given datapoints and $d_i = (x_i, y_i)$ for $i = 1, \ldots, n$ are input-observation pairs. Note, if the space of models $\mathcal{M} = \{M_1, \ldots, M_K\}$, then the formula in (1) can be equivalently written as $p(\Delta|d) = \sum_{k=1}^{K} p(\Delta|d, M_k)p(M_k|d)$ which is a more commonly used notation for BMA. We stick to the notation in (1) to facilitate the developments in section 2.2.

The posterior probability of a model $M$ is given by a simple application of the Bayes’ theorem:

$$p(M|d) = \frac{p(d|M)p(M)}{\sum_{M' \in \mathcal{M}} p(d|M')p(M')}.$$  

(2)

Due to the mixture form of the density (1), determining these probabilities is the key to successful implementation of the BMA framework. To do so, one first needs to assign a suitable prior probability $p(M)$ that $M$ is the true model (assuming there is one such, among the models considered). Hoeting et al. (1999) notes that,

When there is little prior information about the relative plausibility of the models considered, the assumption that all models are equally likely a priori is a reasonable “neutral” choice.
One can, nevertheless, choose informative prior distributions when prior information about the likelihood of each model is available. Eliciting an informative prior is a non-trivial task, but Madigan et al. (1995) provide some guidance in the context of graphical models that can be applied in other settings as well.

The second component of model’s posterior probability is the model’s marginal likelihood, also known as model evidence,

\[
p(d|M) = \int p(d|\theta_M, M)p(\theta_M|M) \, d\theta_M,
\]

where \( \theta_M \) is the set of model-specific parameters (\( \theta_M = (\beta, \sigma) \) in regression problems), \( p(\theta_M|M) \) is their prior distribution, and \( p(d|\theta_M, M) \) is the model’s data likelihood. The evaluation of model evidence is the main reason why BMA becomes challenging in practice, because a closed form solution is available only in special scenarios for the exponential family of distributions with conjugate priors, and thus the integral (3) requires approximation. Some problem-specific algorithms have been developed for direct sampling from BMA posterior density (1) such as the Markov chain Monte Carlo (MCMC) model composition for linear regression models (MC3) (Raftery et al., 1997).

A vast body of literature was produced over the past 30 years on the topic of model evidence approximation, with the simplest approach being the Monte Carlo (MC) integration. The advantage of MC integration is in the method’s ease of implementation, however, one typically needs to generate a large number of samples to achieve reasonable convergence. Another popular method is the Laplace approximation. This corresponds to a second order Taylor expansion of the log-likelihood around its maximum, which makes the likelihood normal. Laplace method is efficient for well behaved likelihoods. We refer the reader to Kass and Raftery (1995) for a complete survey of classical approximation methods for the model evidence. Additionally, the more recently proposed Nested Sampling algorithm by Skilling (2006) and expanded by Feroz et al. (2009) provides another alternative to these classical approaches.

Despite its computational challenges, BMA has a long history of use in both natural sciences and humanities because of a superior predictive performance that is theoretically guaranteed (Bernardo and Smith, 1994). Geweke (1999) introduced BMA in economics and later in other fields such as political and social sciences. See the recent review on
the use of BMA in Economics by Steel (2020). BMA has also been applied to the medical sciences (Balasubramanian et al., 2014; Schorning et al., 2016), ecology and evolution (Silvestro et al., 2014; Hooten and Hobbs, 2015), genetics (Wei et al., 2011; Wen, 2015), machine learning (Clyde et al., 2011; Hernández et al., 2018; Mukhopadhyay and Dunson, 2020), and lately in nuclear physics (Neufcourt et al., 2019, 2020a,b; Kejzlar et al., 2020).

In this paper, we present a Variational Bayes Inference (VBI) approach to BMA. VBI is a machine learning algorithm that approximates a target density through optimization as opposed to the sampling-based approximation via MCMC. Statisticians and computer scientists (starting with Peterson and Anderson (1987); Jordan et al. (1999)) have been widely using variational techniques because they tend to be faster and easier to scale to massive datasets. Our method is based on the black box variational inference algorithm developed by Ranganath et al. (2014) which can be applied to wide class of models with minimum additional derivations. The proposed approach, which we shall call black box variational BMA (BBVBMA), is a one step procedure that simultaneously approximates model evidences and posterior distributions of individual models while enjoying all the advantages of VBI. Here we note that this is not the first time a VBI is used in the context of BMA. For instance, Latouche and Robin (2016) developed a variational Bayes approach to averaging of graphon functions, and (Jaureguiberry et al., 2014) use VBI and BMA for audio source separation, however, the BBVBMA is a general algorithm that can be applied directly to a wide class of models.

1.1 Outline of this paper

In section 2, we provide a brief overview of VBI and derive our proposed BBVBMA algorithm. Then, in section 3, we present a collection of classical examples that include standard linear regression, logistic regression, and Bayesian model selection to illustrate the utility of our methodology. We compare BBVBMA with direct sampling BMA via MC³ and with posterior approximation and evidence computed using MC integration. A fully documented Python code with our algorithm and examples is available at https://github.com/kejzlarv/BBVBMA. Lastly, in section 4, we discuss machine learning applications of the proposed methodology.
2 BMA via Variational Bayes Inference

2.1 Variational Bayes Inference

VBI strives to approximate a target posterior distribution through optimization. One first considers a family of distributions $q(\theta | \lambda)$, indexed by a variational parameter $\lambda$, over the space of model parameters and subsequently finds a member of this family $q^*$ closest to the the posterior distribution $p(\theta | d)$. The simplest variational family is the mean-field family which assumes independence of all the components in $\theta$ but many other families of variational distributions exist; see Wainwright and Jordan (2008); Hoffman and Blei (2013); Ranganath et al. (2016); Tran et al. (2015, 2017) for more examples. The approximate distribution $q^*$ is chosen to minimize the Kullback-Leibler divergence of $q(\theta | \lambda)$ from $p(\theta | d)$:

$$q^* = \arg \min_{q(\theta | \lambda)} KL(q(\theta | \lambda) || p(\theta | d)). \quad (4)$$

Finding $q^*$ is done in practice by maximizing an equivalent objective function (Jordan et al., 1999), the evidence lower bound (ELBO):

$$\mathcal{L}(q) = \mathbb{E}_{q(\theta | \lambda)} \left[ \log p(d, \theta) - \log q(\theta | \lambda) \right]. \quad (5)$$

The ELBO can be optimized via the standard coordinate- or gradient-ascent methods. However, these techniques are inefficient for large datasets, and so it has become the common practice to use the stochastic gradient ascent (SGA) algorithm. SGA updates $\lambda$ at the $t^{th}$ iteration according to

$$\lambda_{t+1} \leftarrow \lambda_t + \rho_t \tilde{l}(\lambda_t), \quad (6)$$

where $\tilde{l}(\lambda)$ is a realization of the random variable $\tilde{\mathcal{L}}(\lambda)$ which is an unbiased estimate of the gradient $\nabla_\lambda \mathcal{L}(\lambda)$. The gradient of the ELBO can be expressed as the following expectation with respect to the variational distribution $q(\theta | \lambda)$ (Ranganath et al., 2014):

$$\nabla_\lambda \mathcal{L}(q) = \mathbb{E}_{q(\theta | \lambda)} \left[ \nabla_\lambda \log q(\theta | \lambda) (\log p(d, \theta) - \log q(\theta | \lambda)) \right]. \quad (7)$$

The expectation (7) does not have a closed form in general, nevertheless, one can use MC samples from $q(\theta | \lambda)$ to construct the unbiased estimate of ELBO gradient

$$\nabla_\lambda \tilde{\mathcal{L}}(\lambda) = \frac{1}{S} \sum_{s=1}^{S} \left[ \nabla_\lambda \log q(\theta[s] | \lambda) (\log p(d, \theta[s]) - \log q(\theta[s] | \lambda)) \right], \quad (8)$$
where $\theta[s] \sim q(\theta|\lambda)$. Note that since the gradient of the variational log-likelihood and the sampling needs to be derived only once for variety of models, the method is black box in nature \cite{Ranganath2014}. The estimate \cite{8} can be conveniently used in SGA algorithm which converges to a local maximum of $\mathcal{L}(\lambda)$ (global for $\mathcal{L}(\lambda)$ concave \cite{Bottou1997}) when the learning rate $\rho_t$ follows the Robbins-Monro conditions \cite{Robbins1951}:

\begin{align}
\sum_{t=1}^{\infty} \rho_t &= \infty, \\
\sum_{t=1}^{\infty} \rho_t^2 &< \infty.
\end{align}

Choosing an optimal learning rate $\rho_t$ can be challenging in practice. Ideally, one would want the rate to be small in situations where MC estimates of the ELBO gradient are erratic (large variance) and large when the MC estimates are relatively stable (small variance). The elements of variational parameter $\lambda$ can also differ in scale, and the selected learning rate should accommodate these varying, potentially small, scales. The ever-increasing abundance of stochastic optimization in machine learning applications spawned development of numerous algorithms for element-wise adaptive scale learning rates. We use the adaptive gradient (AdaGrad) algorithm, Chapter 3 \cite{Duchi2011}, which is a popular and easy-to-implement adaptive rate algorithm. However, there are many other frequently used algorithms such as the ADADELTA \cite{Zeiler2012} or the RMSProp \cite{Tieleman2012}.

Below, we extend the standard VBI that approximates a distribution of model parameters to a scenario where a distribution over the model space needs to be approximated as well.

### 2.2 Black Box Variational BMA

For any quantity of interest $\Delta$, such as a future observation or an effect size, the BMA posterior density $p(\Delta|d)$ corresponds to the mixture of posterior densities of the individual models $p(\Delta|d, M)$ weighted by their posterior model probabilities $p(M|d)$ as in equations \cite{1}, \cite{2} and \cite{3}.

In order to facilitate variational inference, we reformulate the problem of BMA as follows

\begin{equation}
\int p(\Delta|d, M, \theta_M)p(M, \theta_M|d) \, d\mu(M, \theta_M)
\end{equation}
where \( \mu \) is the product measure of counting and Lebesgue. Note, the expression (10) indeed summarizes the equations (1), (2) and (3) in one step. In practice, the most difficult quantity to compute is \( p(M, \theta_M|d) \). We shall now consider the joint posterior distribution of the model \( M \) and its corresponding parameter \( \theta_M \) as our parameter of interest. As explained in Section 2.1, there has been a plethora of literature in using variational inference to obtain the posterior distribution \( \theta \) for a given model. In this section, we adapt the variational inference to obtain the joint distribution of the model and the parameter together in one stroke.

We next assume a variational approximation to the posterior distribution \( p(M, \theta_M|d) \) of the form \( q(M, \theta_M|\lambda_M) = q(M)q(\theta_M|M, \lambda_M) \), where \( \lambda_M \) is the variational parameter of the family for \( \theta_M \) under the model \( M \). Thus, the optimal variational distribution \( q^* \) is given by

\[
q^* = \text{argmin}_q KL(q(M, \theta_M|\lambda_M)||p(M, \theta_M|d)).
\]  

Note that in the KL expression above, we assume that \( M \) is a random variable whose values are the individual models in the model space \( \mathcal{M} \). As explained in section 2.1, finding \( q^* \) is obtained in practice by maximizing an equivalent objective function [Jordan et al., 1999], the ELBO

\[
\mathcal{L}(q) = \mathbb{E}_{q(M, \theta_M|\lambda_M)} \left[ \log p(d, M, \theta_M) - \log q(M, \theta_M|\lambda_M) \right],
\]

this time, subject to constraint \( \sum_{M \in \mathcal{M}} q(M) = 1 \). Using Lagrange multipliers, we optimize

\[
\mathcal{L}(q) = \mathbb{E}_{q(M, \theta_M|\lambda_M)} [\log p(d, M, \theta_M) - \log q(M, \theta_M|\lambda_M)] - \varrho (\sum_{M \in \mathcal{M}} q(M) - 1).
\]

The ELBO can be simplified further

\[
\mathbb{E}_{q(M, \theta_M|\lambda_M)} [\log p(d, M, \theta_M) - \log q(M, \theta_M|\lambda_M)] - \varrho (\sum_{M \in \mathcal{M}} q(M) - 1)
\]

\[
= \mathbb{E}_{q(M, \theta_M|\lambda_M)} [\log p(d|M, \theta_M) + \log p(\theta_M|M) + \log p(M) - \log q(\theta_M|M, \lambda_M) - \log q(M)] - \varrho (\sum_{M \in \mathcal{M}} q(M) - 1)
\]

\[
= \sum_{M \in \mathcal{M}} q(M) \mathbb{E}_{q(\theta_M|M, \lambda_M)} [\log p(d|M, \theta_M) + \log p(\theta_M|M) + \log p(M) - \log q(\theta_M|M, \lambda_M) - \log q(M)] - \varrho (\sum_{M \in \mathcal{M}} q(M) - 1).
\]
Further, $\nabla_{\lambda M} \mathcal{L}(q) = q(M)G_M$ where

$$G_M = \mathbb{E}_{q(\theta_M|M,\lambda_M)}[\nabla_{\lambda M} \log q(\theta_M|M,\lambda_M)(\log p(d|M,\theta_M) + \log p(\theta_M|M) - \log q(\theta_M|M,\lambda_M))].$$

To estimate the quantity $G_M$, we can generate multiple samples from the distribution $q(\theta_M|M,\lambda_M)$ and then use the MC estimate

$$\hat{G}_M = \frac{1}{S} \sum_{s=1}^{S} [\nabla_{\lambda M} \log q(\theta_M[s]|M,\lambda_M)(\log p(d|M,\theta_M[s]) + \log p(\theta_M[s]|M) - \log q(\theta_M[s]|M,\lambda_M))].$$

For updating of $q(M)$, note that

$$\nabla_{q(M)} \mathcal{L}(q) = \mathbb{E}_{q(\theta_M|M,\lambda_M)}[(\log p(d|M,\theta_M) + \log p(\theta_M|M) - \log q(\theta_M|M,\lambda_M))]$$

$$+ \log p(M) - \log q(M) - 1 - \varrho,$$

where $\mathcal{L}_M$ is nothing but the ELBO under a fixed model $M$. Equating the above derivative to 0, we get a closed form expression for $q(M)$ as

$$q(M) = \exp(\mathcal{L}_M + \log p(M) - 1 - \varrho) \propto \exp(\mathcal{L}_M + \log p(M)).$$

It only remains to generate the quantity $\mathcal{L}_M$, which we get by multiple samples from the distribution $q(\theta_M|M,\lambda_M)$ and then use the Monte Carlo estimate

$$\hat{\mathcal{L}}_M = \frac{1}{S} \sum_{s=1}^{S} [\log p(d|M,\theta_M[s]) + \log p(\theta_M[s]|M) - \log q(\theta_M[s]|M,\lambda_M)].$$

This allows us to get Algorithm 1 for BBVBM.

### 2.2.1 Implementation Details and Variational Families

The general form of BBVBM algorithm allows the user to select variational family that is most appropriate for the problem at hand. As we noted in Section 2.1, there is a vast pool of candidate families that vary by their expressiveness and ability to capture complex structure of unknown parameters. In the subsequent applications, we shall consider mean-field variational families with normal distributions for real valued variables and gamma
Algorithm 1 Black Box Variational BMA

Start with an initial choice of \((\lambda_M, q(M))_{M \in M}\) and a learning rate \(\rho\).

repeat

By generating \(\theta_M[1], \cdots, \theta_M[S]\) from \(q(\theta_M | M, \lambda_M)\), calculate

\[
\hat{G}_M = \frac{1}{S} \sum_{s=1}^{S} \nabla_{\lambda_M} \log q(\theta_M[s] | M, \lambda_M) \left( \log p(d | M, \theta_M[s]) \\
+ \log p(\theta_M[s] | M) - \log q(\theta_M[s] | M, \lambda_M) \right)
\]

Update \(\lambda_M\) as

\[
\lambda_M = \lambda_M + \rho q(M) \hat{G}_M
\]

By generating \(\theta_M[1], \cdots, \theta_M[S]\) from \(q(\theta_M | M, \lambda_M)\), calculate

\[
\hat{L}_M = \frac{1}{S} \sum_{s=1}^{S} \left[ \log p(d | M, \theta_M[s]) + \log p(\theta_M[s] | M) - \log q(\theta_M[s] | M, \lambda_M) \right]
\]

Update \(q(M)\) as

\[
\tilde{q}(M) = \exp(\hat{L}_M + \log p(M))
\]

and \(q(M) = \tilde{q}(M) / \sum_{M \in M} \tilde{q}(M)\).

until Convergence of \(\hat{L}(q)\) where

\[
\hat{L}(q) = \sum_{M \in M} q(M) \hat{L}_M
\]

distributions for positive variables. Despite its simplicity, mean-field variational family can approximate a wide class of posteriors and is good enough to achieve consistency for the variational posterior for a wide class of models (Wang and Blei, 2018; Zhang and Gao, 2020; Bhattacharya and Maiti, 2021). Moreover, all the strictly positive variational parameters \(\lambda\) will be transformed as

\[
\tilde{\lambda} = \log(e^\lambda - 1)
\]
to avoid constrained optimization. See Appendix A for the details on the reparametrization of normal and Gamma mean-field families.

Besides the choice of suitable variational family for BBVBMA, another practical consideration needs to be made regarding the updation of variational parameter given by $\lambda_M = \lambda_M + \rho q(M) \hat{G}_M$. Since each step directly depends on the variational approximation of the posterior model probabilities $q(M)$, the updates can be computationally unstable unless the ELBO of each individual model is close to convergence. We therefore recommend setting $q(M) := 1$ until the variation approximation of the posterior model probabilities stabilizes. Additionally, we recommend to compute the final values of $\tilde{q}(M)$, and $q(M)$ respectively, as an average of the last several hundred iterations of the Algorithm for a greater reliability of the estimates.

3 Examples

Below, we provide a suite of illustrative real data examples to demonstrate how BBVBMA serves as a viable alternative to approximate the BMA posterior distribution. First, we analyze the U.S. crime data under the standard linear regression model. Second, we consider a logistic regression model for a heart disease dataset. Lastly, we show that BBVBMA also provides a convenient solution to the Bayesian model selection with Bayes factors. Each of the examples looks at a situation with several competing models without any prior knowledge of which is better; thus we set the prior model weights to be uniform over the model space.

3.1 Bayesian Linear Regression

In this example, we compare BBVBMA with the MCMC algorithm MC$^3$ using the aggregated crime data on 47 U.S. states of Vandaele (1978) which has been considered by Raftery et al. (1997) to illustrate the efficiency of BMA in regression scenario with multitude of candidate models. For simplicity, we concentrate only on a minimal subset of 2 out of 15 predictors of the crime rate and following Raftery et al. (1997), we log transformed all the continuous variables (predictors were also centered).
Given the response variable \( y \), we consider models of the form
\[
y = \beta_0 + \sum_{j=1}^{p} \beta_j x_j + \epsilon, \tag{14}
\]
where \( x_1, \ldots, x_p \) is a subset of a set of candidate predictors \( x_1, \ldots, x_k \). In this specific example, we consider two predictors: \( x_1 \) corresponding to the percentage of males age 14-24, and \( x_2 \) corresponds to the probability of imprisonment. We assign \( \epsilon \) a normal distribution with mean zero and precision \( \phi \). The \( \epsilon \)'s are assumed to be independent for distinct cases. For the parameters in each model (14), we use Zellner’s g-prior (Zellner, 1986; Raftery et al., 1997)
\[
\begin{align*}
\phi & \propto 1/\phi, \\
\beta_0 & \propto 1, \\
\beta_1, \ldots \beta_p & \propto N(0, g(X'X)^{-1}/\phi),
\end{align*}
\]
where \( g = n \) and \( X \) is the design matrix. Zellner’s g-prior is one of the most popular conjugate Normal-Gamma prior distributions for linear models that is convenient and provides Bayesian computation with marginal likelihoods that can be evaluated analytically.

3.1.1 Results

| Inclusion | \( p(M|d) \) |
|-----------|---------------|
| Model     | Intercept | \( x_1 \) | \( x_2 \) | \( p(M|d) \) | \( p(M|d) \) |
| 0         | *         |         |         | 0.03 | 0.06 |
| 1         | *         | *       |         | 0.78 | 0.78 |
| 2         | *         |         | *       | < 0.01 | < 0.01 |
| 3         | *         |         | *       | 0.19 | 0.15 |

Table 1: Linear regression: Posterior model probabilities

Table 1 shows the estimates of model posterior probabilities obtained with BBVBMA and through the MCMC algorithm \( \text{MC}^3 \). The BBVBMA results are based on running the
algorithm for $3 \times 10^4$ iterations for each model and 130 MC samples from the variational distributions to estimate the ELBO gradient. The displayed probabilities were determined as the average over the last $10^3$ iterations of the algorithm to ensure stability of the estimates. The MC$^3$ results were computed with R package BAS (Clyde et al., 2011). Clearly, the BBVBMA based values closely match the MC$^3$ with small deviations for the models with lower posterior probabilities. However, this difference does not impact the data analysis.

For completeness, Figure 1 shows the converged ELBOs for all the four competing models.

Figure 1: Linear regression: Converging ELBOs for all the 4 models on the set of two predictors.

![Converging ELBOs for all the 4 models](image)

Besides the model posterior probabilities, one can assess the fidelity of BBVBMA using the posterior distributions of regression coefficients based on the model average. Figure 2 shows the posterior distributions for the coefficients of the percentage of males 14-24 and the probability of imprisonment based on the model averaging results. The figure additionally displays $\mathbb{P}(\beta = 0|d)$ obtained by first summing the posterior model probabilities across the models for each predictor and then subtracting the value from one. We can see that the means of the posterior distributions based on BBVBMA coincides with those obtained
with MC\(^3\). However, the variational posterior distributions underestimate the uncertainty of the regression coefficients. This is a well known flaw of mean-field families that typically does not affect model’s predictive performance and can be avoided by using more complex variational family that does not assume independence of unknown parameters (Blei et al., 2017; Wang and Blei, 2018).

Figure 2: Linear regression: Posterior distributions for \(\beta_1\) and \(\beta_2\) based on MC3 and BBVBMA. The density is scaled so that the maximum of the density is equal to \(\mathbb{P}(\beta \neq 0|d)\). The spike corresponds to \(\mathbb{P}(\beta = 0|d)\).

### Predictive Performance

Similar to Raftery et al. (1997), we assess the predictive ability of BBVBMA by randomly splitting the U.S. crime data into a training and a testing dataset. A 50-50 split was chosen here due to a relatively small size of the dataset. We subsequently re-run the BBVBMA (and MC\(^3\)) using the training dataset. The predictive performance was measured through coverage of 90% predictive intervals (equal-tails). A
(1 − α) × 100% prediction interval is a posterior credible interval within which a (predicted) observation falls with probability (1 − α). An equal-tail interval is chosen so that the posterior probability of being below the interval is as likely as being above it, Gelman et al. (2013). Table 2 shows that for both BBVBMA and MC^3 88% of the observations in the testing set fell in the 90% prediction intervals. This also demonstrates that the lost due to the underestimated uncertainty of the regression parameters was negligible from the prediction perspective. Additionally, we compare the model averaging predictions with those obtained by the best models according to the adjusted $R^2$ and Mallows’ $C_p$ under both BBVBMA and MC^3. Both of these model selection strategies under-performed the model averaging.

Table 2: Linear regression: Predictive coverage of the test set based on the 90% predictive credible intervals. Model averaging is compared with the performance of the models chosen by two model selection method (Adjusted $R^2$ and Mallows’ $C_p$).

| Method              | Model                  | MC3 | BBVBMA |
|---------------------|------------------------|-----|--------|
| Model averaging     |                        | 0.88| 0.88   |
| Adjusted $R^2$      | $\beta_0 + \beta_1 x_1 + \beta_2 x_2$ | 0.84| 0.84   |
| Mallows’ $C_p$      | $\beta_0 + \beta_2 x_2$       | 0.84| 0.84   |

### 3.2 Bayesian Logistic Regression

Unlike the standard linear regression, generalized linear models such as logistic regression exemplify the slew of challenges that one can encounter when implementing BMA. First, the evaluation of the evidence integral does not have an analytic form and can be high-dimensional. Additionally, direct sampling from the BMA posterior through MC^3 algorithm is not available. One therefore needs to approximate the evidence integral and consequently approximate the BMA posterior with MC samples from the mixture of the posteriors of each of the individual models.

Here we illustrate the utility of BBVBMA on the analysis of a heart disease data
(Dua and Graff, 2017) to assess the factors that contribute to risk of heart attack. The models used are logistic regression models with logit link function of the form

$$\log \left( \frac{P(y = 1)}{P(y = 0)} \right) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j,$$

(15)

where $y = 1$ corresponds to subjects with higher chance of heart attack, and $y = 0$ to those with a smaller chance of heart attack. In this example, we shall consider three predictors, namely $x_1$ is the serum cholesterol in g/dl, $x_2$ is their resting blood pressure on admission to the hospital, and $x_3$ is the biological sex. All the continuous variables were again log transformed and centered. For the parameters in each model (15), we use independent normal prior distributions.

### 3.2.1 Results

Table 3: Logistic regression: Posterior model probabilities

| Model | Intercept | $x_1$ | $x_2$ | $x_3$ | $p(M|d)$ | $p(M|d)$ |
|-------|-----------|-------|-------|-------|----------|----------|
|       |           |       |       |       | MC       | BBVBMA   |
| 0     | *         |       |       |       | < 0.01   | < 0.01   |
| 1     | *         |       | *     |       | 0.15     | 0.15     |
| 2     | *         |       |       | *     | < 0.01   | < 0.01   |
| 3     | *         |       |       | *     | 0.20     | 0.18     |
| 4     | *         |       | *     |       | < 0.01   | < 0.01   |
| 5     | *         |       | *     |       | 0.09     | 0.10     |
| 6     | *         |       | *     | *     | < 0.01   | < 0.01   |
| 7     | *         |       | *     | *     | 0.69     | 0.70     |

Table 3 shows the estimates of model posterior probabilities obtained with BBVBMA as compared to those computed using MC integration. The BBVBMA results are based on running the algorithm for $1.2 \times 10^4$ iterations for each model and 220 MC samples from the variational distributions to estimate the ELBO gradient. The MC estimates are based on $75 \times 10^5$ samples. This large number of samples was necessary in order to achieve reasonable
convergence. We again observe a close match of the BBVBMA model posteriors with the MC model posteriors.

Figure 3 shows the posterior distribution of regression coefficients based on the model average. The MCMC results were obtained with No-U-Turn sampler (Homan and Gelman, 2014) implemented in Python package for Bayesian statistical modeling PyMC3 (Salvatier et al., 2016). Analogically to the linear regression example above, BBVBMA algorithm captures the means of the posterior distributions well but underestimates the uncertainty of $\beta_3$, which is the consequence of assumed independence of the components in the mean-field variational family.

Figure 3: Logistic regression: Posterior distributions for $\beta_1$, $\beta_2$, and $\beta_3$ based on MCMC and BBVBMA. The density is scaled so that the maximum of the density is equal to $P(\beta \neq 0|\mathbf{d})$. The spike corresponds to $P(\beta \neq 0|\mathbf{d})$.

### 3.3 Bayesian Model Selection

Lastly, we demonstrate that the BBVBMA algorithm can be conveniently applied in the generalization of Bayesian hypotheses testing, that is, model selection with Bayes factors.
Instead of averaging, suppose that we wish to compare the two Bayesian models,

\[ M_0 : \mathbf{d} \sim p(\mathbf{d} | \mathbf{\theta}_0), \mathbf{\theta}_0 \sim p(\mathbf{\theta}_0), \quad M_1 : \mathbf{d} \sim p(\mathbf{d} | \mathbf{\theta}_1), \mathbf{\theta}_1 \sim p(\mathbf{\theta}_1), \]

where the definition of the parameter \( \mathbf{\theta} \) may differ between models. Then the posterior probability of model \( M_0 \) can be written as

\[ p(M_0 | \mathbf{d}) = \frac{p(M_0) B_{01}}{p(M_0) B_{01} + p(M_1)}, \]

where \( B_{01} \) is the Bayes factor in support of model \( M_0 \) given by

\[ B_{01} = \frac{p(\mathbf{d} | M_0)}{p(\mathbf{d} | M_1)} = \frac{p(M_0 | \mathbf{d}) p(M_1)}{p(M_1 | \mathbf{d}) p(M_0)}. \]

The quantity \( B_{01} \) is the ratio of the posterior odds of model \( M_0 \) to its prior odds and represents information about the evidence provided by the data in favor of model \( M_0 \) as opposed to \( M_1 \) (Kass and Raftery, 1995). It should be clear from the definition of (17) that the Bayesian model selection suffers from exactly the same computational challenges as BMA. To this extent, BBVBMA directly approximates posterior probabilities of individual models and Bayes factors can be conveniently computed as a byproduct of the algorithm without the need of approximating the model evidence (3).

### 3.3.1 Linear and Logistic Regression examples

To illustrate the Bayesian model selection via BBVBMA, we consider the following hypotheses for both linear and logistic regression examples above and compare the BBVBMA based results with their MC counterparts.

\[ H_0 : \theta_1 = 0, \quad H_1 : \theta_1 \neq 0. \]

For the linear regression case, this corresponds to comparing models \( M_1 \) and \( M_3 \). For the logistic regression example, we need to compare models \( M_3 \) and \( M_7 \). Table 4 presents the respective Bayes factor approximations. For both linear and logistic regression examples, BBVBMA approximations qualitatively agree with the MC based approximations. The results show that the U.S crime data favor the linear regression model with \( \theta_1 = 0 \), and the heart disease data favor logistic regression model with \( \theta_1 \neq 0 \).
Table 4: Bayes factors obtained via BBVBMA approximation and MC methods. Models $M_1$ and $M_3$ are considered for the linear regression example and models $M_3$ and $M_7$ for the logistic regression example.

| Example          | MC  | BBVBMA |
|------------------|-----|---------|
| Linear regression| 4.11| 5.2     |
| Logistic regression| 0.29| 0.26   |

4 Discussion

We presented a VBI approach to BMA that avoids some of the practical challenges that burdens the standard MCMC based approaches to approximate the BMA posterior, especially numerical evaluation of the evidence integral. The fidelity of the method was demonstrated on a series of pedagogical examples including the averaging of linear and logistic regression models and Bayesian model selection via Bayes factors.

The proposed procedure is “black box” in the sense that it can be readily applied to wide range of models with minimal additional derivations needed. For instance, BBVBMA can be conveniently applied to nonconjugate models including generalized linear models, Bayesian neural networks, and Deep latent Gaussian models (Blei et al., 2017).

Additionally, BBVBMA is a general VBI algorithm and the presented implementation with the AdaGrad learning rate and the mean-field variational family is just one of many implementations. One can consider any adaptive learning rate and other variational family available in the literature. BBVBMA can also be simply modified for greater scalability in the scenarios with complex machine learning models that need to be fitted to massive datasets. First, one can subsample from the data to construct computationally cheap noise estimates of ELBO gradients. Secondly, the nature of BBVBMA allows for immediate parallelization across the models. To achieve a faster convergence of the algorithm, BBVBMA can be augmented with Rao-Blackwellization (Casella and Robert, 1996), control variates (Ross, 2006), and importance sampling (Ruiz et al., 2016) to reduce the variance of noisy gradient estimators. A fully documented Python code with the basic implementation

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Appendix A  Parametrization of Variational Families

A.1 Normal Variational Family

Let us consider a real valued parameter $\theta$ with normal variation family $q(\theta | \mu, \sigma^2)$ parametrized by the mean $\mu$ an variance $\sigma^2$. Under the transformation (13), we get the following expressions for the log likelihood of the variational distribution

$$
\log q(\theta | \mu, \lambda) = -\frac{1}{2} \log[\log(e^{\lambda \theta} + 1)] - \frac{1}{2} \log 2\pi - \frac{1}{2}\frac{\theta - \mu)^2}{2\log(e^{\lambda \theta} + 1)},
$$

and the gradient of the log likelihood

$$
\nabla_\mu \log q(\theta | \mu, \lambda) = \frac{\theta - \mu}{\log(e^{\lambda \theta} + 1)},
$$

$$
\nabla_\lambda \log q(\theta | \mu, \lambda) = \frac{1}{2}\frac{e^{\lambda \theta}}{e^{\lambda \theta} + 1} \left[ \frac{(\theta - \mu)^2}{(\log(e^{\lambda \theta} + 1))^2} - \frac{1}{\log(e^{\lambda \theta} + 1)} \right]
$$

A.2 Gamma Variational Family

For a positive-valued parameters, we shall consider a gamma variational family $q(\theta | m, \tau^2)$ parametrized by the mean $m$ and variance $\tau^2$:

$$
\log q(\theta | m, \tau^2) = \frac{m^2}{\tau^2} \log(m) - \frac{m^2}{\tau^2} \log(\tau^2) + \left( \frac{m^2}{\tau^2} - 1 \right) \log(\theta) - \frac{m}{\tau^2} \theta - \log \Gamma\left( \frac{m^2}{\tau^2} \right).
$$

Using (13) we get the following parametrization of the variational distribution

$$
\log q(\theta | m, \lambda) = \frac{(\log(e^{\lambda m} + 1))^2}{\log(e^{\lambda r} + 1)} \log[\log(e^{\lambda m} + 1)] - \frac{(\log(e^{\lambda m} + 1))^2}{\log(e^{\lambda r} + 1)} \log[\log(e^{\lambda r} + 1)]
$$

$$
+ \left( \frac{(\log(e^{\lambda m} + 1))^2}{\log(e^{\lambda r} + 1)} - 1 \right) \log(\theta) - \frac{\log(e^{\lambda m} + 1)}{\log(e^{\lambda r} + 1)} \theta
$$

$$
- \log \Gamma\left( \frac{(\log(e^{\lambda m} + 1))^2}{\log(e^{\lambda r} + 1)} \right)
$$
and the gradient of the log likelihood

\[
\nabla_{\lambda_m} \log q(\theta|\lambda_m, \lambda_r) = -\frac{e^{\lambda_m}}{\log(e^{\lambda_r} + 1)(e^{\lambda_m} + 1)} \left\{ \theta + \log(e^{\lambda_m} + 1) \left[ -1 - 2 \log[\log(e^{\lambda_m} + 1)] + 2 \log[\log(e^{\lambda_r} + 1)] + 2 \psi\left( \frac{(\log(e^{\lambda_m} + 1))^2}{\log(e^{\lambda_r} + 1)} \right) \right] \right\},
\]

\[
\nabla_{\lambda_r} \log q(\theta|\lambda_m, \lambda_r) = -\frac{\log(e^{\lambda_m} + 1)e^{\lambda_r}}{(\log(e^{\lambda_r} + 1))^2(e^{\lambda_r} + 1)} \left\{ \theta + \log(e^{\lambda_m} + 1) \left[ -1 - \log[\log(e^{\lambda_m} + 1)] + \log[\log(e^{\lambda_r} + 1)] + \psi\left( \frac{(\log(e^{\lambda_m} + 1))^2}{\log(e^{\lambda_r} + 1)} \right) - \log(\theta) \right] \right\},
\]

where \( \psi(x) = \frac{d}{dx} \log(\Gamma(x)) \).

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